일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **PLEN-1**
발표분야: 기조강연
발표종류: 특별강연, 발표일시: 목 16:00, 좌장: 박한오

Discovery Process of Cancer Drug Zelboraf: Broader Implications of Chemical Approaches to Cancer Therapy

Sung-Hou Kim

Department of Chemistry, University of California, Berkeley, CA, USA

The process of discovery and development of a “tergeted” cancer drug, Zelboraf, will be briefly described. The process taken by Plexxikon, a Berkeley biotech company, involved a new approach, “Scaffold-based method”, to shorten the time and to reduce the cost for discovering chemical drug leads, for optimization of the drug leads, and for obtaining multiple drug candidates to enter clinical trials. The process revealed the dynamic interplay of how basic science opens the first door to a problem and clinical results point the directions to many more doors for basic science to be opened to understand complexities of cancer resistance, one of the greatest challenges ahead.

Although this approach was successfully used for the discovery of Zelboraf, similar approaches can be used to find chemical drugs that can regulate activities of checkpoint proteins, which are the targets of immunotherapy of cancer.

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장소: 대구 EXCO
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 11:00, 좌장: 황광연

Development of a chemical-based potent anti-bacterial agent and a novel small molecule-based theragnostic agent for disease

윤문영

한양대학교 화학과

In anti-bacterial agent research, we have focused on enzymatic mechanism of acetohydroxyacid synthase (AHAS) and development of their potent inhibitors. The AHAS as a novel target is known to catalyze at the first stage for biosynthesis of an essential branched chain amino acid (BCAA) synthesized by plants and bacteria not by animals. In our research, we have identified and characterized functional and structural features of AHAS from various bacteria (*M. tuberculosis*, *H. influenzae*, *B. anthracis*, *E. coli*, *S. sonnei*, *P. aeruginasae*, and *E. faecalis*) and screened a chemical inhibitors via high-throughput screening (HTS) technique. The most of found inhibitors are exhibited a strong inhibitory effect in bacterial strains, thus the AHAS could be a potent anti-bacterial target. In addition, we have studied a novel theragnostic agent based on small molecular probe such as peptide and aptamer produced by phage display and SELEX technique. In order to evaluate the probes as a therapeutic agent, we have developed peptide/aptamer against a various target molecules as biomarkers in a particular disease; Tuberculosis (AHAS), Anthrax (anthrax toxins), Citrus canker (FtsZ), and Phytophthora blight (tubulins). The most of probes did not only exhibit a strong binding ability, but also the potent inhibition effect in their target. At a time, we have also focused on development of diagnostic probes against various diseases; Anthrax, Alzheimer's disease, Cancer, Foodborne pathogens, Antibiotics, and Endocrine disrupters. In order to enhance a probe-sensitivity and selectivity, we have further developed a polyvalent directed probe polymer (PDPP) and applied a novel biological sensor systems for early diagnosis of diseases with a diverse convergence techniques. Consequently, we suggest that the peptide or aptamer would be prospected a potent candidate and could be used in disease therapy and diagnosis.

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장소: 대구 EXCO
발표코드: **POLY1-1**
발표분야: Polymers for Drug Delivery System
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김동하

Eutectic Growth of Organic Semiconductors

김주은 <u>강영종</u>*

한양대학교 화학과

Organic semiconductors have been extensively investigated as promising materials for cost-effective flexible electronic devices. The performance of the devices are highly dependent on the crystallinity of semiconductors as well as intrinsic molecular structure. Vacuum deposition and solution deposition techniques are often adopted for growing crystals. Nerverless, it is known that highly crystalline organic semiconductors are hard to prepare by simple vapor evaporation or by solution growh. Furthermore, crystallization of polymeric semiconductors with high molecular weights is often hindered by difficulty of vaporization and poor solubility in most common solvents.

Herein, we report controlled growth of single-crystalline organic semiconducting nanowires using crystallizable solvents as templates. In this work, we utilized the melting temperature depression induced by eutectic mixtures of organic semiconductors and crystallizable solvents. Due to the formation of eutectic mixtures, organic semiconductors which originally have high melting temperature (> 350 °C) melted at moderately low temperature (~62 °C). Upon cooling, eutectic mixtures of organic semiconductors and crystallizable solvents form various thermodynamic micro- or nanostructures including lamellae, cylinders or spheres by eutectic reaction, a phase transition between liquid and mixture of solid phases. During the eutectic reaction, the crystallizable solvents templates the crystal structure of organic semiconductors.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY1-2**
발표분야: Polymers for Drug Delivery System
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김태일

Photodegradable Hydrogels for Cell Sorting and Single Cell Research

신동식

숙명여자대학교 의약과학과

In this study, a method for capture, analysis, and sorting of live cells using a photodegradable hydrogel (photogel) functionalized with antibodies will be demonstrated. Photogel substrates used to first isolate human CD4 or CD8 T-cells from a heterogeneous cell suspension and then to release desired cells or groups of cells by UV-induced photodegradation. Flow cytometry analysis of the retrieved cells revealed approximately 95% purity of CD4 and CD8 T-cells, suggesting that this substrate had excellent specificity. To demonstrate the possibility of sorting cells according to their function, photogel substrates that were functionalized with anti-CD4 and anti-TNF-a antibodies were prepared. Single cells captured and stimulated on such substrates were identified after immunofluorescent staining and could be retrieved by site-specific exposure to UV light through a microscope objective. The use of a photodegradable gel allows the detection of cells of interest based on their function and the release of these cells for downstream analysis, which could entail gene expression studies or continued cultivation.

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발표코드: **POLY1-3**
발표분야: Polymers for Drug Delivery System
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 김태일

Polysaccharide-Based Nanoparticles Responding to Tumor Microenvironments

박재형

성균관대학교 화학공학부

Self-assembled polymeric nanoparticles have received attention as anticancer drug carriers because they can circulate in blood for long periods of time, followed by selective accumulation into tumor tissue via the enhanced permeation and retention effect. However, delivery of the drug into the intracellular compartments of the cancer cell is often insufficient due to the slow release of the drug from nanoparticles. In our group, various polysaccharide-based nanoparticles, responsive to cancer-specific stimuli, have been investigated as the drug carrier for cancer therapy. When such nanoparticles are administered into tumor-bearing mice, they selectively accumulated into the tumor site. Their in vivo tumor targetability were achieved via passive or active targeting mechanism. Once they reach the tumor site, the drug was rapidly released, primarily owing to the characteristic stimuli of tumor such as the low pH, reductive envionment, and hypoxic condition. Overall, the stimuli-sensitive polysaccharide nanoparticles might have promising potential as the carrier of the anticancer drugs.

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발표코드: **POLY1-4**
발표분야: Polymers for Drug Delivery System
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 김태일

PEGylated Poly(amidoamine) Dendrimers for Drug Delivery

나동희

경북대학교 약학대학/약학과

Poly(amidoamine) (PAMAM) dendrimers are well-defined, highly branched, and globular-shaped macromolecules that have been used for many diverse biomedical applications, such as drug or gene delivery and medical imaging, but they are shown to exhibit cytotoxicity and hemolytic toxicity, depending on the surface charge and generation. In order to reduce toxicity, modification of surface amino groups of PAMAM dendrimers with PEG (PEGylation) has been often performed. Fully PEGylated PAMAMs have been studied, but in some cases partly PEGylated forms are necessary because the positive surface charge of the nanocarrier is helpful for cellular uptake. Since the number and size of PEG attached affect the usefulness of PAMAM dendrimers, the PEGylation degree and physicochemical properties should be well characterized. In this presentation, novel chromatographic methods for the determination of PEGylation degrees and purity characterization of PEGylated PAMAM dendrimers. In addition, microchip electrophoretic method for investigating difference in electrophoretic mobility between partially and fully PEGylated PAMAM dendrimers. Finally, solubilization strategy for water-insoluble or poor soluble drugs using PAMAM or PEGylated PAMAM dendrimers is presented.

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발표코드: **POLY1-5**
발표분야: Polymers for Drug Delivery System
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 서지훈

Nanoparticles for sustained delivery of protein

육순홍

고려대학교 약학대학 약학과

Sustained delivery of exenatide was demonstrated using nanoparticles (NPs) with a core/shell structure. Exenatide, a glucagon-like peptide-1 (GLP-1) agonist, was approved by the Food and Drug Administration (FDA) in 2005 as a twice daily subcutaneous injection to treat type 2 diabetes .For this purpose, the interactions between lipid bilayers and Pluronic F-68 were utilized to form core/shell NPs using a layer-by-layer approach. With the addition of alternating Pluronic F-68 and lipid bilayers onto the NPs, the release pattern and antidiabetic activity showed that they were sustainable, indicating that the in vivo functionality of the NPs could be controlled through manipulating the NP nanostructure. Although the antidiabetic effects of exenatide-loaded NPs have been demonstrated in an animal model, the attempt was made to demonstrate the extended duration of antidiabetic effects, which was accomplished by localizing the exenatide-loaded NPs in muscular areas in the body through the gelation of Pluronic F-127. NPs/Pluronic F-127 mixtures were designed and characterized based on the sol-gel transition of Pluronic F-127 aqueous solution at body temparature. In vitro release pattern and in vivo antidiabetic activity of exenatide from the NPs/Pluronic F-127 mixtures showed that they were sustainable and exhibited the therapeutic effect for extended period of time.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **POLY1-6**
발표분야: Polymers for Drug Delivery System
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 서지훈

Immune modulation by BBB-permeable peptide to control autoimmune diseases

최제민

한양대학교 생명과학과

Immune diseases such as autoimmune and allergic diseases are based on the abnormal regulation of immune system. The most of the immunosuppressant has undesirable side effects and still there is high unmet need for various immune diseases although antibody based biologic drugs are emerging currently. Here we will introduce a cell penetrating peptide (CPP) application technology, which enables intracellular therapeutic protein delivery to control cell's behavior. We have identified several novel CPPs derived from human proteins which are naturally exist implies none toxic or immunogenic effect. CPPs could deliver a protein into various tissues including liver, spleen, intestine, and even into the brain in the mice. Moreover, it could be translocated into the cytoplasm and the nucleus in vitro and in vivo. Then, we designed T cell specific immune modulatory recombinant proteins by using BBB-permeable CPP and CTLA-4 protein to apply them in immune diseases. BBB-permeable peptide conjugated Cytoplasmic domain of CTLA-4 (ctCTLA-4) could enter into T cells and inhibit proximal signaling, cytokine production, and proliferation in activated mouse and human T cells. In addition, it could modulate Th1 or Th17 cells to inhibit autoimmune encephalitis, and human allo-response against skin graft. Collectively these results suggest protein based intracellular signaling modulation approach by using BBB-permeable peptide would increase clinical potentials and much broaden biologic drug targets. Our therapeutic proteins will be further studied as a novel drug development pipeline in autoimmune diseases such as MS.

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장소: 대구 EXCO
발표코드: **POLY2-1**
발표분야: Organic Materials for Solar Cell Applications
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 장성연

Nanomaterial-Based Interfacial Layers for Organic Solar Cells

윤진문

한국원자력연구원 첨단방사선연구소 공업환경연구부

In the past few years, bulk-heterojunction organic solar cells (OSCs) have been intensively studied due t the potential for the low cost, solution process, and high-throughput manufacturing via a roll-to-roll printing technique. Power conversion efficiencies of OSCs have been improved by the novel synthesis of innovative materialsfor the three primary layers or optimization of processing conditions. Nevertheless, long-term stability of the OSCs, which is highly depends on the interfacial materials, still remains a serious drawback for widespread commercialization of OSCs. In particular, representative materials, PEDOT:PSS, showed a poor device stability, which is attributed to a high acidity and a hygroscopic property. To solve these problems, low dimensional nanomaterials (graphene, graphene analog, nanoparticles), which have an unique optical, electrical, and electronic properties, were used as efficient interfacial layers for highly efficient and stable OSCs.

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장소: 대구 EXCO

발표코드: **POLY2-2**

발표분야: Organic Materials for Solar Cell Applications

발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 장성연

Lead Chalcogenides Nanocrystal Quantum Dots for Solar Cell Applications

정소희

한국기계연구원 나노기계연구본부

Lead chalcogenides nanocrystal quantum dots (PbS, PbSe, PbTe) provide a tunable bandgap in infrared region suiting for photovoltaic applications. A noticeable photoconversion efficiency of nanocrystal quantum dot solar cells has been achieved recently, reaching around 10 %. Achieving higher efficiencies with enhanced stability in quantum dot solar cells require understanding and controlling over the surface of nanocrystal quantum dots. In this presentation, our recent efforts on a fundamental aspects of efficient nanocrystal quantum dots-based photovoltaics focusing on the surface chemistry of nanocrystal quantum dots will be discussed. Shape originated size-dependent stability and facet specific atomic layer passivation enhancing ambient stability will be presented. Also, various approaches on increasing devices performances via organic/inorganic surface modifications will be introduced.

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장소: 대구 EXCO
발표코드: **POLY2-3**
발표분야: Organic Materials for Solar Cell Applications
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 장성연

Nano-template for spectrum conversion technology

고두현

경희대학교 응용화학과

We describe a metal nanodisk?insulator?metal (MIM) structure that enhances lanthanide-based upconversion (UC) and downshifting (DS) simultaneously. The structure was fabricated using a nanotransfer printing method that facilitates large-area applications of nanostructures for optoelectronic devices. The proposed MIM structure is a promising way to harness the entire solar spectrum by converting both ultraviolet and near-infrared to visible light concurrently through resonant-mode excitation. The overall photoluminescence enhancements of the UC and DS were 174- and 29-fold, respectively.

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발표코드: **POLY2-4**
발표분야: Organic Materials for Solar Cell Applications
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 고두현

Crystalline Low Band Gap Polymers for Organic Photovoltaics

우한영

부산대학교 나노과학기술대학 나노융합공학과

Over the past few decades, polymer solar cells (PSCs) have made a significant progress, showing their potential in low-cost, flexible, light weight, portable and large-area energy-harvesting devices. We present a series of crystalline low band gap polymers which were designed by considering the backbone planarity, noncovalent intra- and interchain coulomb interactions, chain curvature and solution processibility, etc. The detailed molecular design and resulting morphological, electrical and device properties will be discussed.

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장소: 대구 EXCO
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발표분야: Organic Materials for Solar Cell Applications
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 고두현

Efficient planar heterojunction perovskite solar cells employing PCBM electron transport layer

서장원

한국화학연구원 광에너지융합소재연구센터

Hybrid organic/inorganic perovskite material, $CH_3NH_3PbI_3$ (=$MAPbI_3$) has received a great deal of attention due to their intrinsic properties such as appropriate band gap, high absorption coefficient, long hole-electron diffusion length. This feature allows for diversity in its device architecture. So far, significant progresses in solar cell performance have been established by virtue of improvement in device structures, including meso-superstructured, mesostructured, planar and bi-layer architecture, reporting certified power conversion efficiency (PCE) of 20.1%. In this talk, we will present our results on efficient planar heterojunction hybrid solar cells employing $MAPbI_3$ and phenyl-C61-butyric acid methyl ester (PCBM) with a PCE over 17%. This is achieved through fundamental understanding of the control of the morphology, the optimization of electron and hole selective contacts, and the introduction of buffer layer between organic/electrode. Furthermore, this presentation will also cover our recent progress in bi-layer perovskite solar cells using $NH_2CH{=}NH_2PbI_3$ (=$FAPbI_3$).

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일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY3-1**
발표분야: Conjugated Polymers for Organic Thin Film Transistors
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 노용영

New Organic Semiconducting Materials for Organic Electronics

김윤희

경상대학교 화학과

Organic semiconductors have been studied extensively with regards to their charge transport ability and have recently been demonstrated to be a viable option for large-area, commercial electronic devices and photonics. Thus far, various synthetic strategies for organic semiconductors have been reported that enhance their charge carrier transport characteristics for OTFT, enhance high efficiency and color purity for OLED, and enhance the efficiency for organic solar cell. Recently, we have reported various organic semiconducting materials for organic electronics. In this presentation, it will be introduced the new organic semiconducting materials for organic thin film transistors, organic light emitting display, and organic solar cells.

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장소: 대구 EXCO

발표코드: **POLY3-2**

발표분야: Conjugated Polymers for Organic Thin Film Transistors

발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 노용영

Highly ordered liquid crystalline organic semiconductors for OTFT applications

김윤호

한국화학연구원 고기능고분자연구센터

Development of high-performance printed semiconductor devices is highly desired with the expectation for the next generation technologies of “printable electronics” providing simply fabricated, flexible, large-area, low-cost, and environmentally friendly electronic products such as paper-like flexible displays.Here, we fabricated highly ordered organic semiconductor micropatterns of the liquid crystalline small molecule, C10-BTBT, by using a simple method based on template-assisted self-assembly (TASA). The self-alignment properties of the smectic liquid crystal phase of C10-BTBT enable the solvent-free processing of well-defined micropatterns for printed OFETs. The orientation of the liquid crystalline OSC material was directed by using a topographically pre-patterned polymeric template. The nucleation and directional growth of C10-BTBT via TASA was investigated with X-ray diffraction as well as optical and electron microscopy. We then fabricated high-performance organic transistors with a mobility of ~1.7 cm2/V·s based on the highly ordered small molecule micropatterns. We used a polyimide organic dielectric layer in the FETs instead of typical SiO2 gate insulators to realize all-organic FET devices.

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장소: 대구 EXCO

발표코드: **POLY3-3**

발표분야: Conjugated Polymers for Organic Thin Film Transistors

발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 노용영

PEDOT:PSS-Based Bio-Electronic Interfaces and Water-Stable Electrochemical Transistors

윤명한

광주과학기술원(GIST) 신소재공학부

In this work, we report the fabrication of water-stable high-performance flexible PEDOT:PSS electrodes and active channels for versatile underwater bio-electronic interface applications. The G-PEDOT:PSS films with highly-ordered fibrillar structures were prepared via crystallization treatment and deposited onto on flexible plastic substrates by dry transfer. The G-PEDOT:PSS films transferred onto flexible polyethylene terephthalate substrates, exhibit exceptional electrical performance and outstanding mechanical stability in aqueous media over several weeks without film dissolution or delamination. The comparative investigation of electrical properties reveals that electrical conductivity and electrochemical impedance of transfer-printed PEDOT:PSS films substantially surpass those of other water-stable PEDOT:PSS films prepared by the previously reported methods. Finally, we demonstrate that these flexible cellular electrodes exhibit long-term neuronal culture viability on top and promising potential as efficient cellular interfaces for both electrical recording and stimulation.

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장소: 대구 EXCO
발표코드: **POLY3-4**
발표분야: Conjugated Polymers for Organic Thin Film Transistors
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 김윤호

High-Performance Flexible Sensors Based on Engineered Organic Semiconductors

오준학

포항공과대학교(POSTECH) 화학공학과

Nanoscopically engineered organic semiconducting materials have attracted great interest recently as they are promising building blocks for various electronic and optoelectronic applications. In addition, multicomponent semiconducting materials such as p-n junctions or core-shell structures are of great importance both in modern electronic applications and in understanding other semiconductor devices. They can potentially realize novel or improved chemical and physical properties that cannot be obtained from the single component system or their bulk materials. Furthermore, the physical structure of an organic solid is strongly affected by the surface of underlying substrate. Controlling this interface has always been an important issue to improve device performance in organic electronics. In this study, unconventional organic semiconducting nanomaterials including branched nanowires, nanoporous organic semiconducting films, and core-shell structured 1-D nanomaterials have been fabricated, and applied in high-performance flexible and wearable sensors such as photodetectors, chemical and biological sensors. In addition, the fundamental charge transport and photophysical phenomena of organic semiconducting nanomaterials have been investigated. Furthermore, an approach that utilizes an organic heterointerface to improve the crystallinity and control the morphology of organic thin film has been developed. Our approach opens a new way for the fabrication of nanostructured semiconducting layers towards high-performance organic electronics.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **POLY3-5**

발표분야: Conjugated Polymers for Organic Thin Film Transistors

발표종류: 심포지엄, 발표일시: 금 15:50, 좌장: 김윤호

Polymer Gate Insulators for Solution-Processed Flexible Organic & Oxide TFTs

장광석

한국화학연구원 그린화학소재연구본부

플렉서블 디스플레이 구현을 위해서는 플렉서블 박막트랜지스터(thin-film transistor) 기술이 필수적으로 필요하며 폭넓은 관련 기술이 개발되었거나 활발히 연구되는 단계에 있다. 박막트랜지스터에는 전도체, 반도체, 절연체 등의 다양한 전기적 특성을 가지는 소재들이 사용된다. 이 중에서도 기판, 게이트 절연체, 보호층 등에 사용되는 절연체 소재는 보다 넓은 면적 또는 전 면적에 활용되기 때문에 소재 자체의 유연성이 더욱 중요시되고 있다. 최근에는 유연성, 공정성 등의 장점을 가지고 있는 고분자 게이트 절연체에 관한 연구가 활발히 진행되고 있다. 무기 게이트 절연체와 비교하여, 고분자 게이트 절연체는 더 유연한 특성을 가지고 있을 뿐만 아니라 낮은 온도에서 인쇄공정을 통해 유연기판 위에 쉽게 코팅할 수 있다는 장점을 가지고 있다. 고분자 게이트 절연체는 주로 유기 박막트랜지스터에 적용되어 왔으며, 우수한 소자특성을 나타내는 용액공정 유기 박막트랜지스터 소자에 관한 연구가 활발히 진행되고 있다. 본 발표에서는 전기절연성, 내열성 및 내화학성이 우수한 폴리이미드 게이트 절연체 소재를 소개하고, 폴리이미드 게이트 절연체가 적용된 용액공정 유기 및 산화물 박막트랜지스터에 관한 연구동향을 소개하고자 한다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY3-6**
발표분야: Conjugated Polymers for Organic Thin Film Transistors
발표종류: 심포지엄, 발표일시: 금 16:05, 좌장: 김윤호

Multi-Functional Organic Field-Effect Transistors for Flexible/Printed Flash Memory

백강준

부경대학교 인쇄정보공학과

As the market of flexible device technologies grows, the integration of solution-processible unit elements for printed chip becomes decisive for the device performance and the reliability. Unfortunately, common solid-state devices are not compatible with flexible substrates because these devices must use vapor deposition processes in vacuum condition, which increases the complexity and cost of production. Moreover, flexible and portable flash memories have been proposed as key components of personal digital appliances. These memory devices have been researched to improve device flexibility using polymer materials, which have the potential to deform their layered platform structure to curved shape while maintaining signal performance. Here I present a new approach to realize high-density organic flash memory devices based on printed and flexible organic field-effect transistors.

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장소: 대구 EXCO

발표코드: **INOR1-1**

발표분야: Designer Molecules and Assemblies for Energy Conversion and Signal Transduction

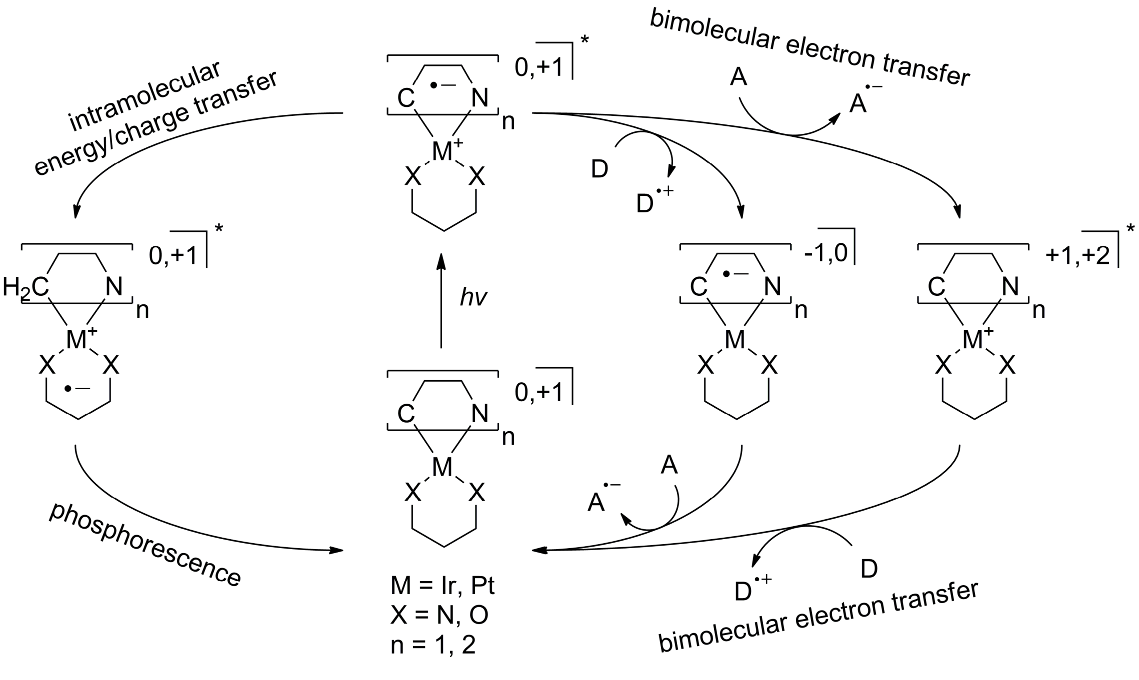
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이동환

Mechanism and Applications of Excited-State Energy and Electron Transfer Involving Cyclometalated Transition Metal Complexes

유영민

이화여자대학교 화학신소재공학부

Cyclometalated complexes of the late transition metals provide unique photofunctionality, as they exhibit ultrafast spin-orbit coupling and wide tailorability in the electronic structures. We have exploited the photofunction of Ir(III) and Pt(II) complexes. Studies, including organic/organometallic syntheses, photophysical characterization, electrochemical measurements, and DFT/TD-DFT calculations, enabled precise control of the excited-state processes. In particular, intramolecular energy transfer and photoinduced electron transfer have been investigated and employed as a useful means to create electrophosphors, phosphorescence bioprobes, and photoredox catalysts.



일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **INOR1-2**

발표분야: Designer Molecules and Assemblies for Energy Conversion and Signal Transduction

발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 이동환

TAILORING PHOTOPHYSICAL PROPERTIES OF BODIPY DYES AND THEIR APPLICATIONS

김영미

단국대학교 화학과

The design of highly sensitive and selective molecular sensory materials having easily detectable recognition events is of great interest in chemical, biological, and pharmaceutical sciences. To this end, fluorescence-based sensors have received a great deal of attention due to their highly sensitive optical transduction modes including fluorescence intensity modulation, wavelength shifts, or changes in fluorescence lifetime upon analyte binding. 4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) dyes are ubiquitous in multiple areas of materials science thanks to their high chemical and photochemical stabilities, relatively large molar absorption coefficients, narrow emission bands and high fluorescence quantum yields.[1-2] However, while many BODIPY dyes exhibit high fluorescence quantum yields in dilute solutions (quantum yield > 0.5) they scarcely emit in the solid state as a result of emission quenching upon aggregation, which remains a major challenge in the application of BODIPY dyes.[3] In this talk, we present a systematic study of the substituents at the periphery of BODIPY dyes, in particular that of the *meso* substituent, to elucidate the factors that govern the formation of emissive aggregates in this family of fluorophores. We also present the design of BODIPY-based fluorescence sensory materials by the modulation of photophysical properties of BODIPY fluorophore.[1] Ulrich, G.; Ziessel, R.; Harriman, A. Angew. Chem., Int. Ed. 2008, 47, 1184.[2] Loudet, A.; Burgess, K. Chem. Rev. 2007, 107, 4891.[3] Tleugabulova, D.; Zhang, Z.; Brennan, J. D. J. Phys. Chem. B 2002, 106, 13133

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO

발표코드: **INOR1-3**

발표분야: Designer Molecules and Assemblies for Energy Conversion and Signal Transduction

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이동환

Photofunctional porphyrin derivatives for energy transduction

장우동* 임다정 이호수위

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. Based on above distinct properties of porphyrins, we recently have designed several porphyrin-based bio-inspired functional materials. In this symposium, I would like introduce recent advances in our researches to mimic natural light harvesting antenna.

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장소: 대구 EXCO

발표코드: **INOR1-4**

발표분야: Designer Molecules and Assemblies for Energy Conversion and Signal Transduction

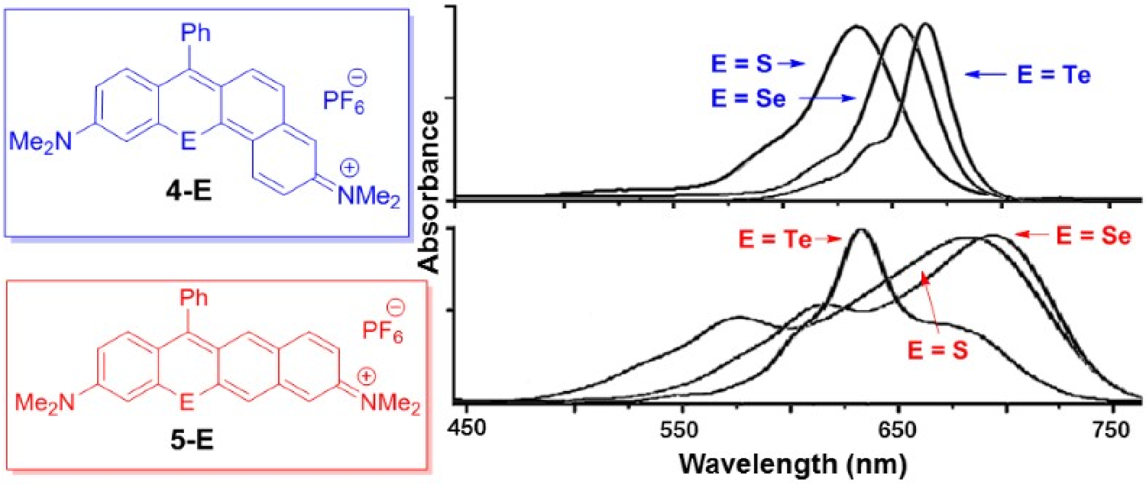
발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 이동환

A Highly Regioselective, Directed Metalation Approach to Extended Chalcogenorhodamine Dyes

Michael R. Detty

Department of Chemistry, University at Buffalo, USA

Extended rhodamines were prepared by inserting an additional fused benzene ring into the rhodamine xanthylium core. The synthesis of “bent” dyes 4-E began with regioselective lithiation of the 1-position of N,N-diisopropyl 6-dimethylamino-2-naphthamide with n-BuLi/TMEDA (≥ 25:1 1- vs. 3-lithiation) followed by addition of a dichalcogenide electrophile. The synthesis of “linear” dyes 5-E began with regioselective lithiation of the 3-position of N,N-diethyl 6-dimethylamino-2-naphthamide with lithium tetramethylpiperidide (≥ 50:1 3- vs. 1-lithiation) followed by addition of a dichalcogenide electrophile. Both 4-E and 5-E absorb at longer wavelengths than their tetramethylrosamine counterparts. Dyes 4-E generate singlet oxygen upon irradiation while dyes 4-S and 5-S are highly fluorescent. Dyes 4-S and 4-Se are effective photosensitizers for the harvesting of light in the solar spectrum for use in dye-sensitized solar cells.


Ph
PF6
Me2N
E
NMe2
4-E
Ph
PF6
Me2N
E
NMe2
5-E
E = S
E = Se
E = Te
E = Te
E = Se
E = S
Absorbance
450
550
650
750
Wavelength (nm)

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **INOR2-1**
발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 박기영

Advanced EPR Investigation of Copper-Amyloid beta Peptides Relevant to Alzheimer’s Disease

<u>김선희</u>

한국기초과학지원연구원 서울서부센터

Redox-active copper ions have been proposed to play an important role in Alzheimer’s disease pathogenesis via an oxidative stress pathway. This inspired us to explore the coordination environment of the copper ion site because the elucidation of the structural details of the copper coordination is essential in understanding the molecular mechanisms of amyloid fibrilization. To probe the atomic structural details of metal-amyloid peptides, we employed multi-frequency, multi-technique pulsed EPR. This includes 34 GHz ENDOR (Electron Nuclear Double Resonance), 9 GHz HYSCORE (Hyperfine Sublevel Correlation) and ESEEM (Electron Spin Echo Envelope Modulation) techniques along with specific isotopic labelings. In addition, the application of advanced EPR spectroscopy to other bio-inorganic chemistry areas will be also presented.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO

발표코드: **INOR2-2**

발표분야: Recent Trends in Bioinorganic Chemistry

발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 박기영

Oxidation of zinc fingers and their binding events to nucleic acids

이승재

전북대학교 화학과

Zinc finger proteins use zinc as a structural co-factor to function, typically by binding to nucleic acids with sequence specificity. Although zinc is typically thought to be the physiologically relevant metal ion for zinc finger protein function there is evidence that other metal ions, including iron, may replace zinc under certain conditions. Studies on iron binding to two zinc finger proteins, NZF-1 and ST-18 will be presented. Neural Zinc Finger-1 has two zinc binding domains each of which is composed of three cysteine and one histidine residues (Cys2His1Cys1) that bind zinc. ST-18 is a non-classical zinc finger protein that contains six zinc binding domains of the form Cys2His1Cys1. Peptides corresponding to the zinc binding domains of NZF-1 and ST-18 were prepared and their zinc, iron and DNA binding properties were determined. These results will be further applied for the development of new inhibitors of neuronal diseases.

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장소: 대구 EXCO
발표코드: **INOR2-3**
발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 박기영

Biomimetic Reactivity of Metal-O_2 Adducts

조재홍

대구경북과학기술원(DGIST) 신물질과학

The reactivity of mononuclear metal-O_2 adducts has long fascinated researchers in many areas due to the significance of diverse biological and catalytic processes. Herein, a set of nickel(III)-peroxo complexes bearing tetraazamacrocyclic ligands, $[Ni(TBDAP)(O_2)]^+$ and $[Ni(CHDAP)(O_2)]^+$, were prepared by reacting $[Ni(TBDAP)(NO_3)]^+$ and $[Ni(CHDAP)(NO_3)]^+$, respectively, with H_2O_2 in the presence of triethylamine. The mononuclear nickel(III)-peroxo intermediates were fully characterized by various physicochemical methods, such as UV-vis, ESI-MS, resonance Raman, EPR and X-ray analysis. The spectroscopic and structural characterization clearly shows that the NiO_2 cores are almost identical where the peroxo ligand is bound in a side-on fashion. However, the different steric properties of the supporting ligands were confirmed by X-ray crystallography where the CHDAP ligand gives enough space around the Ni core compared to the TBDAP ligand. In the aldehyde deformylation reaction, the nucleophilic reactivity of the nicke(III)-peroxo complexes was highly dependent on the steric properties of the macrocyclic ligands, with the reactivity order of $[Ni(TBDAP)(O_2)]^+ < [Ni(CHDAP)(O_2)]^+$. This result provides fundamental insight into the mechanism of the structure-reactivity relationship of metal-peroxo intermediates.

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발표코드: **INOR2-4**
발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 10:15, 좌장: 박기영

Direct Hydroxylation of Benzene to Phenol Using Hydrogen Peroxide Catalyzed by Nickel Complexes Supported by Pyridylalkylamine Ligands

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Osaka University, Japan

Methods for the selective functionalization of aromatic C-H bonds under mild conditions have synthetic applications in the research fields ranging from fine chemistry to industrial scale chemistry. However, direct introduction of oxygen atom into aromatic ring is one of the most challenging chemical reactions due to its notoriously high stability. Thus, development of an efficient method for direct aromatic oxygenation has remained a focal point for extensive research efforts.We report herein aromatic ring hydroxylation with H_2O_2 employing nickel complexes supported by pyridylalkylamine ligands as catalysts. Among the complexes examined, $[Ni^{II}(tepa)(OAc)](BPh_4)$ (tepa: tris(2-pyridyl-ethyl)amine, AcO: acetate) has the highest catalytic efficiency for the oxygenation reaction to produce phenol with 21% yield based on benzene. Negligible amount of over oxidation products such as hydroquinone or benzoquinone was yielded, and selectivity for phenol reached to 99% in the system. In endurance test, the catalyst shows the turn over number of 748 in 240 h. A tepa derivative, bepa (*N*,*N*-bis[2-(2-pyridyl)ethyl]-2-phenylethylamine) was also found to facilitate this benzene hydroxylation reaction, and we succeeded to observed putative reactive species, dinickel(III)-bis(μ-oxide) complex supported by bepa under low temperature conditions (-60ºC). Adding to this catalytic benzene hydroxylation reaction, we will also discuss substrate scope, effect of the supporting ligand on the efficiency and selectivity of the reaction, and reaction mechanisms in the presentation.

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발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 임미희

Nickel Nitrosyl Complexes Supported by a PEP ligand

곽진성 이윤호*

한국과학기술원(KAIST) 화학과

The reactivity of transition metal nitrosyl complexes is of particular interest in our research. This is due in part to the extensive roles of nitric oxide (NO) in biology, which involves an integral part of immune response, vasodilatation, and neurotransmission. Recent researches have revealed that reactive nitrogen species (RNS) might be generated from the interaction of NO with various reactive oxygen species (ROS) mediated by transition metal ions in biological systems. Our investigation has focused on the chemistry of metal nitrosyl in particular with nickel. To date, structurally characterized nickel nitrosyl complexes reported in literature feature only an Enemark-Feltham configuration of $\{Ni(NO)\}^{10}$. Despite this lack of diversity, recent works have shown that nickel nitrosyl complexes can exhibit a diverse range of reactivity such as dissociation, disproportionation, and reduction.Recently we have synthesized dinuclear nickel dinitrogen complexes $\{(PP^RP)Ni\}_2(?\text{-}N_2)$ with tridentate PP^RP ligands; $PP^RP = P(R)(2\text{-}P\mathit{i}Pr_2\text{-}C_6H_4)_2$, (R = Ph and Me), well-characterized by various physical methods such as NMR and IR spectroscopies as well as X-ray crystallography. A series of 4-coordinate nickel nitrosyl complexes $[(PP^RP)Ni(NO)][BF_4]$ were prepared by the reaction of dinuclear nickel N_2 complexes with nitrosonium ion ($NOBF_4$). A neutral paramagnetic nickel nitrosyl species $(PP^RP)Ni(NO)$ featuring an unusual $\{Ni(NO)\}^{11}$ configuration was chemically prepared by the chemical reduction of $[(PP^RP)Ni(NO)][BF_4]$. As closely analogous complexes, square planar 4-coordinate nickel nitrosyl complexes (PNP)Ni(NO) with a tridentate PNP^- ligand; ($PNP^- = N[2\text{-}P\ \mathit{i}Pr_2\text{-}4\text{-}Me\text{-}C_6H_3]_2^-$) was also prepared by oxygen atom transfer reaction. A series of these nickel nitrosyl complexes were characterized by various spectroscopic techniques. Details of nickel nitrosyl species will be presented especially describing their structural parameters and electronic character.

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장소: 대구 EXCO
발표코드: **INOR2-6**
발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 10:43, 좌장: 임미희

Modulation of Amyloid-β Aggregation Pathways by Iridium(III) Complexes

강주혜 이신정[1] 권태혁[2,*] 임미희[*]

울산과학기술대학교(UNIST) 자연과학부/화학과 [1]포항공과대학교(POSTECH) 화학과 [2]울산과학기술대학교(UNIST) 친환경에너지 공학부

Iridium(III) complexes are known to have properties to convert triplet dioxygen into singlet dioxygen or superoxide anion upon the treatment with light. These produced reactive oxygen species are shown to oxidize peptides and proteins and further induce their crosslinking. Utilizing such properties, we have applied Ir(III) complexes to modulate the aggregation pathways of amyloidogenic peptides. The aggregated amyloidogenic peptides are found in brains of neurodegenerative disease [*e.g.*, amyloid-β (Aβ) aggregates in the brain of Alzheimer's disease] and are suggested to be linked to neuropathogenesis. Thus, significant efforts on developing chemical reagents capable of controlling the aggregation of amyloidogenic peptides have been recently made. Herein, we will present the synthesis, characterization, and reactivity of Ir(III) complexes, newly designed for regulating Aβ aggregation based on their photophysical properties. Some mechanistic studies for the anti-amyloidogenic activity of our Ir(III) complexes will also be discussed.

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발표분야: Recent Trends in Bioinorganic Chemistry
발표종류: 심포지엄, 발표일시: 금 10:46, 좌장: 임미희

Reactivity Comparison of Cobalt(III)-Peroxo and Cobalt(III)-Hydroperoxo Complexes

신봉기 조재홍*

대구경북과학기술원(DGIST) 신물질과학

Metal-dioxygen adducts, such as metal-peroxo and -hydroperoxo species, are key intermediates that observed in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. Previously, manganese(III)-hydroperoxo complex, $[Mn(III)(TMC)(OOH)]^{2+}$ (TMC=1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane) was characterized and reactivity of this intermediate has been shown electrophilic character. In this work, using Me_3-TPADP (Me_3-TPADP=3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane) ligand, $[Co(Me_3\text{-TPADP})(CH_3CN)_2]^{2+}$ was synthesized and characterized by various physicochemical methods. Cobalt-peroxo complex, $[Co(Me_3\text{-TPADP})(O_2)]$+, was synthesized with H_2O_2 in the presence of triethylamine. Upon protonation, Co(III)-peroxo complex was converted into a Co(III)-hydroperoxo complex, $[Co(Me_3\text{-TPADP})(OOH)(CH_3CN)]^{2+}$. Interestingly, the Co(III)-hydroperoxo complex shows both nucleophilic and electrophilic reactivity. Nucleophilic reactivity of Co(III)-hydroperoxo complex is higher than that of Co(III)-peroxo complex.

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발표분야: Recent Trends in Inorganic Materials
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 오문현

Calix[4]arene-Based Coordination Polymer Hydrogels and Their Photoluminescent and Rheological Properties

정종화

경상대학교 화학과

Recently, Coordination polymer gels (CPGs) have been exploited for their metal ions which have been reported to show unusual functional properties, such as redox responsiveness, catalysis, phosphorescent behaviour, spin-crossover phenomenon. Furthermore, by selectively binding metal ions to gelator molecules one can affect self-assembly modes and finely tune gelation conditions. Much like in supramolecular chemistry, chemists have begun to rationally design CPG ligands and gelators with suitable coordination geometries for the incoporation of specific metals to generate scaffold containing void spaces. These cavities amongst the polymers can thus accommodate additional solvent molecules in the gel state. I will present the preparation and applications of gels formed from the functional calix[4]arene-based ligand and metal ions to sensing, drug-delivery and catalysis that have been developed over the past five to seven years. Calix[4]arene-based ligands include pyridine, tetrazole, carboxyl acid and amino acid moieties which bind to metal ions to form coordination polymer gels in organic solvents or water, and are characterized by their indiscrete structure which self-assemble to form fibrillar networks.

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발표코드: **INOR3-2**
발표분야: Recent Trends in Inorganic Materials
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 오문현

Nanoporous Hexagonal TiO_2 Superstructure Obtained from Coordination Polymers: New Physical Properties and Their Implications in Energy Applications

방진호

한양대학교 바이오나노학과, 응용화학과

Designing an innovative titanium dioxide (TiO_2) nanostructure that can overcome its current limitations in energy applications remains a great challenge. With a novel synthesis strategy using coordination polymers and a judicious control in annealing process, an exotic TiO_2 nanostructure is synthesized and new physical properties are endowed to this TiO_2 nanostructure. In-depth physical characterizations combined with theoretical simulation studies provide new insights into the physical properties of TiO_2. Superior performances of this TiO_2 in solar cells and lithium-ion batteries are revealed by electrochemical investigation. Implication of the new physical properties in these energy applications is discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR3-3**
발표분야: Recent Trends in Inorganic Materials
발표종류: 심포지엄, 발표일시: 금 15:20, 좌장: 오문현

Synthesis of New Class of Metal Nanostructures: Nanorigns and 3-Dimensional Metal Nanoframes

박성호

성균관대학교 화학과

Herein, we report a general synthetic pathway to various shapes of Au two- and three-dimensional (3-D) nanoframes embedded with a Pt skeleton for structural rigidity. The synthetic strategy consisted of serial reactions involving site-selective growth of Pt on the rim of Au nanoplates, subsequent etching of Au nanoplates, followed by regrowth of Au on the Pt rim. In this synthetic method, Au3+ionsexhibiteddualfunctionalityasanetchantandametalprecursor.The resultant product, Pt@Au nanorings and Au 3-D nanoframes exhibited unique localized surface plasmon resonance (LSPR) bands originating from the Au nanoframes. The synthetic method described here will open new avenues toward many new kinds of metal nanoframes.

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장소: 대구 EXCO

발표코드: **INOR3-4**

발표분야: Recent Trends in Inorganic Materials

발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 오문현

Catalytic Ionic Hydrogenation by Intra-zeolite Frustrated Lewis Pairs

최용남* 이희주[1] 임대운 조인화 윤경병[2]

한국원자력연구원 중성자과학연구부 [1]서강대학교 물리학과 [2]서강대학교 화학과

Catalytic ionic hydrogenation (CIH)1) is achieved by a successive transfer of a proton and a hydride ion from catalytic support to the reactants. Zwitterionic compounds possessing both proton (H^+) and hydride ion (H^-) at sterically hindered position can facilitate ionic hydrogenation of unsaturated organic compounds such as ketones, aldehydes, alkenes/alkynes and so on. Zeolites loaded with platinum nanoparticles by a physical method, sputtering and vacuum annealing, form *frustrated Lewis pairs* (FLPs), protic sites + hydridic sites, within the nanopores.2) These intra-zeolite FLPs do catalytic ionic hydrogenation at milder conditions than other catalytic reactions. Some demonstrative CIH reactions on ketones and alkenes will be presented and discussed with possible mechanisms. These intra-zeolite FLP compounds may open a new era of size- and shape-selective CIH reactions.1). R. Morris Bullock, *Chem. Eur. J.*, 2004, 10, 2366-2374.2). Heeju Lee *et. al.*, *Angew. Chem. Int. Ed.*, 2015 (in press). DOI: 10.1002/anie.201506790.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **PHYS1-1**
발표분야: Advances in Spectroscopic Investigation of Molecules and Clusters
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 장준경

Gas phase laser spectroscopic and computational studies of jet-cooled small molecule-water clusters

최명룡

경상대학교 화학과

Gas phase spectroscopy has been a powerful tool to investigate the intrinsic properties (such as structure or stability) and explore the potential energy surfaces of the isolated individual molecules. The conformational structures of jet-cooled small molecules have been investigated by resonant 2-photon ionization (R2PI) and UV-UV hole-burning (UV-UV HB) spectroscopy. R2PI spectroscopy provides detailed information of the electronic excited states of interest. In order to obtain further information about the conformer specific electronic spectra from the R2PI spectra, a UV-UV HB spectroscopy is employed to discriminate the electronic transitions originating from different conformers. Moreover, gas phase studies can provide critical information for the test of the accuracy of theoretical predictions in the ground (S_0) and excited (S_1) states, in which those of the latter for the systems are much more challenging. In this talk, general gas phase spectroscopic techiques will be presented for the conformational analysis of small molecules and the conformation-specific structural assignment of the conformers is compared and discussed with theoretical calculations.

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장소: 대구 EXCO
발표코드: **PHYS1-2**
발표분야: Advances in Spectroscopic Investigation of Molecules and Clusters
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 윤상운

virbronic state selective reaction dynamics: structure matters a lot

김상규

한국과학기술원(KAIST) 화학과

Relationship between molecular structure and chemical reactivity has not yet been established. One of the main obstacles is the difficulty in selection and/or varation of the molecular structure of reactant. Vibrational excitation of the ground state is not universal as the energy radomization is so efficient to wipe out any mode-selective chemistry afterwards. For excited states, however, vibronic selection in the very low vibrational energy region is quite handy. Especially for predissociation reactions where chemical reaction occurs on excited states exclusively, initial preparatioin of the reactive flux on the specific nuclear configurations is plausible, and this allows for the study of reaction dynamics without energy randomization into all degrees of freedom. Herein, we will discuss several successful cases in this endeavor.

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발표코드: **PHYS1-3**

발표분야: Advances in Spectroscopic Investigation of Molecules and Clusters

발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 윤상운

Circular dichroism spectroscopy of cold chiral molecules and clusters in the gas phase

김남준

충북대학교 화학과

Circular dichroism (CD) spectroscopy is a powerful tool to determine the configurations of chiral compounds in solution. The CD spectroscopy measurement of a chiral compound in solution yields an average CD value derived from all of the conformations of a chiral molecule. By contrast, CD spectroscopy measurement of cold chiral molecules in the gas phase distinguishes specific conformers of a chiral molecule, but the weak CD effect for gas-phase molecules has limited the practical application of this technique. Here, we report the first resonant two-photon ionization CD and laser-induced fluorescence CD spectra of cold chiral molecules, as determined using a supersonic jet with circularly polarized laser pulses. The spectra exhibited well-resolved CD bands that were specific for the conformations and vibrational modes of each enantiomer. The CD signs and magnitudes of the jet-cooled chiral molecules were very sensitive to their conformations and thus offered crucial information on the three-dimensional structures of chiral species, as conducted in combination with quantum chemical calculations.

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발표코드: **PHYS1-4**

발표분야: Advances in Spectroscopic Investigation of Molecules and Clusters

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김명화

Novel Double-Resonance Laser Spectroscopy Technique in a Cold Quadrupole Ion Trap and Its Application to Protonated Adenine Dimer

강혁

아주대학교 화학과

A novel method for double-resonance photofragmentation spectroscopy in a cold quadrupole ion trap has been developed and applied to the spectroscopy of a cold protonated adenine dimer. A burn laser generates a population hole of a certain conformer of the dimer stored in a cold quadrupole ion trap, and an auxiliary dipolar RF is applied to eject the photofragments produced by the burn laser from the trap. A probe laser detects depletion of a certain conformer by the burn laser, and a conformer-specific UV or IR spectrum of a cold ion is obtained by scanning the wavelength of the burn or the probe laser. This simple and versatile method is applicable to any type of double-resonance photofragmentation spectroscopy in a cold quadrupole ion trap. To demonstrate its capability, it was applied to UV-UV hole-burning spectroscopy of a protonated adenine dimer. It is proved that a cold protonated adenine dimer has at least two hydrogen-bonding geometries and each has multiple electronically excited states with significantly different spectral bandwidths, possibly due to different excited state dynamics.

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장소: 대구 EXCO
발표코드: **PHYS1-5**
발표분야: Advances in Spectroscopic Investigation of Molecules and Clusters
발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 김명화

Excited-state intramolecular proton transfer studied by time-resolved electronic and vibrational spectroscopy

방윤수

광주과학기술원(GIST) 물리화학부

Fluorophores which form the intramolecular hydrogen bonds often exist in two tautomeric forms and an excited state intramolecular proton transfer (ESIPT) can be observed with large Stokes shifts. 1,2-Dihydoxyanthraquinone (alizarin) forms an intramolecular hydrogen bond between a carbonyl and a hydroxyl group in the ground and excited states. Upon photoexcitation, the ESIPT from the hydroxyl to the carbonyl group occurs in ultrafast (< 100 fs) time scales and the dual emission from the locally excited tautomer and the proton-transferred tautomer is observed, especially in nonpolar solvents. In polar solvents, the energy barrier of ESIPT becomes lower thus the emission from the proton transferred tautomer is dominant.In this work, the ESIPT of alizarin and related molecules in various solutions were investigated by steady-state and time-resolved absorption and emission measurements. Femtosecond stimulated Raman spectroscopy was also used to monitor the instantaneous structural changes of molecules in the excited state.

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일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **PHYS2-1**

발표분야: Computational Materials Design

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 이근식

Large-scale Computational Screening of Porous Materials and Big Data Analysis

김지한

한국과학기술원(KAIST) 생명화학공학과

Porous materials such as zeolites and metal-organic frameworks have garnered significant amount of attention in the past decade due to their potential applications in variety of energy and environmental related applications. In this talk, we will discuss about computational methods that can be utilized to create hypothetical porous materials, in silico, and multi-scale methods to characterize these materials. Traditionally, the resulting big data for porous materials screening is use to (a) identify the best materials for a given application and (b) identify structure-property relationships that might be amiss from analyzing just a few data points. In this talk, we will discuss about a novel way to utilize the generated big data that can shed new insights onto phenomena such as structural deformation.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **PHYS2-2**
발표분야: Computational Materials Design
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 이근식

Development of Chiral Surfaces and their Modifications for Enantiospecific Separation Processing

한정우

서울시립대학교 화학공학과

The extremely different bioactivity of two enantiomers of a chiral species in biological systems has created an enormous demand for enantiopure chemicals in pharmaceutical manufacturing. This has also raised fundamental questions about the origin of biological homochirality in living organisms. It is therefore important to understand chiral environments which can differentiate two enantiomers of a chiral molecule. Solid surfaces can potentially be used for creating chiral environments that are applicable to chiral processing. There are a variety of routes for creating such chiral solid surfaces. Surfaces of materials whose bulk crystal structure is enantiomorphic can be used as one type of chiral solid surfaces. Chirality can also be imparted onto surfaces by irreversibly adsorbing chiral organic species on otherwise achiral surfaces. Alternatively, metal surfaces that are intrinsically chiral due to the presence of kinked surface steps provide another route for creating chiral solid surfaces. These surfaces can be created by cutting a single crystal along certain high Miller index directions. A number of previous studies have proved the enantiospecific adsorption difference of chiral molecules on those surfaces. To further enhance the enantiospecificity, step decoration, that is doping the kink site of chiral metal surface with second metal, can be a way. It may induce one enantiomer adsorbed on the surface more stable than the other, inducing the larger enantiospecific energy difference. In this talk, we will discuss the enantioselective process to efficiently separate chiral molecules on these types of asymmetric interfaces using density functional theory calculations.

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발표분야: Computational Materials Design
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 이근식

Computational Materials Science for Lithium Ion Battery Materials

이상욱

한양대학교 응용화학과

“Computational materials science” has drawn much attention in several R&D fields because experimentally exploring large numbers of combinations of organic and inorganic materials is both time-consuming and economically expensive. Therefore, computer-aided design and first principles atomic scale simulations are tools of paramount importance in the hand of researchers. Especially, in the commercial field, it has been well known that the average developing time of commercialization of new concept through R&D is around 18 years. In the case of Lithium Ion Battery (LIB), the concept was born at 1976, but the first commercial product came at 1991 by SONY. So, recently, it becomes essential to reduce developing time in the commercial field. In this regard, we have investigated LIB materials from the viewpoint of computational materials science. We have mainly deal with cathode and electrolyte materials pursuing high performance LIB.

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발표코드: **PHYS2-4**
발표분야: Computational Materials Design
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이근식

Computational study on the interfacial interactions between layered materials and metal substrates

정재훈

울산대학교 화학과

Interfacial interaction has long served as a key element to get fundamental insights into surface science and related chemical phenomena. Understanding interfacial interaction is, therefore, of great importance to achieve robust predictability and high controllability in a variety of applications. Herein, we discuss the role of interfacial interaction in (i) fabricating a well-ordered molecular superstructure on metal surface, such as fluorinated fullerene molecules on Au(111) [1a] and diarylethene molecules on Cu(111) [1b], (ii) controlling chemical reactivity for the water dissociation on ultrathin oxide film supported by metal substrate, i.e., MgO/Ag(100) [2,3], and (iii) introducing a novel functional group, i.e., enolate, to the basal plane of graphene grown on metal substrate [4]. Computational studies based on density functional theory (DFT), in close conjunction with scanning tunneling microscopy (STM) experiment, have been mainly performed to unveil the influence of interfacial interactions on the geometric and electronic features of a broad range of surface phenomena.

1.(a) T. K. Shimizu[§], J. Jung[§], T. Otani, Y.-K. Han, M. Kawai, and Y. Kim, ACS Nano 6, 2679 (2012). (b) T. K. Shimizu[§] and J. Jung[§], H. Imada, and Y. Kim, Angew. Chem. Int. Ed. 53, 13729 (2014). [§equally contributed]
2.(a) H.-J. Shin, J. Jung, K. Motobayashi, S. Yanagisawa, Y. Morikawa, Y. Kim, and M. Kawai, Nat. Mater. 9, 442 (2010); (b) J. Jung, H.-J. Shin, Y. Kim, and M. Kawai, Phys. Rev. B 82, 085413 (2010).
3.(a) J. Jung, H.-J. Shin, Y. Kim, and M. Kawai, J. Am. Chem. Soc. 133, 6142 (2011); *ibid.*, 134, 10554 (2012).
4.J. Jung, H. Lim, J. Oh, and Y. Kim, J. Am Chem. Soc. 136, 8528 (2014).

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장소: 대구 EXCO
발표코드: **PHYS2-5**
발표분야: Computational Materials Design
발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 장준경

From “Nanoions” to All-Nanoparticle Electronics

Bartosz Grzybowski

UNIST IBS첨단연성물질연구단/화학과

Nanoscopic objects stabilized with charged organics exhibit properties fundamentally different from either molecular or macromoleculer ions, and can combine ionic-like properties with electronic and ionic conductivity and/or photoexcitability. By careful control of electrostatic interactions, ”nanoions” of various shapes and material compositions can be assembled into functional nanomaterials including 3D supracrystals, ”layered” crystals, or extended films. Depending on the properties of the charged organics, these nanomaterials can act as chemical amplifiers, photoconductors, diodes, transistors, or even full-fledged electronic circuits containing no semiconductors. This last set of constructs can integrate on the nanoparticles electronic function with chemical sensing. Key References: 1. A.M. Kalsin, M. Fialkowski, M. Paszewski, S.K. Smoukov, K. J.M. Bishop & B.A. Grzybowski Electrostatic self-assembly of binary nanoparticle crystals with a diamond lattice, Science, 312, 420 (2006).2. H.Nakanishi, K.J.M. Bishop, B.Kowalczyk, E.A. Weiss, A. Nitzan, K.V. Tretiakov, M.M. Apodaca, R. Klajn, J.F. Stoddart & B.A. Grzybowski* Photoconductance and inverse photoconductance in films of functionalized metal nanoparticles Nature 460, 371-375 (2009).

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장소: 대구 EXCO
발표코드: **PHYS3-1**
발표분야: Physical Chemistry in Low Dimensions
발표종류: 분과기념강연, 발표일시: 금 14:30, 좌장: 장준경

Molecular Structural Dynamics Visualized by Time-Resolved X-ray Diffraction

이효철

한국과학기술원(KAIST) 화학과

The pump-probe X-ray diffraction and scattering techniques have now been fully established as a powerful method to investigate molecular structural dynamics [1-5]. We have employed the techniques to study structural dynamics and spatiotemporal kinetics of many molecular systems including diatomic molecules, haloalkanes, organometallic complexes and protein molecules over timescales from ps to milliseconds. X-ray crystallography, the major structural tool to determine 3D structures of proteins, can be extended to time-resolved X-ray crystallography with a laser-excitation and X-ray-probe scheme, but has been limited to a few model systems due to the stringent prerequisites such as highly-ordered and radiation-resistant single crystals. These problems can be overcome by applying time-resolved X-ray diffraction directly to protein solutions rather than protein single crystals. To emphasize that structural information can be obtained from the liquid phase, this time-resolved X-ray solution scattering technique is named time-resolved X-ray liquidography (TRXL) in analogy to time-resolved X-ray crystallography where the structural information of reaction intermediates is obtained from the crystalline phase. We will present our recent results including the achievement of femtosecond TRXL by using an X-ray free electron laser.[1] Nature, 2015, 518, 385.[2] Nat. Chem., 2013, 5, 212.[3] Acc. Chem. Res., 2009, 42, 356.[4] Nat. Methods, 2008, 5, 881.[5] Science, 2005, 309, 1223.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **PHYS3-2**
발표분야: Physical Chemistry in Low Dimensions
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 김형민

Friction Properties of Graphene; The Effect of Chemical Modification and Water Intercalation

박정영

KAIST EEWS 대학원

The material properties of large-scale synthesized graphene and other two-dimensional atomic sheets are greatly influenced by atomic-scale defects, mechanical deformation, and microstructures. For graphene-based applications, it is, therefore, essential to uncover the role of atomic-scale defects and domain structures of two-dimensional layers. This talk highlights recent studies of friction and nanomechanical properties of graphene, addressing the role of chemical modification and water intercalation. Because of intrinsic structural differences, two-dimensional atomic sheets give rise to unique nanomechanical properties (e.g., thickness dependence, changes after chemical modification) that are in contrast to the three-dimensional continuum medium. We found that hydrogenated, fluorinated, and oxidized graphenes exhibit, 2-, 6-, and 7-fold enhanced nanoscale friction on their surfaces, respectively, compared with pristine graphene, based on friction force microscopy measurements. We associate the measured nanoscale friction with the adhesive and elastic properties of the chemically modified graphenes. In addition, we studied the behavior of water intercalated between graphene and the hydrophilic surface. Atomic force microscopy showed that while the hydrophilic substrates determine the structure of the water near its surface, graphene guides its diffusion, favoring growth of intercalated water domains along the C-C bond zigzag direction. Using atomic force microscopy, we show that intercalated water increases the friction force ~3 fold relative to “dry” graphene over mica, an unexpectedly large increase. We explain this by the softening of the flexural modes of graphene and by stronger phonon coupling between graphene and mica.

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발표분야: Physical Chemistry in Low Dimensions

발표종류: 심포지엄, 발표일시: 금 15:20, 좌장: 김형민

Interlayer Orientation Dependent Light Absorption and Emission in Monolayer Semiconductor Stacks

조문호

포항공과대학교(POSTECH) 신소재공학과

Two-dimensional (2D) stacks of dissimilar hexagonal transition metal dichalcogenide (h-TMDC) monolayers (MLs) exhibit unusual electronic, photonic, and photovoltaic responses that arise from substantial interlayer excitations. Interband excitation phenomena in individual h-TMDC MLs occur in states at band edges (valleys) in the hexagonal momentum space; therefore low-energy interlayer excitation in the h-TMDC ML stacks can be directed by the 2D rotational degree of each ML crystal. However, this rotation-dependent excitation is largely unknown, due to lack in control over the relative ML rotations, thereby leading to momentum-mismatched interlayer excitations. Here, we report that light absorption and emission in MoS2/WS2 ML stacks can be tunable from indirect- to direct-gap transitions in both spectral and dynamic characteristics, when the constituent ML crystals are coherently stacked without in-plane rotation-misfit. Our study suggests that the interlayer rotational attributes determine tunable interlayer excitation as a new set of basis for the h-TMDC 2D optical phenomena.

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발표코드: **PHYS3-4**

발표분야: Physical Chemistry in Low Dimensions

발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 김형민

Close Encounters: When Two Plasmonic Nanoparticles Meet

윤상운

단국대학교 화학과

금이나 은나노입자는 빛에 의해 전도성 전자들이 집단적으로 움직이는 표면플라즈몬(surface plasmon)이라는 독특한 성질을 갖는다. 이러한 표면플라즈몬이 유도되는 공명파장은 개별 나노입자의 크기, 모양, 재질 등에 의해 달라지는데 나노입자 조립체를 이용하면 나노입자들 사이의 상호작용을 통해 이를 더욱 정밀하게 조절할 수 있다. 본 발표에서는 최근 우리 그룹이 새로이 개발한 나노입자 이합체(dimer) 조립 방법을 소개하고, 이합체를 이루는 나노입자간 거리가 수 nm 에서 1 nm 이하로 가까워질 때 나타나는 플라즈몬 커플링 특성의 변화에 대해 논의하고자 한다.

참고문헌

- Cha, H.; Yoon, J. H.; Yoon, S. *ACS Nano* 2014, *8*, 8554.
- Lee, D.; Yoon, S. *J. Phys. Chem. C* 2015, *119*, 7873.
- Cha, H..; Lee, D.; Yoon, S. 2015, submitted.
- Jung, H.; Lee, D.; Yoon, S. 2015, submitted.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **PHYS3-5**
발표분야: Physical Chemistry in Low Dimensions
발표종류: 심포지엄, 발표일시: 금 16:00, 좌장: 김형민

Novel Graphene Based Nano-photocatalysts Development and Application to Waste-water Remediation

김태규

부산대학교 화학과

Rapid industrial growth with lack of proper pollution control measures is effectively leading to environmental damage by the release of organic and inorganic pollutants into the air and water resources. In particular, pollution of natural water is a significant health risk and continues to threaten both human quality of life and the eco-system. Drinking water contaminated with organic dye stuffs, which is likely to cause deadly diseases to human beings like cancers, is also quite common. To resolve this issue photocatalysis has been widely applied because of its potential for the degradation of organic-dye molecules present in waste-water into harmless substances. So far, numerous semiconductor photocatalysts, such as sulfides (ZnS, CuS, Bi2S3, etc.) and oxides (ZnO, TiO2, etc.), have been investigated as photocatalyst for the degradation of toxic organic pollutants in waste-water. However, individual semiconductor nanostructures have an inherent limitation to achieving high photocatalytic efficiency because the recombination of electron-hole pairs is faster than the surface redox reaction. In addition, nanosized materials are normally unstable, easily agglomerated, and difficult to recover after use. Among the many ways to resolve these problems, a novel controlled synthesis of nanocomposites, i.e., graphene coupled with different components, is one of promising methods of improving the photocatalytic performance. These are expected to be highly efficient photocatalysts with good photo stability, due to the formation of hierarchical electron transfer cascade channels among its components and it can suppress electron?hole recombination via delocalization of electrons through the π network, which ultimately enhances the photocatalytic performance. In view of this, we report facile synthesis of various nanocomposites like ZnS-Ag2S/RGO, ZnO-RGO/RuO2, AgI-RGO, AgI-RGO aerogels, CuI-RGO nanocomposites with superior photocatalytic properties. Our detailed structural, optical, and photocatalytic measurements demonstrated that the nanocomposite photocatalytic performance of synthesized nanocomposites is significantly higher than that of bare nanostructures. Overall, our presentation provides new insight into the synthesis of graphene based nanocomposites and the developed composites are highly active photocatalysts with stable cycling that can be exploited in environmentally friendly applications.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ANAL1-6**

발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA

발표종류: 분과기념강연, 발표일시: 목 15:15, 좌장: 김성환

Nanoparticle-enhanced Bioaffinity Sensing Platforms for Biomedical and Environmental Applications

이혜진

경북대학교 화학과

In this talk, I will highlight the extensive efforts made by my research group on the development of highly sensitive and selective bioaffinity sensing platforms in conjunction with gold nanomaterials for a wide range of biological and environmental applications. These efforts involve a concerted approach focusing on the preparation of a diverse range of nanoparticle-biomolecule conjugates alongside the integration of surface enzyme reactions and the introduction of new bioaffinity sandwich assays. The first part of my talk will mainly focus on the development of a surface-based antibody-aptamer sandwich assay in conjunction with the surface plasmon resonance (SPR) detection of various biomarkers important for disease diagnostics. The second part of my talk will switch to the development of electrochemical sensors incorporating biofunctionalized nanoparticles, liquid/liquid interfaces and enzyme reactions to detect environmentally toxic reagents.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

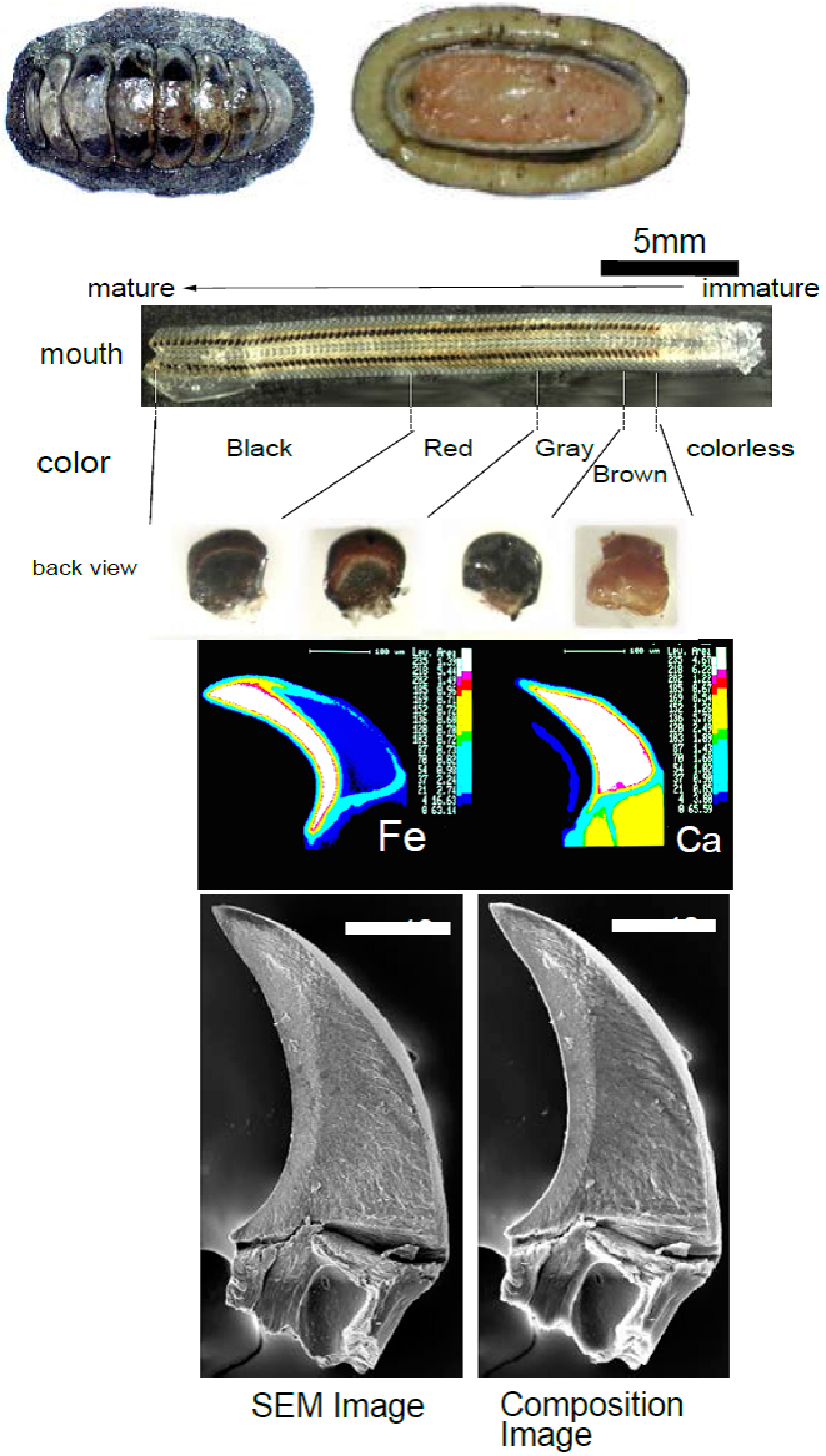
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL1-1**
발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA
발표종류: 심포지엄, 발표일시: 목 13:00, 좌장: 김성환

Evaluation of teeth of chiton accumulating magnetite (Fe_3O_4) as a major material

Chiya Numako

Chiba University, Japan

Chitons are well known to have special strong teeth accumulating iron oxides, especially magnetite (Fe3O4), and calcium phosphates as major components. In the case of Japanese chiton *Acanthopleura japonica*, about 80 pairs of the iron teeth (ca. 400 x 200 x 500 mm3) locate on a radula with their maturation sequence which can be divided into five stages from their mineral composition and appearance. The teeth was soft with organic flame work consist of chitin in the first maturation stage, and their color turns into reddish-brown with amorphous iron (III) components in the flame at the second stage. The posterior edge of a tooth where is main place for feeding accumulates magnetite abruptly at the thierd stage, and its abundance of magnetite increased until 60th teeth on a radular teeth, the fourth stage. Other mineral components can be observed in the later maturation stages; at third stage with red color, goethite (α-FeOOH) and lepidocrocite (γ-FeOOH) are stored at posterior surface of the tooth, and finally the posterior part of the tooth is filled with hydroxyapatite (Ca10(PO4)6(OH)2) at final maturation stage. The hardness of the teeth was much higher than those of other marine creature at intertidal zone because of the magnetite. In this study, nano-indentation technique was applied in order to evaluate of the mechanical property of the teeth of chiton and their variation through the teeth maturation on a radular teeth. Meterial scientific properties of the teeth of chiton has been investigated with ICP-AES, EPMA, FE-SEM, X-ray diffraction, IR, Mossbauer, Raman and X-ray Absotption spectroscopy.


5mm
mature
immature
mouth
color
Black
Red
Gray
Brown
colorless
back view
Fe
Ca
SEM Image
Composition Image


대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL1-2**
발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA
발표종류: 심포지엄, 발표일시: 목 13:25, 좌장: 김성환

In needle Microextraction with PDMS-based Coatings for Polar and Nonpolar Volatile Compounds

배선영

서울여자대학교 화학과

Volatile organic compounds are generally small molecules and emitted from various sources including food, cosmetics, environment and many different mediums. They can be considered as a significant indicator of freshness, quality control, and/or level of pollution. Needle-based headspace extraction methods have been investigated and a novel in-needle micro-extraction (INME) with polydimethylsiloxane (PDMS)-based coatings has been proposed. INME needle is easy to handling and inexpensive to fabricate. Depending coating materials in needle, the selectivity and extraction efficiency of both polar and non-polar compounds were enhanced. In addition, the micro-bore tunnel generated from filling the needle with the coating materials enhanced the sorption of compounds. The various PDMS-based coating materials were investigated to optimize the conditions for target compounds. Through this study, the coating phase/sample distribution constant, the volume of coating phase, the coating thickness, the diameter of the micro-bore tunnel, and length of the coating phase in the needle, and extraction time were found to be significant parameters for optimization of needle design and extraction efficiency. The proposed INME method with various coating materials was properly validated.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL1-3**
발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA
발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 김성환

Imaging Mass Microscopy for high spatial resolution analysis

Koretsugu Ogata

Shimadzu Corporation, Japan

Matrix-assisted laser desorption/ionization-mass spectrometry imaging (MALDI-MSI) is a powerful technique for visualizing the distribution of molecules and drugs in organs. In particular, iMScope *TRIO* is an "imaging mass microscope" instrument that is equipped with an optical microscopy, an atmospheric pressure ion-source chamber for MALDI and a quadrupole ion trap time-of-flight (QIT-TOF) analyzer. This instrument is capable of narrowing down the laser diameter to minimum of 5 μm for high spatial resolution MS imaging.

We performed IMS using that dosed tissue sections were surgically removed from mouse liver after treatment with drugs. Samples were frozen in dry ice acetone and, then sectioned at a thickness of 10 μm and transferred to an ITO slide glass (Sigma).

We succeeded the MS and MS/MS imaging performed with high spatial resolution (5 μm). Compared to the result acquired at 25 μm resolution, the number of positions that gave signal appears smaller at higher resolution. On magnification view of the overlaid image, revealed that the positions of detected signals were localized to narrow intercellular spaces. This result suggests that drug accumulates outside of cells or on cell membrane.

In conclusion, iMScope *TRIO* demonstrated a clear picture of drug imaging which showed that the target molecule is presumably localized on cell membrane or in intercellular spaces and not contained within the hepatocytes. Such observation was only possible at 5 μm spatial resolution. This level of spatial resolution achieved is indispensable for unraveling the physiology of pharmacokinetics at cellular level. Moreover, the above observation was only noticeable after superimposing the MS/MS image onto the optical image. The optical microscope incorporated in the instrument is giving iMScope*TRIO* its unique and important features that magnification and resolution of optical imaging is high.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ANAL1-4**

발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA

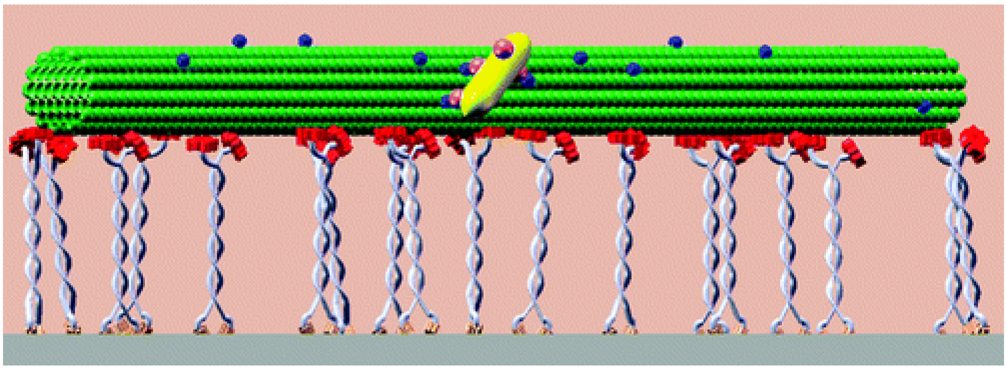
발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 김성환

Resolving rotational motions of single gold nanorods with differential interference contrast microscopy

<u>하지원</u>

울산대학교 화학과

Rotational tracking is of great importance for scientists to understand certain functions and mechanisms of biomolecules, such as RNA folding, rotational motion of ATPase, and structural and rotational dynamics of myosin V. Plasmonic gold nanorods (AuNRs) have been gaining much attention as ideal probes in a variety of imaging tools for orientation sensing due to their anisotropic shape, photo-stability, and biocompatibility. In this talk, I present that the dynamic rotational motion of AuNRs in the 3D space can be disclosed with Nomarski-type differential interference contrast (DIC) microscopy. By using the combination of gold nanorod probes and DIC microscopy, we are able to resolve rotational motions of nano-cargoes transported by motor proteins at video rate not only on engineered surfaces but also on cytoskeleton tracks in live cells.



일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL1-5**
발표분야: Diverse Technologies in Spectroscopy - Joint Symposium with JAIMA
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김성환

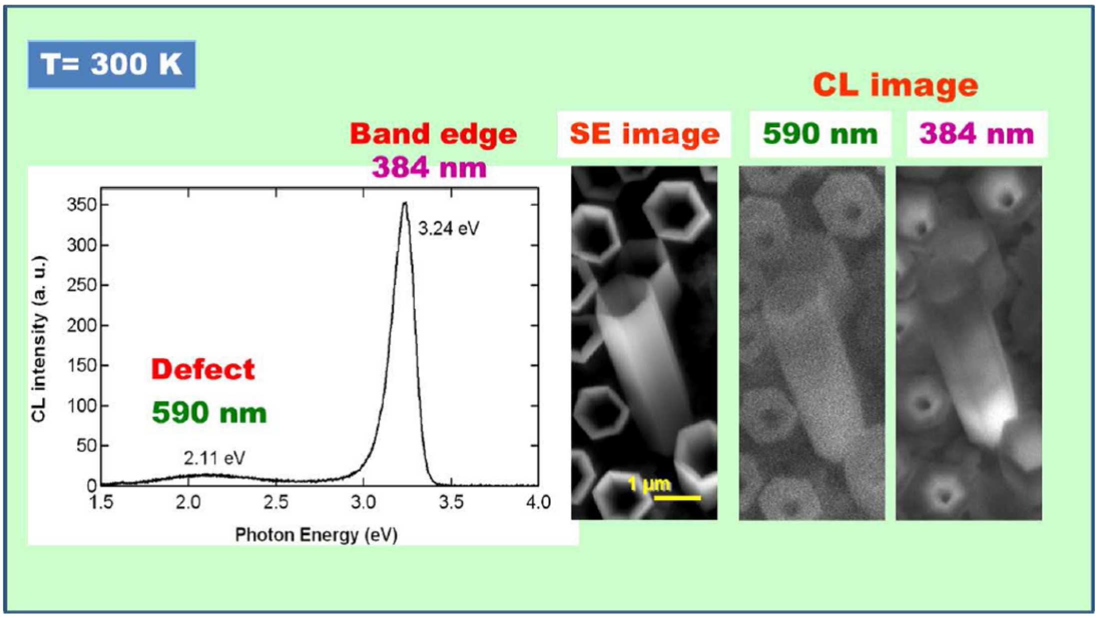
Microscopic Evaluation of Nanomaterials using Cathodoluminescence

Ken Nakagawa

Horiba, Ltd., Japan

The light emitted from a specimen in response to electron beam irradiation is called cathodoluminescence (CL), and it is possible to use this luminescence to evaluate the physical properties of microscopic areas of the specimen. It can be used for many different purposes, such as observing and evaluating the structures under a surface, evaluating wide-gap materials, and making evaluations about defects and impurities.It is used across a wide range of fields such as semiconductors, oxides, dielectrics, ceramics and living organisms. In addition, as it uses electron beam as a means of excitation, it can be used for complex evaluations in the same location as detection means such as an EBIC or EDS. It uses a field emission electron gun as an excitation source, allowing evaluation with a high spatial resolution of nanometer scale. I introduce CL and CL application including nanomaterials in the meeting.

Spatial Distribution of Impurities in ZnO Nanotubes Characterized by Cathodoluminescence



일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ANAL2-5**

발표분야: Material Sciences in Analytical Chemistry

발표종류: 분과기념강연, 발표일시: 금 10:30, 좌장: 김태영

Analytical Technology in Chemical Industry

옥종화

LG화학기술연구원

최근 화학기업은 기술과 가격의 무한 경쟁, 고객 요구수준의 다양화 등 여타 기업의 경영환경 변화에 더해 화평법, 화관법 등으로 대표되는 생산과정 및 제품의 안전에 대한 책임 등 점점 더 기업환경이 어려워지고 있다. 변화하는 환경에 따라 화학기업의 분석은 전통적인 재료/공정/제품 검사 및 제품 개발을 위한 분석 고유의 역할을 넘어 특허기술 확보, 환경 및 안전성 관련 분석 등으로 확대되고 있으며 분석 수요 또한 날로 증가하고 있다.

최근의 화학기업에서의 분석기능은 새로운 물질 및 특성을 분석할 수 있는 신기술의 확보와 더불어, 신속하고 정확한 분석결과 제공하고 대량의 분석시료를 짧은 시간 및 적은 비용으로 처리할 수 있는 기기 및 시스템을 확보하고 제품 및 공정문제 해결에 필요한 Solution 제공하는 역할을 하여야 한다.

LG 화학에서는 석유화학 기능소재, 정보전자소재, 이차전지 및 미래 혁신소재에 대한 분석이 진행되고 있으며 이 발표에서는 LG 화학을 포함한 화학기업에서의 연구개발, 생산, 마케팅활동에서의 분석기술 활용사례들을 소개하고 분석이슈들에 대하여 논의하고자 한다.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL2-1**
발표분야: Material Sciences in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 임재민

Development of a Non-invasive Probing Method for Pharmaceutical Analysis Using Spatially Offset Raman Spectroscopy

김형민

국민대학교 생명나노화학과

Vibrational spectroscopies, such as Infrared spectroscopy and Raman spectroscopy, should be a better solution for obtaining all information from large batch, since they only examine small volume of the sample. Furthermore, these spectroscopic methods are available for gathering molecular information including functional groups, chirality and tautomerism. They provide much valuable information, comparing with other sample selection ? and detecting methods, such as high performance liquid chromatography.Recently, an emerging new technique, spatially offset Raman spectroscopy (SORS) is a promising tool for the pharmaceutical analysis. SORS can provide more information than conventional Raman spectroscopy because it covers much larger sample size and wide depth. Also, it is non-destructive analysis tool through containers, such as bottles, sacks, and polymers. In this work, we developed SORS setup for probing mixing process of pharmaceutical ingredients. We improved the sampling and analysis speed and presented spectra with better signal to noise ratio, since this technique increases Raman signals. Also, for pharmaceutical industry, uniformity of all tablet components is essential to keep the patients' health. So, we demonstrated this technique as an analysis tool for proving the uniformity of the tablets.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ANAL2-2**

발표분야: Material Sciences in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 임재민

Probing Structural Dynamics of Intrinsically Disordered Amyloid Proteins using SAXS Spectroscopy and Ion Mobility Mass Spectrometry

김준곤

고려대학교 화학과

Information of structural dynamics and interactions of intrinsically disordered amyloid proteins is quite limited despite its importance to establish a principle for developing therapeutics for the associated degenerative diseases. Electrospray ionization ion mobility mass spectrometry (ESI-IM-MS) has been successfully applied to assess the structural analysis of proteins with its unique ability to separate, isolate, and characterize each conformer of protein. However, correlation between the structures of proteins in the gas phase and in solution has been yet to be understood clearly. In our laboratory, we have been utilized synchrotron solution small angle X-ray scattering (SAXS) spectroscopy and ESI-IM-MS for identification of conformers of intrinsically disordered proteins (IDPs) in solution and the gas phase, respectively. In this presentation, I will discuss our approach for characterizing the conformational dynamics and intermolecular interactions of IDPs using these two techniques. For example, beta-amyloid peptide (Ab) undergoes complexation with human serum albumin (HSA). We probed specific binding sites of Ab1-40 in HSA and structural conversion of Ab1-40 upon complexation. Additional examples of structural dynamics and aggregations of amyloid proteins will be further discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL2-3**
발표분야: Material Sciences in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 임재민

Element-based Absolute Quantification using ICP-OES and ICP-MS

임용현

한국표준과학연구원(KRISS) 분석화학표준센터

An element-based reductive approach provides an effective means of realizing International System of Units (SI) traceability for high-purity organic and biological standards. In this presentation, KRISS' approach to establish SI-traceable of pure nucleic acids and protein standards will be introduced. For protein stanards, a novel quantification method using double isotope dilution (ID) inductively-coupled plasma mass spectrometry (ICP-MS) combined with microwave-assisted acid digestion was developed for the first time. The method was validated and applied to certify candidate protein reference material (RM) of human growth hormone (hGH). The concentration of hGH was determined by analyzing the total amount of sulfur in hGH. Next, the size-exclusion chromatography method was used with ICP-MS to characterize and quantify sulfur-containing impurities. By subtracting the contribution of sulfur-containing impurities from the total sulfur content in the hGH CRM, SI-traceable certification value was obtained. The quantification result obtained with the present method based on sulfur analysis was in excellent agreement with the result determined via a well-established protein quantification method based on amino acid analysis using conventional acid hydrolysis combined with an ID liquid chromatography-tandem mass spectrometry. The developed method was applied for accurate analysis of protein drugs and standards including hGH, human thyroglobulin (hTG) and insulin. The element-based quantification methods developed here can be generally used for SI-traceable absolute quantification of pure organic- and bio-molecule standards.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ANAL2-4**
발표분야: Material Sciences in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 김태영

Quantitative analysis of nuclear materials in ultra-trace levels using thermal ionization mass spectrometry and its application to particle analysis

박종호* 송규석 임상호

한국원자력연구원 원자력화학연구부

A highly accurate and precise quantitative analysis of nuclear materials in ultra-trace levels plays an essential role in monitoring undeclared nuclear activities of corresponding facilities. Isotope dilution mass spectrometry coupled with thermal ionization mass spectrometry (ID-TIMS) was utilized to develop the analytical techniques and procedure for bulk analysis. The procedure is initiated with sample recovery by complete combustion of a sample and followed by dissolution of the recovered nuclear materials with nitric acid. Uranium (U) and plutonium (Pu) in the solution were separated with high purity by sequential ion chromatography using UTEVA resin. The quantities of U and Pu were determined by the isotopic measurements of TIMS and the amounts of reference materials added into solution as spikes. The analytical results for the nuclear materials in a simulated sample, which was prepared by blending known amounts of U and Pu reference materials, were in good agreement with the certified values. ID-TIMS was also applied to determine both of the quantity and the isotopic ratios of uranium in a micro-particles simultaneously. The verification of the application was performed using U030 particles

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **BIO-1**

발표분야: Protein biochemistry and biotechnology

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 하상수

Functional oligonucleotides for diagnostics and therapeutics

김동은

건국대학교 생명공학과

Oligonucleotides are attractive molecules as therapeutic biologic agents specifically targeting pathogenic genes and as diagnostic tools. RNA-cleaving antisense oligodeoxyribozymes, known as DNAzyme, is an attractive therapeutic oligonucleotide which enables cleavage of mRNA in a sequence specific manner and thus, silencing target gene. DNAzymes were designed to specifically target and cleave leukemogenic BCR-ABL fusion transcript sequence and the site of the point mutation (T315I), conferring imatinib resistance in BCR-ABL mRNA. DNAzymes significantly induced apoptosis and inhibited proliferation in wild-type and T315I-mutant BCR-ABL-positive cells. Next, I will present applications of RNA aptamer targeting prostate cancer cells as well as viral proteins. For example, anticancer drug (Doxorubicin)-encapsulating liposome was conjugated with an RNA aptamer specific to the prostate specific membrane antigen (PSMA), which is expressed on the surface of prostate cancer cells. The RNA aptamer-conjugated liposome (i.e. aptamosome) encapsulated with Dox were significantly more toxic to the targeted cancer cells than to nontargeted cancer cells. Dox-encapsulating aptamosomes administered to prostate cancer xenograft nude mice were selectively retained in tumor tissue with an antitumor efficacy. In the later part of the talk, I will show recent accomplishments regarding a simple diagnostic platform for detection of mutant DNA and RNA using graphene oxide. Hence, nucleic acids can be harnessed in a diverse way for diagnosis and therapeutics, especially when combined with functional nano-sized materials.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **BIO-2**
발표분야: Protein biochemistry and biotechnology
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 하상수

A helix-loop-helix motif of amphipathic alpha-helical peptides can deliver drugs in pico-molar concentration

유재훈

서울대학교 화학교육과

Since Tat peptide from a virus origin has been known as a membrane transduction domain, many cell penetrating peptides (CPPs) have been discovered and developed as carriers for drugs that could not be translocated into cells by themselves. However, the arginine based CPPs showed enough translocation efficiency only if the peptides exceed over micro-molar concentrations, giving severe cytotoxicity. Unlike those arginine-based CPPs, we have developed dimer bundles of alpha-helical amphipathic peptides with two disulfide bonds as the first generation of CPPs in our laboratory. These dimer bundle peptides are translocated into cells in their low nano-molar concentrations, facilitating to deliver a variety of drugs as low as a single digit nano-molar concentration. These 1st generation CPPs, however, possess an intrinsic limitation for the conjugation of drugs, because disulfide bonds were already used for the generation of the carrier. To trouble shoot this problem and to maintain excellent cell penetrating ability, we try to design and synthesize helix-loop-helix or helix-turn-helix motifs as decedents of 1st generation CPPs. One of them showed substantial amount of peptides got into cells in sub-nanomolar concentration as well as showed alleviated cytotoxicity. We can use these motifs as tools for delivering drugs as low as their pico-molar concentrations.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **BIO-3**
발표분야: Protein biochemistry and biotechnology
발표종류: 심포지엄, 발표일시: 목 14:35, 좌장: 하상수

DNA aptamer that specifically binds to the influenza NS1 protein suppresses interferon antagonism

정용주

국민대학교 생명나노화학과

Non-structural protein 1 (NS1) of the influenza A virus blocks the host's innate immune response by suppressing the induction of interferons. Therefore, blocking NS1 activity can be a potential strategy in the development of antiviral agents. In the present study, we selected a single-stranded DNA aptamer specific to the influenza NS1 protein after 15 cycles of systematic evolution of ligands by exponential enrichment (SELEX) procedure and examined the ability of the selected aptamer to inhibit the function of NS1. The selected aptamer binds to NS1 with a Kd of about 20 nM and RNA binding domain of NS1 is determined to be critical for the aptamer binding. The aptamer has a G-rich sequence in the random sequence region and forms a G-quadruplex structure. The localization of the aptamer bound to NS1 in cells was determined by confocal images, and flow cytometry analysis further demonstrated that the selected aptamer binds specifically to NS1. In addition, luciferase reporter gene assay, quantitative RT-PCR, and ELISA experiments demonstrated that the selected aptamer had the ability to induce interferon-β by suppressing the function of NS1. Importantly, we also found that the selected aptamer was able to inhibit the viral replication without affecting cell viability. These results indicate that the selected DNA aptamer has strong potential to be further developed as a therapeutic agent against influenza virus.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **BIO-4**

발표분야: Protein biochemistry and biotechnology

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 하상수

Ultrasensitive Biosensors Using Redox Cycling

양해식

부산대학교 화학과

High signal amplification is essential for ultrasensitive detection of biomolecules. In recent years, we have developed new redox cycling schemes combined with enzymatic amplification that allow high signal amplification along with low background levels. To minimize unwanted side reactions, a new concept that outer-sphere-reaction-philic species can react slowly with inner-sphere-reaction-philic species was applied. In this presentation, the signal amplification based on (i) electrochemical-chemical (EC) redox cycling using a reducing agent, (ii) electrochemical-chemical-chemical (ECC) redox cycling using a reducing agent and an oxidizing agent, and (iii) electrochemical-enzymatic (EN) redox cycling using a redox enzyme will be introduced.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **BIO-5**
발표분야: Protein biochemistry and biotechnology
발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 하상수

Unnatural Amino Acid Mutagenesis-Based Enzyme Engineering

윤형돈

건국대학교 특성화학부

Traditionally, enzyme engineering relies upon the substitution of one amino acid with other 19 natural amino acids to change the functional properties of an enzyme. However, in the past decade, the power of unnatural amino acid (UAA) incorporation method and its advancements have been harnessed for the development of various efficient biocatalysts. Enzyme engineering via in vivo residue-specific and site-specific incorporation methods has become established as a new route for producing enzymes with altered and improved functional properties. In this talk, in vivo UAA incorporation methodologies and applications for enzyme engineering will be briefly reviewed, and its future prospects will be discussed. Also our efforts in engineering omega-transaminase with UAA incorporation for improving the functional properties will be discussed

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장소: 대구 EXCO

발표코드: **ORGN1-1**

발표분야: Division of Organic Chemistry Symposium I

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 윤주영

Catalytic and Traceless Approaches to Complex Chemical Synthesis

이철범

서울대학교 화학부

Our laboratory has been interested in the development of synthetic tools and networks of reactions for efficient and selective chemical synthesis. In particular, we have been engaged in the chemistry of transition metal vinylidene complexes for catalytic alkyne functionaliztion. For the past several years, we have developed a range of reactions that are of broad potential utility in organic synthesis, which include carboxylative, alkylative, and hydrate cyclization reactions, and cycloisomerization reactions. In addition to these reactions, further explorations of a new mechanistic motif of metal-carbene oxidation have also led to the discovery of novel oxygenative alkyne addition reactions. The scope, mechanism and utility of the new processes will be discussed. Also presented in this talk will be our recent effort in the development of traceless C-C bond formations using organosulfur compounds. The new reaction forms C-C bonds stereoselectively by taking advantage of the reactivity of sulfone and allylic sulfinic acid functionalities, without leaving hints of the functional group unlike the traditional auxiliary chemistry. The details our studies will be described in this presentation.

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발표분야: Division of Organic Chemistry Symposium I
발표종류: 심포지엄, 발표일시: 목 14:05, 좌장: 조천규

SYNTHESIS WITH CYCLOBUTANES THE CHALLENGE OF MAKING AND BREAKING SMALL RINGS

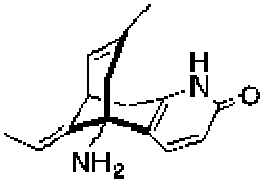
James D. White

Department of Chemistry, Oregon State University, Corvallis, Oregon

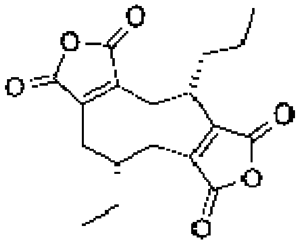
The cyclobutane ring contains approximately the same amount of strain (*ca.* 26 kcal.mol^{-1}) as the cyclopropane ring but application of the strain energy in a cyclobutane to the synthesis of less strained structures is much less well known than is the case with cyclopropanes. This lecture will focus on the synthesis of cyclobutanes using [2+2]-photocycloaddition of two alkene units and on subsequent fragmentation of the strained four-membered carbocycle in structural environments that afford a novel entry to certain natural products.

Several examples from our natural product work will be presented which illustrate the construction and controlled fragmentation of a cyclobutane intermediate as the pivotal step in a total synthesis. The examples include syntheses of byssochlamic acid, where a [2+2]-photoaddition-cycloreversion is used to create the nine-membered ring, elacomine, where a tandem intramolcular cycloaddition-retro-Michael sequence is the key step, and huperzine A, where two successive [2+2]-cycloadditions are followed by fragmentation of a cyclobutylcarbinyl cation generated by an intramolecular aza-Prins reaction.

Elacomine



Huperzine A



Byssochlamic Acid

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **ORGN1-3**
발표분야: Division of Organic Chemistry Symposium I
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 조천규

Total Synthesis of Inostamycin A

강성호

한국과학기술원(KAIST) 화학과, 한양대학교 화학과

Inostamycin A has been isolated from the culture broth of a microorganism pertaining to the genus *Streptomyces sp.* MH816-AF15.[1] In the isolation process, inostamycins B and C have also been found together. Their structures were assigned by NMR spectroscopy and later inostamycin A was confirmed by X-ray crystallography of its sodium salt. While inostamycin A has ethyl group at C2, inostamycin B is one-carbon less homolog with methyl substituent instead of the ethyl and inostamycin C corresponds to decarboxylated inostamycin A. Inosamycin A sodium salt is folded around the sodium ion coordinated with its two carboxyl oxygens, two hydroxyl oxygens at C9 and C17, carbonyl oxygen at C11, and ether oxygen between C13 and C16. The folding conformation is believed to be responsible for its various potent physiological properties as an ionophoric polyether antibiotic. Inostamycin A displays inhibitory activity against phosphatidyl inositol turnover and inositol transferase to prevent cell proliferation and transformation, antibacterial activity against Gram-positive bacteria, anti-HIV activity, and reversing effect on multidrug resistance in cancer cells. It also potentiates paclitaxel cytotoxicity, and induces arrest of cell growth at G1 and apoptosis in human small cell lung carcinoma Ms-1 cells.[2] Intrigued by its structural complexity and promising biological activities, we have been engaged in synthetic studies on inostamycin A. In this seminar, we present the first total synthesis of the natural product.

References

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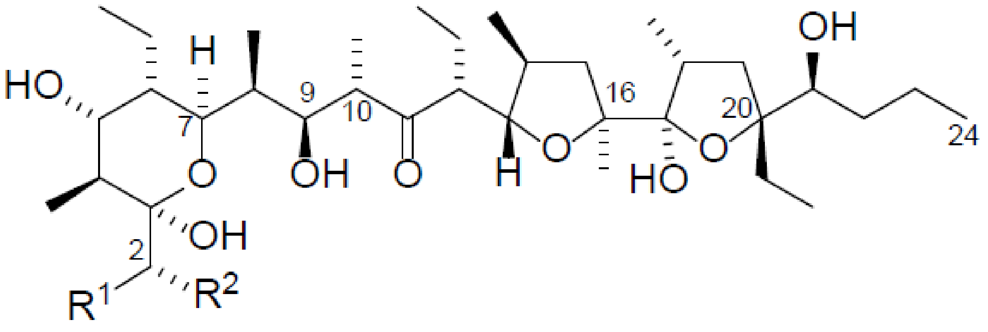
2. M. Kawatani, M. Uchi, S. Simizu, H. Osada, M. *Imoto, Exp. Cell Res.* 2003, *286,* 57.



Inostamycin A (reported) : $R^1 = CO_2H$ $R^2 = Et$
Inostamycin A (corrected) : $R^1 = Et$ $R^2 = CO_2H$
Inostamycin B : $R^1 = CO_2H$ $R^2 = Me$
Inostamycin C : $R^1 = Et$ $R^2 = H$

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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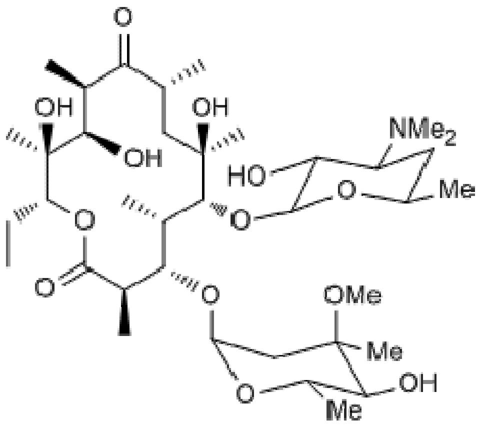
발표코드: **ORGN1-4**
발표분야: Division of Organic Chemistry Symposium I
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 조천규

Pikromycin and the Beyond: A Case of Natural Product Synthesis

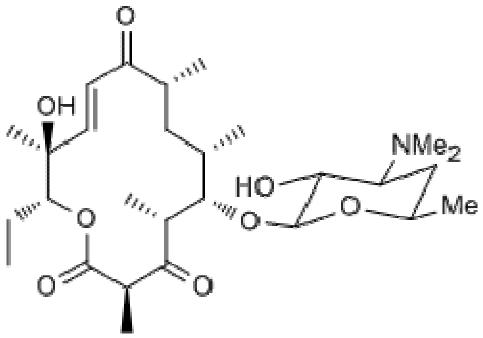
강한영

충북대학교 화학과

Macrolide antibiotics are a group of compounds that contains a macrolactone ring to which one or more sugars are attached. Although erythromycin has played a leading part in macrolide research, pikromycin is actually the first isolated macrolide antibiotics. Pikromycin is similar to erythromycin in structure because, it possesses a 14-membered macrolactone, pikronolide. However, it has only a single sugar, that is, desosamine attached to one of the hydroxy groups of the macrolactone ring. Pikromycin has recently regained attention as a promising target for biosynthetic studies due to fact that during its biosynthetic pathway, a series of macrolides are produced. Because as many as eight possible macrolides are produced by the polyketide synthase in Streptomyces venezuelae, it has emerged as an ideal target system for the biosynthetic study in relation to combinatorial biosynthesis. Inspired by the genetic study on the pikromycin biosynthesis, we have been involved in the total synthesis of macrolides appeared in the pikromycin biosynthesis with an aim of facilitating the biosynthetic research. As a result, total synthesis of pikromycin and related macrolides has been successfully achieved. Because the main reason that pikromycin and the related macrolides are relatively unknown might be ascribed to their low antibacterial activity, we have also made an effort to improve their biological activity.



Erythromycin A



Pikromycin

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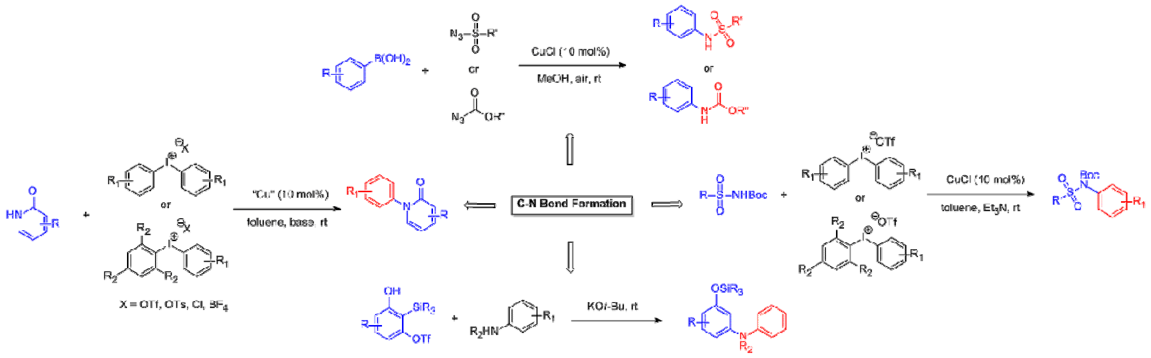
장소: 대구 EXCO
발표코드: **ORGN2-1**
발표분야: Division of Organic Chemistry Symposium II
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 홍석원

C-N Bond Formation Employing Transition Metal or Charge Transfer Method

김원석

이화여자대학교 화학 나노과학과

We have been developed a mild and efficient method for the synthesis of *N*-arylsulfonamide and *N*-arylcarbamate moieties, which are widely encountered in the structure of biologically active compounds, employing azides and boronic acids in an open flask at room temperature without any base, ligand, or additive. As an alternative way to synthesize *N*-arylsulfonamide derivatives, we also have demonstrated a new and mild synthetic method employing various tert-butyl *N*-sulfonylcarbamates and diaryliodonium salts as the coupling partner under copper-catalyzed conditions at room temperature. Furthermore, to explain the viability of diaryliodonium salts as an electrophilic coupling partner, we here reported copper-catalyzed C-N bond formation using 2-pyridone derivatives at room temperature.In addition, we employed the benzyne intermediate formed by 1,3-silyl group migration on the aryl moiety to demonstrate metal-free C-N bond formation. This base-promoted benzyne formation method would be used for the synthesis of 3-aminophenol or acridone derivatives, which are the scaffold of some synthetic compounds with various pharmacological activities.



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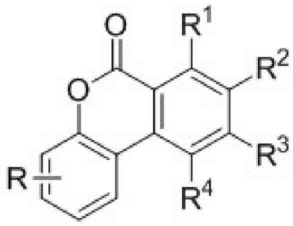
장소: 대구 EXCO
발표코드: **ORGN2-2**
발표분야: Division of Organic Chemistry Symposium II
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 홍석원

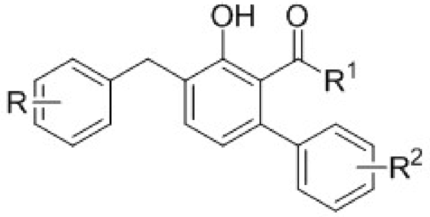
Construction of Diverse Aromatics and Heteroaromatics via Transition-Metal-Free Tandem Annulation

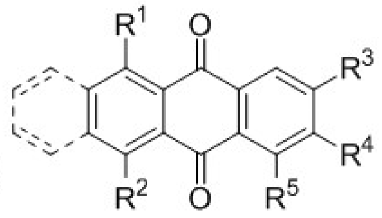
<u>이용록</u>

영남대학교 화학공학부

Tandem annulation has attracted great interest owing to their exceptional synthetic efficiency. This reaction plays a pivotal role in construction of aromatics and heteroaromatics for the use of pharmacological and highly advanced materials. Particularly, transition-metal-catalyzed tandem annulation reactions are now well-established, but most of these methods, if not all, suffer from certain drawbacks including the necessity of complex and expensive metal catalysts and harsh reaction conditions. Therefore, more environmentally benign and mild tandem annulation approaches are highly desirable to improve on these shortcomings. Herein, I present unique transition-metal-free tandem annulation for the construction of various functionalized and diverse aromatics and heteroaromatics such as benzo[c]chromenones, biaryls, anthraquinones, pyridines, and 2-pyridones. This protocol offers several significant advantages, such as catalyst-free, low toxicity, ease of handling, excellent functional group tolerance, and environmental benignity, under mild reaction conditions.


O
R1
R2
O
R3
R
R4


OH
O
R1
R
R2


R1
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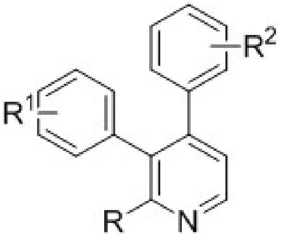
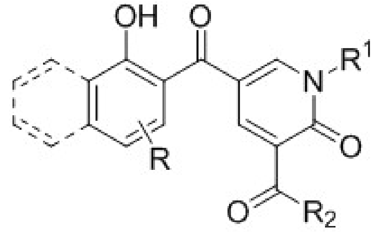

R2
R1
R
N


OH
O
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R2

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발표코드: **ORGN2-3**
발표분야: Division of Organic Chemistry Symposium II
발표종류: 심포지엄, 발표일시: 금 15:20, 좌장: 홍석원

Toward Sustainable Chemical Synthesis: Ruthenium-Catalyzed C-N Bond Formation Reactions Using Methanol as C1 Source

홍순혁* 김승효 강병준

서울대학교 화학부

Development of useful, practical, and selective synthetic methods that generate minimal by-product is of critical importance in both academic and industrial research. The research of our group seeks to develop practical and environmentally friendly synthetic methodology using transition metal catalysts. Specifically, we have explored novel C-N bond formation reactions from primary alcohols and various N-sources, chemical synthesis using CO_2 and methanol as C1 feedstock, and development of organometallic catalysts based on N-heterocyclic carbene ligands. In this symposium, we will present our recent development utilizing methanol, an environmentally benign and economical molecule, as C1 source.

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발표분야: Division of Organic Chemistry Symposium II
발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 홍석원

Towards Sub-ppm Level Loading Asymmetric Hydrogen-Bond Catalysis

송충의

성균관대학교 화학과

The field of organocatalysis has blossomed over the past few decades, becoming an alternative to transition-metal catalysis or even replacing the realm of transition-metal catalysis. However, a truly powerful organocatalyst with a high turnover number and turnover frequency while retaining high enantioselectivity is yet to be discovered. Despite many efforts, the current limit of catalyst loading for asymmetric organocatalysis is usually in the range of 0.1-1 mol% for overriding of the non-selective background pathway. Similar to metal catalysis, thus, extremely low catalyst loading (ppm or ppb levels) is the ultimate goal of the organocatalysis community. In this symposium, I will present our recent contributions in this context.[1-4] For examples, quite recently, we developed ppm level loading asymmetric hydrogen bond catalysis by designing a in-situ repairable catalyst system[3] or by employing a hydrophobically directed catalyst system.[4]

References
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3. Park, S. Y.; Lee, J.-W.; Song, C. E. *Nature Communications* 2015, 7, 7312.
4. Bae, H. Y.; Song, C. E. *ACS Catal.* 2015, 5, 3613.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **BI&OR-1**
발표분야: Joint Symposium between Organic and Life Chemistry Divisions: Biomolecules and Biomimetics
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 임현석

Handedness Control of Unconventional Peptide Helices

최수혁

연세대학교 화학과

?Beta-peptide helices are among the most extensively studied secondary structures of unnatural peptides. Cis-2-aminocyclohexanecarboxylic acid (cis-ACHC) is known to promote mixed helices such as the beta-peptide 12/10-helix and the alpha/beta-peptide 11/9-helix in solution. The crystal structures of the 11/9-helix have recently characterized. However, no atomic resolution structures of the 12/10-helix has been reported to date. We successfully characterized the crystallographic structure data of the 12/10-helix from racemic mixtures of cis-ACHC oligomers with alternating chirality. The crystal structure suggested that those oligomers could adopt two types of 12/10-helical conformations with the opposite handedness. Various-temperature NMR experiments indicated that there are at least two sets of different conformations that are in equilibrium. X-ray crystallographic analysis and further NMR experiments confirmed that they are indeed 12/10-helices with opposite handedness. The handedness of these beta- and alpha/beta-peptide helices is dependent on the residue types, the capping groups of either terminus, or solvent conditions. The incorporation of a single residue can override all these conditions and control the handedness of the unconventional helices.

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발표분야: Joint Symposium between Organic and Life Chemistry Divisions: Biomolecules and Biomimetics
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 임현석

변형핵산 및 올리고뉴클레오티드 합성을 이용한 DNA 이차구조에 관한 연구

서영준

전북대학교 화학과

DNA 와 RNA 의 이차 구조(G-quadruplex, i-motif, B-Z-DNA, CNG 반복염기서열)의 다이나믹스와 관련된 탐지 시스템에 관련한 연구는 DNA 와 RNA 의 이차구조가 유전자의 발현 조절 및 각종 암과 정신 질환등 다양한 질병과도 관련하여 중요한 역할을 한다는 것이 최근에 밝혀짐에 따라 후생유전학에서 가장 중요한 연구의 한 분야가 되고 있다. 본인은 이러한 DNA 와 RNA 의 이차 구조에 관한 연구를 위해 합성핵산 과 합성 올리고뉴클레오티드를 이용하여 이러한 구조의 다이나믹스를 연구하고 있다. 본 연구를 통해 DNA 의 Telomere 에서 처음 발견 되어지고 사람의 나이와 상관관계가 있으며 최근에는 유전자의 promoter 영역에서 유전자의 발현 조절 과정에도 중요한 역할을 하는것으로 밝혀진 G-quadruplex DNA 이차구조 에 관련한 연구를 진행 하였다. 특히 대표적인 유전자의 변형인 TT dimerization 이 G-quadruplex 의 구조의 안정성에 미치는 영향 및 상관 관계를 알아 보고 그 모니터링 시스템을 개발하고자 하였으며 연구 결과를 통해 TT dimerization 이 G-quadruplex 의 구조의 안정성에 지대한 영향을 미치는 것을 확인할 수 있었고 이를 탐지하는 시스템을 개발할 수 있었다. 또한 이러한 모델 시스템에 대한 연구를 생체내 실제 시스템에 접목하고자 DNA 중합효소가 인식가능한 형광성 인공 핵산을 개발하여 이러한 이차구조를 가진 DNA 에 도입하고자 하는 노력을 소개하고자 한다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **BI&OR-3**
발표분야: Joint Symposium between Organic and Life Chemistry Divisions: Biomolecules and Biomimetics
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 임현석

Design and Evaluation of Soluble Glycosphingolipid Immunostimulants

김상희

서울대학교 약학대학/약학과

It has been of considerable interest to identify the lipid antigens that can be presented by CD1 molecules of antigen-presenting cells. The identified CD1-presented glycolipid antigens have diverse molecular architectures, but they share the common characteristics of containing a long straight alkyl chain moiety in their lipid structures. Due to the presence of this moiety along with their amphiphilic properties, most CD1 lipid ligands have very poor solubility, which limits their usefulness in basic and medical research. We have designed and synthesized various types of non-stereotypical glycolipid derivatives that have improved solubility, based on the X-ray crystal structures of antigen-presenting CD1 molecules. One example is branched chain-containing glycosphingolipid derivatives of the prototypical CD1d ligand KRN7000. Another example is ω-hydroxyl group containing KRN7000 analogs. We wish to discuss our own findings on this subject.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **BI&OR-4**
발표분야: Joint Symposium between Organic and Life Chemistry Divisions: Biomolecules and Biomimetics
발표종류: 심포지엄, 발표일시: 금 10:05, 좌장: 서지원

Self-Assembling Peptides as Mega-Modulators/Detectors of Biomacromolecular Interactions

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 nanomaterials as mega-modulators & detectors of biomacromolecular interactions, will be presented.

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장소: 대구 EXCO
발표코드: **BI&OR-5**
발표분야: Joint Symposium between Organic and Life Chemistry Divisions: Biomolecules and Biomimetics
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 서지원

Structure-Based Design and Efficient Synthesis of Kinase Inhibitors via Catalysis

홍승우

한국과학기술원(KAIST) 화학과

Transition-metal-catalyzed direct and regioselective C?H bond activation/functionalization is a highly efficient and straightforward tool that is useful in the field of organic synthesis and total synthesis. Driven by the need for a more efficient synthetic route to the kinase inhibitors, we have explored one-pot catalysis of tandem processes for generating molecular complexity from simple starting materials by employing a single catalyst in a single reaction vessel. Cyclopropane is also widely used as a conformational restricting framework in medicinal chemistry, and arylated cyclopropanes are a privileged class of structures found in many biologically active molecules. In this regards, transition-metal-catalyzed asymmetric C?H arylation of cyclopropanes has been the focus of great research interest. We hypothesized that an appropriate chiral bidentate directing group embedded in the substrate could induce high levels of stereocontrol during C?H functionalization via a steric repulsion. With efficient synthetic routes in hand, we have studied application of the structure-based design to identify potent kinase inhibitors and ultimately streamline late-stage drug modification. Ongoing results in this direction and future plan will be presented and discussed.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **MEDI-1**

발표분야: Current Trends for Infectious Disease

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 한수봉

Discovery an Antiviral Agent Targeting the Influenza Viral M2 Protein from Target-free Screening of a Chemical Library

김미현

한국화학연구원 바이러스시험연구그룹

A cytopathic effect-reduction assay was performed to discover anti-influenza viral agents from a chemical library composed of 2,000 existing drugs and natural products. Among the hit compounds, compound X inhibited the infection of influenza A viruses A/Puerto Rico/8/34 (PR8) (H1N1), A/Hong Kong/8/68 (H3N2) and B/Lee/40 with half maximal effective concentrations of 0.5, 0.4, and 1.6 μM, respectively. Its half maximal cytotoxicity concentration in Madin-Darby canine kidney cells was about 22.9 μM. The antiviral efficacy was further confirmed by the plaque inhibition assay and Western blot analysis, resulting in the reduction of both influenza viral plaque titers and protein expression by compound X in a dose dependent manner. Confocal microscopy showed obvious accumulation of the viral nucleoprotein (NP) in the cytoplasm of the influenza virus-infected cells at 5 h post-infection, when treated with compound X, while NP was efficiently localized into the nucleus without the compound. Measurement of proton conductance across influenza A matrix 2 protein (M2) incorporated into the lipid bilayer of virus-like particles (VLPs) suggested that compound X inhibited proton movement across the M2 channel. In conclusion, we propose that compound X potentially targets the viral entry step by blocking the proton channel function of M2.

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장소: 대구 EXCO
발표코드: **MEDI-2**
발표분야: Current Trends for Infectious Disease
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 한수봉

Anti-viral drug discovery targeting 3C, 3C-like proteases and neuraminidase

Po-Huang Liang

Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan

A novel coronavirus causing severe acute respiratory syndrome (SARS) spread to more than 30 countries, infecting nearly 8000 people and causing around 800 fatalities in 2002-2003. After 10 years of silence, a newly emerged Middle East respiratory syndrome coronavirus (MERS-CoV) causes SARS-like disease. We and others have developed inhibitors for the 3C-like protease, a valid target for anti-SARS agents, which seem to be also effective against MERS 3C-like protease. Particularly, using a compound bank from Korea Research Institute of Chemical Technology, we identified a dual inhibitor of picornavirus 3C and coronavirus 3C-like proteases. Using this collection, we recently identified an inhibitor for the neuraminidase of H5N1 avian flu virus.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MEDI-3**
발표분야: Current Trends for Infectious Disease
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 오태권

Autophagy: a New Paradigm for Protective Immunity in Tuberculosis

조은경

충남대학교 미생물학교실

Tuberculosis remains a major public health problem worldwide. In developing countries, tuberculosis remains highly endemic, and the global incidence is increasing as a consequence of the human immunodeficiency virus epidemic. Mycobacterium tuberculosis (Mtb) is a successful pathogen that enhances its own intracellular survival by arresting phagolysosomal fusion. Autophagy is an essential process for lysosomal degradation to eliminate protein aggregates and damaged organelles, thus maintaining intracellular homeostasis against various stress conditions. It is now becoming clear that autophagy is crucial in host immune defense against infection with intracellular bacteria, including Mtb, through enhancement of phagosomal maturation. Emerging evidence has shown that autophagy is involved in potential therapeutics for various human disorders, including metabolic conditions, neurodegenerative diseases, cancers, and infectious diseases. Last several years, we have focused on the roles of autophagy and the mechanisms by which autophagy activates innate immunity in Mtb infection. Today, I’ll talk about an overview of the roles and mechanisms by which autophagy activates host protective immunity against mycobacterial infection. Our previous and current data for potential strategies to induce autophagy will be discussed on the basis of development of an antimicrobial therapy against tuberculosis. Advances in our understanding of autophagy will provide a new opportunity to combat mycobacterial infection through to modulation of host-pathogen interaction as a potential therapeutic strategy.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MEDI-4**
발표분야: Current Trends for Infectious Disease
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 오태권

최근 항생제 개발동향과 레고켐바이오사이언스의 항생제 개발현황 소개

조영락

레고켐바이오사이언스 신약연구소

미국 IDSA 에서 2004 년 “Bad Bugs, No Drugs” 라는 제목의 보고서를 내고 2020 년까지 10 개의 새로운 항생제를 확보하자는 캠페인을 시작한지 10 년이 더 지났다. 그 영향인지 최근 1 년 사이 5 개의 새로운 항생제가 승인을 받았다. 그러나 여전히 수퍼박테리아에 대항할 치료제 부족에 대한 우려는 전세계적인 이슈로 떠오르고 있으며 새로운 계열의 약물개발은 최근에 모두 실패로 돌아갔다. 더우기 작년에 만들어진 Longitude prize 는 170 억원에 상당하는 상금을 걸고 항생제 내성증가를 방지할 수 있는 진단 시스템을 찾는 쪽으로 방향을 잡았다. 결국 글로벌 관심은 새로운 신약의 개발보다 진단쪽으로 쏠리는듯 해 보이며 신약개발은 점차 어려운 환경에 직면해 있는 실정이다.이러한 어려운 상황속에서 레고켐은 현재 가장 문제시 되고 있는 병원균에 대해 3 개의 항생제를 개발 중에 있다. 먼저 LCB01-0371 은 MRSA, VRE 등 그람양성균 뿐 아니라 MDR-TB 에도 우수한 약효를 보여주며 장기투여가 가능한 약물로 현재 임상 1 상을 마치고 임상 2 상을 준비 중이다. LCB01-0699 는 리네졸리드 내성 MRSA 균에도 탁월한 효과를 보이는 화합물로 현재 중국회사와 공동으로 전임상 시험을 진행중이며 내년에 IND filing 을 할 계획이다. LCB10-0200 은 그람음성균에 효과적인 세파계 항생제로 특히 MDR-P.aeruginosa 에 탁월한 효과를 가진 물질로 현재 전임상 시험중이며 내년에 임상 1 상을 계획 중이다. 이번 발표에서는 이들 파이프라인에 대한 간략한 소개와 앞으로 항생제 개발방향에 대해 소개하고자 한다.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **MAT1-1**

발표분야: Recent Trends in Materials Research for Emerging Electricity Storage Devices

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 황성주

Intercalation chemistry of divalent ions of Mg, Zn and Ca into transition metal host materials for future batteries

홍승태

대구경북과학기술원(DGIST) 에너지시스템공학

Li ion batteries (LIB) are one of the most successful energy storage devices for portable electronics application, electrical vehicles, and utility grids. However, there are still strong needs for higher energy density and lower price materials than what the LIB systems can provide. Environmental friendliness, reliability, safety and plentiful sources could be typical advantages of magnesium, zinc and calcium materials over the lithium. A rechargeable battery utilizing intercalation of divalent ions such as Mg^{2+}, Ca^{2+} or Zn^{2+} could be one of the strategies to overcome capacity limit of LIB, and/or to produce lower price batteries. Mg rechargeable batteries have received attention since the reversible Mg intercalation into the Chevrel phase, Mo_6S_8, was demonstrated in 2000. Very recently, zinc or calcium-based rechargeable batteries have also received attention. However, only a few materials have been reported for the successful host materials that can intercalate such divalent ions reversibly. The electrochemical intercalation chemistry is one of newly emerging research fields for future batteries. In the presentation, a recent progress in our exploration for new intercalation chemistry of such divalent ions into various host materials will be presented, utilizing aqueous electrolytes as well as non-aqueous electrolytes.

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장소: 대구 EXCO
발표코드: **MAT1-2**
발표분야: Recent Trends in Materials Research for Emerging Electricity Storage Devices
발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 황성주

Versatile use of graphene in secondary ion batteries

표명호

순천대학교 인쇄전자공학과

In this talk, the benefits of utilization of graphene (oxide) in secondary ion batteries will be presented. Firstly, the effect of graphene oxide (GO) coat on Al current collector on corrosion protection and thereby, the improvement electrochemical properties is discussed. Secondly, the advantage of graphene framework, which physically entraps metallic nanoparticles, is addressed. Various types of anode materials (alloy, conversion, others) will be covered and improvement in both retention and reversible capacities be reported. Thirdly, the control of solid-electrolyte interface on cathodes by spontaneous assembly with graphene is discussed. In addition to these applications of graphene (oxide) in Li-ion batteries, use for cathodes (Prussian blue) in sodium ion batteries will also be briefly covered. Finally, extraction of critical parameters governing energy density of Li-storage cathode materials (layer and spinel) will be unraveled by confirmatory factor analysis.

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장소: 대구 EXCO
발표코드: **MAT1-3**
발표분야: Recent Trends in Materials Research for Emerging Electricity Storage Devices
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 황성주

Fundamental design principles of cathode catalysts for rechargeable Li-O2 batteries

강용묵

동국대학교 융합에너지신소재공학과

A major drawback of lithium-air batteries is its low round trip efficiency resulting from high thermodynamic stability of Li2O2. Various types of materials have been adopted as the catalysts to reduce potential hysteresis and thus attain high round-trip efficiency. In particular, α-MnO2 has received great attention as a catalyst for lithium-air batteries since its superior catalytic activity was introduced by P.G. Bruce et al.. Because the relatively good catalytic activity of α-MnO2 among various metal oxides results from easy accommodation of Li2O2 inside its large 2x2 tunnel structure, many researchers have tried to vary the macrophysical properties such as porosity, surface-to-volume ratio and so on to enhance the electrochemical properties of lithium-air batteries. However, such kind of piecemeal approaches without detailed understanding on the fundamental physical properties governing the catalytic activity of materials failed to make a breakthrough in the development of commercially available catalysts.Hence, we here try to change the crystal structure, surface structure and shape of various catalysts to elucidate their effects on the catalytic activities. The catalysts such as α-MnO2, PdCu, Pt3Co, Pt, etc. have been used to figure out the fundamental design principles of cathode catalysts for Li-O2 batteries. As a result, we knew that surface energy, crystal structure and elemental composition are all important to develop the most optimum metal catalysts to attain high reversibility of Li-O2 batteries.

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장소: 대구 EXCO

발표코드: **MAT1-4**

발표분야: Recent Trends in Materials Research for Emerging Electricity Storage Devices

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 황성주

Multilength-Scale Structural Engineering of Electrode Materials for High Performance Li-Ion Batteries

박병우

서울대학교 공과대학 재료공학부

전기자동차의 상용화에 있어 장벽들은 배터리의 문제점과 직결되는데 특히 전기자동차의 절반이상을 차지하는 비용과 발열문제로 인한 위험성은 전기자동차 배터리에서의 가장 큰 이슈라고 할 수 있다. 이에 높은 안정성과 수명특성을 지니면서 고 에너지 밀도를 가지기 위한 대안 활물질로써 $Li_4Ti_5O_{12}$ 와 $LiMnPO_4$ 를 소개하고자 한다.

음극재 중의 하나인 $Li_4Ti_5O_{12}$ 의 경우 높은 lithiation 전압으로 인해 리튬의 수지상 반응과 solid electrolyte interface 와 같은 부반응을 막아줄 뿐만 아니라 lithiation 과정에서 부피변화가 0.2%에 불과하기 때문에 안정성과 수명특성에 있어 큰 장점을 가지고 있다. 하지만 낮은 전기전도도로 인해 고속 충·방전에서 수명이 저하되고 에너지 밀도가 낮다는 단점을 가지고 있다. olivine 구조를 가지는 양극재인 $LiMnPO_4$ 는 환경친화적인 망간과 그 구조적 안정성으로 인해 큰 관심을 받았지만 낮은 전기 전도도와 1-D diffusion channel 로 인한 낮은 리튬 이온 확산도로 인해 상용화에 큰 어려움이 있었다.

이렇게 앞서 소개한 $Li_4Ti_5O_{12}$, $LiMnPO_4$ 활물질의 단점들을 보안하기 위해 시도한 Multilength-Scale Structural Engineering 을 본 발표에서 말하고자 한다. 우선 음극재의 $Li_4Ti_5O_{12}$ 의 경우 graphene oxide 을 활용한 전구체 TiO_2 에 고체상 반응을 통해, 단결정 $Li_4Ti_5O_{12}$ 에 graphene 을 균일하게 wrapping 함으로써 $Li_4Ti_5O_{12}$ 의 낮은 전기 전도도를 보완하였고, 이로 인해 10 C 에서 ~150 mAh g^{-1} 의 높은 방전용량을 구현하였다. 또한 양극재 $LiMnPO_4$ 의 경우 solvothermal 방법으로 $LiMnPO_4$ aggregates 의 합성을 시도하였고, 약 30 나노 크기의 일차입자로 이루어진 마이크론 크기의 aggregates 는 ~1.2 g cm^{-3} 의 높은 tap density 를 보였다. 여기에 더불어 $LiMnPO_4$ aggregates 표면의 카본코팅으로 전기화학적 특성 향상을 보였다. 이와 같이 본 연구진은 다양한 scale 에서의 구조적 제어를 통해 재료 물성을 변화 시킴으로써 리튬 이온 배터리의 performance 향상에 큰 영향을 보임을

확인하였고, 이를 다양한 분석들을 통해서 정량적으로 파악하였다.

References

[1] Y. Oh, S. Nam, S. Wi, J. Kang, T. Hwang, S. Lee, H. H. Park, J. Cabana, C. Kim, and B. Park, *J. Mater. Chem. A* 2, 2023 (2014).

[2] H. Wang, Y. Yang, Y. Liang, L. F. Cui, H. S. Casalongue, Y. Li, G. Hong, Y. Cui, and H. Dai, *Angew. Chem. Int. Ed.* 123, 7502 (2011).

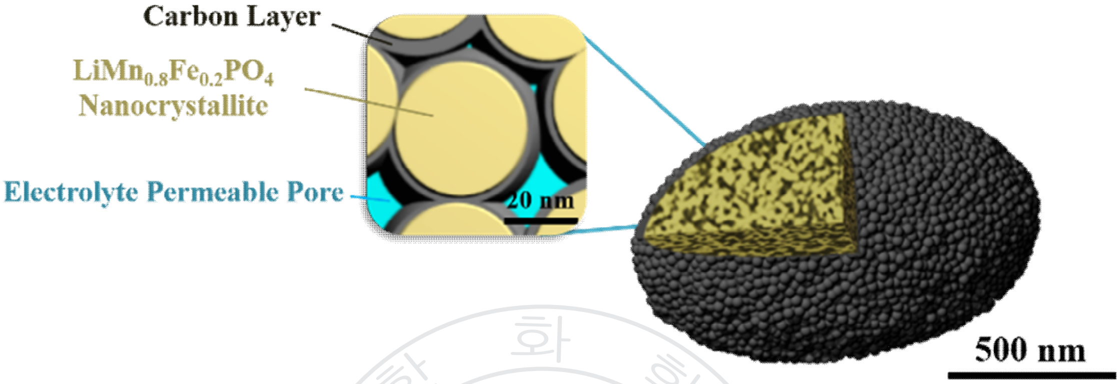

그림 1. $LiMn_{0.8}Fe_{0.2}PO_4$ Aggregates 모식도

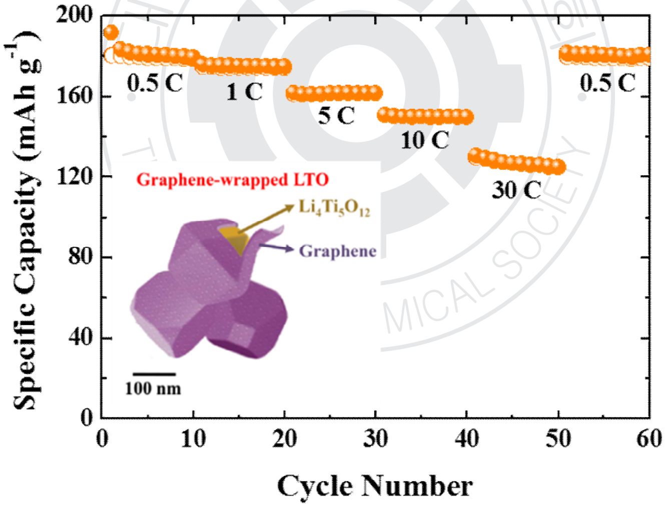

그림 2. Graphene-wrapped LTO의 모식도 및 전기화학적 특성

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT1-5**
발표분야: Recent Trends in Materials Research for Emerging Electricity Storage Devices
발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 황성주

High-Voltage Interfacial Chemistry of 55^{o}C Full-Cell of $Li_{1.13}Mn_{0.463}Ni_{0.203}Co_{0.203}O_2$//graphite

송승완

충남대학교 응용화학공학과

Enabling the high energy density Li-ion batteries requires the use of high-capacity and high-voltage cathode material such as Li-rich layered oxide cathode (xLi_2MnO_3?(1-x)$LiMO_2$ (M=Mn,Ni,Co)). A critical limiting factor for high-voltage battery operation is however the anodic instability of conventional electrolyte that undergoes severe oxidative decomposition and causes a rapid performance fade and safety issue, in particular, at elevated temperature. Overcoming these issues rely on an electrolyte breakthrough and the stabilization of surface films on both cathode and anode, based on a basic understanding of interfacial phenomena and failure mechanism. We have been searching for and evaluating a number of high-voltage electrolyte additives for charging the Li-rich layered oxide cathode to 4.8V *vs.* Li/Li^+ and thus increasing its capacity. This presentation would summarize our recent research results on the performance enhancement of full-cell of $Li_{1.13}Mn_{0.463}Ni_{0.203}Co_{0.203}O_2$//graphite under a harsh condition of charge voltage of 4.7V and elevated temperature of 5555^{o}C through the control of high-voltage interfacial chemistry with functional additive, in contrast to a rapid performance in conventional electrolyte, and the interfacial causes for these performance enhancement and fade.This research was supported by the Korean Ministry of Trade, Industry & Energy (A0022?00725, 10049609), Ministry of Education (2012026203), and Chungnam National University.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT2-1**
발표분야: Recent Advances in Nanocatalysts
발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 박성진

Single-Atom Pt Electrocatalysis: Oxygen Reduction via H_2O_2 formation instead of H_2O

최민기

한국과학기술원(KAIST) 생명화학공학과

High activity and distinct chemoselectivity are expected for single-atom electrocataysis, but its realization has not yet been demonstrated so far because carbon as the most widely used electrocatalyst support cannot stabilize single-atom metal species. In this work, we report for the first time that a sulfur-doped zeolite-templated carbon, simultaneously exhibiting extra-large sulfur content as well as a unique carbon structure (i.e., highly curved 3-dimensional networks of graphene nanoribbons), can stabilize relatively high loading of Pt (5 wt%) as a single-atom species. In oxygen reduction reaction (ORR) as a first model reaction, this single atom catalyst does not follow a conventional 4-electron pathway producing H_2O, but selectively produces H_2O_2 even over extended times without significant degradation of the catalyst activity.

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장소: 대구 EXCO
발표코드: **MAT2-2**
발표분야: Recent Advances in Nanocatalysts
발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 박성진

Triple-Deck 3D Photoanodes with Conformal Interfaces: Enhanced Photoelectrochemical Water Oxidation

박종혁

연세대학교 화공생명공학과

The WO3/BiVO4 system is attractive for photoelectrochemical (PEC) water splitting processes because of the perfect synergistic effects in the heterojunction construction due to their well-matched band edge positions. However, the system suffers from poor charge collection and cannot be efficiently utilized because of non-ideal interfaces. Here, we report a triple-deck three-dimensional (3D) architecture that was designed through the ameliorative swelling-shrinking fabrication process by a polystyrene template, with a promising photocurrent density of 5.1 mA/cm2 at 1.23 V vs. RHE under AM 1.5G illumination. Using the uniformly distributed FeOOH/NiOOH oxygen evolution co-catalyst (OEC) layer as the outer most shell of the WO3/BiVO4/OEC triple-deck 3D structure, the water splitting efficiency was improved dramatically by facilitating the charge transfer process at the electrode/electrolyte interface. The highly open 3D macroporous nanostructure is helpful for the synthesis of the triple-deck 3D photoanodes with layer-by-layer distribution of WO3/BiVO4/FeOOH/NiOOH while promoting the water oxidation kinetics.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT2-3**
발표분야: Recent Advances in Nanocatalysts
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박성진

From 2D Nanosheets to 3D Nanohybrid Photocatalysts

황성주

이화여자대학교 화학·나노과학과

Solar energy is one of the promising renewable energy sources that can fulfill the rising global demand for sustainable energy. One of the most effective approaches to harvest solar energy is the photoinduced production of H_2 and O_2. Despite a great deal of researches, most of inorganic photocatalysts ever-developed is not appropriate for the visible light-induced water splitting because of unsuitable band structure and poor stability. To circumvent this problem, we have tried to synthesize hybrid-type visible light active photocatalysts via self-assembly between two kinds of nanostructured semiconductors including 2D nanosheets and 0D nanoclusters. As building blocks, the 2D nanosheets of layered metal oxide, layered double hydroxide (LDH), and reduced graphene oxide (rGO) are synthesized by the exfoliation process of the pristine layered materials. The obtained 2D inorganic/rGO nanosheets are reassembled with each other or hybridized with other 0D nanoparticles. The band structure and surface area of wide bandgap layered metal oxide can be effectively tailored through the hybridization with LDH 2D nanosheets or transition metal oxide/metal chalcogenide 0D nanoparticles. The obtained nanohybrids show promising photocatalytic activity to effectively decompose organic compounds or to produce H_2 and O_2 gases under the irradiation of visible light.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT2-4**
발표분야: Recent Advances in Nanocatalysts
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 박성진

Nanostructured Carbon-Based Electrocatalysts for Oxygen Reduction Reaction: Enhancing Catalytic Activity and Identifying Active Sites

주상훈

울산과학기술대학교(UNIST) 에너지화학공학부

The development of highly active, durable, and low-cost oxygen reduction reaction (ORR) catalysts is central to making polymer electrolyte fuel cells (PEFCs) commercially viable. In this regard, noble metal-free, nanostructured carbon-based electrocatalysts for the ORR have been of tremendous interests. Yet, the ORR activity of carbon-based catalysts is still lagged behind the Pt-based catalysts. Furthermore, the understanding of critical factors governing the ORR activity of carbon-based catalysts and the identification of their active sites are still not well understood. In this talk, we present the design strategies toward high-performing ORR catalysts based on mesoporous carbons and carbon nanotubes. In addition, our recent efforts for understanding the active sites in the nanocarbon-based ORR catalysts will be also presented.

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장소: 대구 EXCO
발표코드: **MAT3-1**
발표분야: New Visions in Nano-Materials Chemistry
발표종류: 분과기념강연, 발표일시: 금 14:30, 좌장: 유효종

Hybrid Materials of Transition Metal Dichalcogenides and Reduced Graphene Oxide

신현석

울산과학기술대학교(UNIST) 화학과

The rapid progress in graphene research has led to intensive exploration of novel 2D materials. In particular, transition metal dichalcogenides with layered structures have received significant attention because they offer many opportunities for fundamental and technological research in a variety of fields, including catalysis, energy storage, sensing, and electronic devices. In this talk, I demonstrate preparation and characterization of various transition metal chalcogenides/reduced graphene oxide (rGO) hybrid materials such as VS4/rGO, WS2/rGO, and CoS2/rGO by a simple hydrothermal method. In particular, the role of rGO as a support for synthesis of transition metal chalcogenides is explained: rGO induces morphology change or increase of purity of synthesized transition metal chalcogenides. Lastly, I discuss applications of the hybrid materials to an energy storage device and a catalyst for hydrogen evolution reaction.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC1-1**
발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research I
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 방진호

Development of semiconductors for sunlight-driven fuel productions

박현웅

경북대학교 에너지공학부

As the costs of carbon-footprinted fuels grow continuously and atmospheric carbon dioxide concentration increases, solar fuels are receiving growing attention as alternative clean energy carriers. These fuels include molecular hydrogen and hydrogen peroxide produced from water, and hydrocarbons converted from carbon dioxide. For high efficiency solar fuel production, not only light absorbers (oxide semiconductors, Si, inorganic complexes, etc) should absorb most sunlight, but also charge separation and interfacial charge transfers need to occur efficiently. With this in mind, this talk will introduce the fundamentals of artificial photosynthesis, on-going researches, and then discuss in detail on solar CO2 conversion.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC1-2**
발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research I
발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 방진호

Bio-inspired Mn based Catalysts for water oxidation

남기태

서울대학교 재료공학부

Water splitting is regarded as a promising step towards environmentally sustainable energy schemes because electrolysis produces only hydrogen and oxygen, without any by-products. The oxygen evolution reaction (OER), an anodic half-cell reaction that generates an oxygen molecule from two water molecules, generally requires extremely high overpotential due to its slow reaction kinetics. In nature, there exists a water oxidation complex (WOC) in photosystem II (PSII) comprised of the earth-abundant elements Mn and Ca. The WOC in PSII, in the form of a cubical CaMn4O5 cluster, efficiently catalyzes water oxidation under neutral conditions with extremely low overpotential value and a high TOF number. Four Mn atoms are oxo-bridged in asymmetric positions and undergo successive changes in oxidation state, taking part in a so-called Kok cycle. Inspired from the nature, we designed new manganese based water oxidation catalysts, Mn3(PO4)2-3H2O and Li2MnP2O7.We first identified a new crystal structure, Mn3(PO4)2-3H2O, that precipitates spontaneously in aqueous solution at room temperature and demonstrated its superior catalytic performance at neutral pH. The bulky phosphate polyhedron induces a less ordered Mn geometry in Mn3(PO4)2-3H2O. From the combined ex-situ spectroscopic analysis and DFT calculations, we revealed that structural flexibility can stabilize Jahn-Teller distorted Mn(III), and thus facilitate Mn(II) oxidation during catalytic cycle. We also studied a new pyrophosphate based Mn compound, Li2MnP2O7 for water oxidation catalysis. Influence of oxidation state of Mn and asymmetric Mn geometry on water oxidation catalysis was verified using Li2MnP2O7 and its derivatives. We believe higher Mn(III) portion and asymmetric arrangement of Mn atoms which can be seen in the WOC, enhance catalytic water oxidation reaction.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ELEC1-3**

발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research I

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 방진호

Nanostructure electrocatalysts for CO$_2$ conversion

황윤정

한국과학기술연구원(KIST) 청정에너지 연구센터

Electrochemical reduction is a promising pathway of CO2 conversion which can be coupled with photovoltaic cells to realize solar-to-fuel conversion system, but it is still challenging due to a requirement of high overpotential as well as a poor selectivity among various products. In addition, in aqueous solution, poor solubility of CO2 and hydrogen evolution reaction causes additional challenges which encourage development of efficient electrocatalysts. The previous studies have categorized metallic electrodes to four different groups depending on the types of the major products (i.e. H2, CO, formate, and other more reduce products). Au and Ag are known to good electrocatalysts to produce CO from CO2, and their nanostructures have been demonstrated to increase the electrocatalytic activities possessing low overpotential, high selectivity for CO production, improved durability, and etc. However, its origin is still unrevealed. In this talk, we are going to discuss the origin of the improved CO2 reduction activity with our Ag based electrodes through spectroscopic analysis and DFT calculation which supports that subtle modulation of the nanostructures Ag surfaces can cause the changes in the binding energies of the intermediates. Moreover, we are going to demonstrate a nanostructured metal electrode that shows high selectivity from CO2 to formate production and mechanism insights will be discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ELEC1-4**

발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research I

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 방진호

Toward an Efficient Electrochemical CO_2 Conversion: A Theoretical Perspective

<u>김형준</u>

한국과학기술원(KAIST) EEWS대학원

CO_2 conversion is an essential technology to develop a sustainable carbon economy for the present and the future. Many studies have focused extensively on the electrochemical conversion of CO_2 into various useful chemicals. However, there is not yet a solution sufficiently high enough efficiency and stability to demonstrate practical applicability. A key obstacle here is mostly due to the limited performance of the catalysts in terms of activity, stability, etc. To improve and tailor the catalytic properties, it is thus required to understand the operational mechanism of the various possible CO_2 reduction pathways and identify the mechanistic role of catalysts. Using first-principles based multi-scale computational methods, our group aims to achieve such a goal to understand, predict, and design the electrochemical catalysts for CO_2 reduction. In this talk, I will discuss our recent efforts toward this and demonstrate how the atomistic computational simulations can aid understanding complicated electrocatalytic processes.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **ELEC1-5**

발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research I

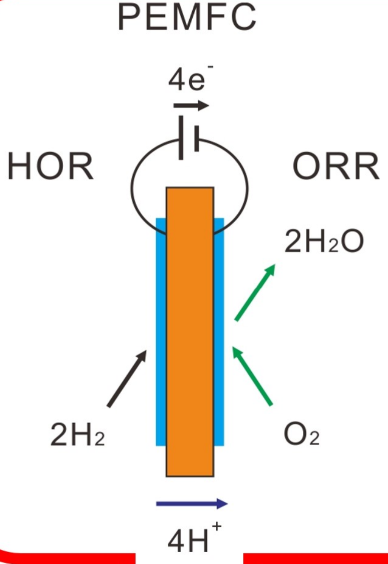
발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 방진호

Novel Platinum-Based Nanocrystals with Enhanced Activity and Durability toward Oxygen Reduction

최상일

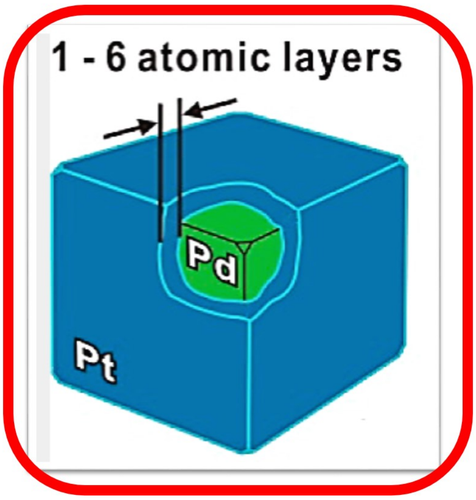
경북대학교 화학과

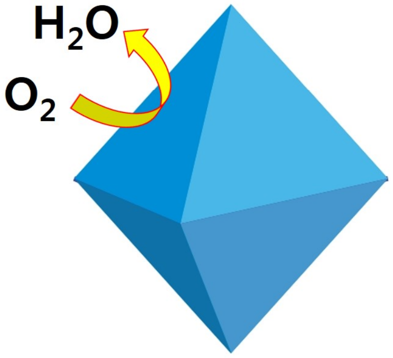
Oxygen reduction reaction (ORR) in a polymer electrolyte membrane fuel cell requires the use of a catalyst based on Pt, one of the most expensive and rarest metals on the Earth. To reduce the use of Pt while to enhance the catalytic performance, multiple strategies, such as formation of Pt-based alloys and deposition of Pt as ultrathin skins on nanoscale substrates made of another metal, have been explored. This presentation will discuss two different routes; one for the synthesis of Pt-Ni alloy octahedra and the other for the conformal deposition of Pt as uniform, ultrathin shells of only a few atomic layers on Pd nanocrystals. By optimizing the catalytic behavior of Pt-based nanocrystals, we obtained the greatly enhanced ORR activity and durability.



CHALLENGES

- Slow kinetics
- Strong OH adsorption
- High cost of platinum


1 - 6 atomic layers


Nanosized Pt-Ni octahedra

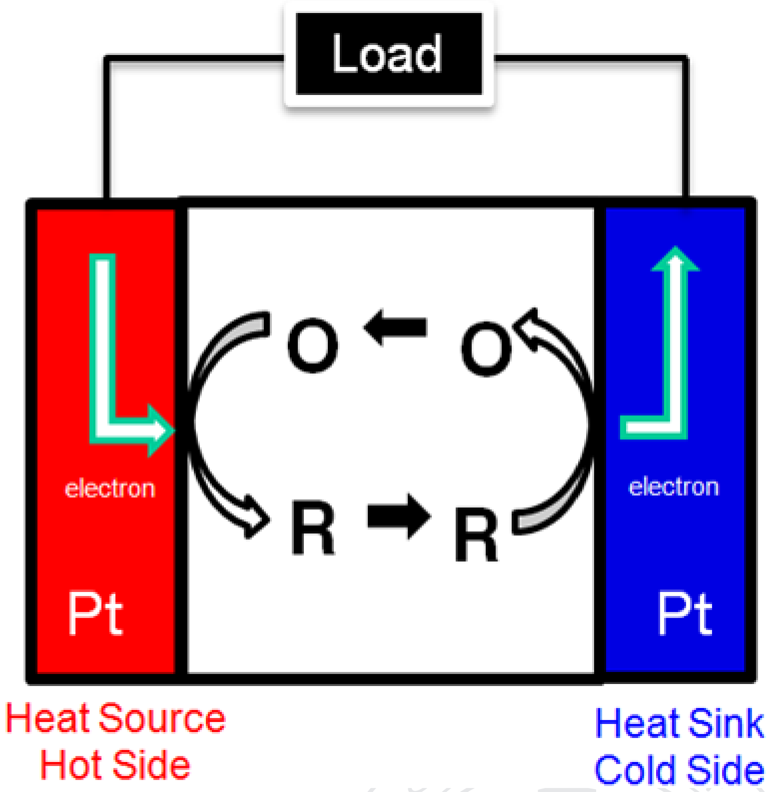
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC2-1**
발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research II
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 황성필

Nonaqueous electrolyte-based thermogalvanic cells for efficient harvesting of low-grade waste heat

이호춘

대구경북과학기술원(DGIST) 에너지시스템공학

The ubiquitous low-grade (less than 100 ^{o}C) waste heat such as industrial/residential waste water streams, or solar thermal energy has been projected as an attractive sustainable energy source. There has been extensive researches on the thermoelectric generators (TEGs) that convert the waste heat into electricity. The conversion efficiency of TEG, however, is still too low to be competitive to other energy conversion technologies. This talk introduces the thermogalvanic (TG) cells an alternative example of the electrochemical energy harvesting device. In particular, our recent achievements in the TG cells based on non-aqueous electrolytes that outperform the conventional cells employing aqueous electrolytes will be presented. First, the superior performances of Li/Li TG cells with glyme-based electrolytes is demonstrated in comparison with conventional Cu/Cu cells with aqueous solutions. Through both the study on the solvation behavior of Li^{+} ion and solvent molecules, and on the electrochemical analysis of the overpotential components, the superior performances of Li/Li cells will be explained in terms of both the thermodynamic and kinetic aspects. Then, the unprecedentedly high thermal conversion efficiency of iodide (I_3^-/I^-) TG cells with carbonate electrolytes is introduced with an emphasis on the positive role of concentation overpential in TG cell performances.


Load
electron
Pt
O
O
R
R
electron
Pt
Heat Source
Hot Side
Heat Sink
Cold Side

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC2-2**
발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research II
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 황성필

Detection of the Sn(III) Intermediate and the Mechanism of the Sn(IV)/Sn(II) Electroreduction Reaction in Bromide Media by Cyclic Voltammetry and Scanning Electrochemical Microscopy

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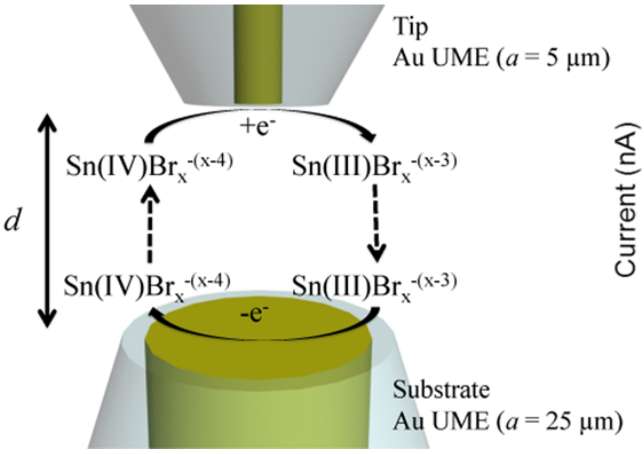
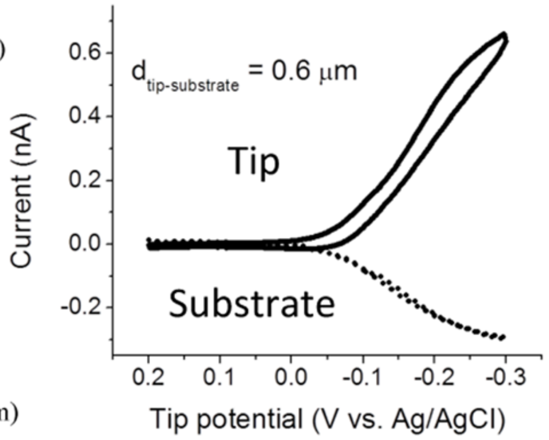
Fast-scan cyclic voltammetry (CV) and scanning electrochemical microscopy (SECM) were used to investigate the reduction of Sn(IV) as the hexabromo complex ion in a 2 M HBr?4 M NaBr medium. CV at scan rates to 100 V/s and SECM indicated the reaction pathway involves ligand coupled electron transfer via an ECEC-DISP process: (1) one electron reduction of $Sn^{IV}Br_6^{2?}$ to $Sn^{III}Br_6^{3?}$; (2) bromide dissociation of the reduced $Sn^{III}Br_6^{3?}$ to $Sn^{III}Br_5^{2?}$; (3) disproportionation of the reduced $2Sn^{III}Br_5^{2?}$ to $Sn^{IV}Br_5^{?}$ and $Sn^{II}Br_5^{3?}$; (4) one-electron reduction of $Sn^{III}Br_5^{2?}$ to $Sn^{II}Br_5^{3?}$; (5) bromide dissociation from $Sn^{II}Br_5^{3-}$ to $Sn^{II}Br_4^{2?}$. The intermediate Sn(III) species was confirmed by SECM, where the Sn(III) generated at the Au tip was collected on a Au substrate in the tip generation/substrate collection mode when the distance between the tip and substrate was a few hundred nanometers.





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Electrochemical SERS Application of Nanostructured Metal Surfaces for Mechanistic Investigation of Electrochemical Energy Conversion

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. Recently, a simple electrochemical deposition of nanostructured metal structures on a clean electrode surface in the absence of additives has received much attention. In this presentation, electrochemical SERS application of electrodeposited Au nanostructures is demonstrated. Highly surface-enhanced Raman scattering (SERS)-active Pt and Pd layers were fabricated using dendritic Au rod (DAR) structures as core substrates. The unique structures of DAR with sharp edge sites and long-range enhancement caused by the underlying DAR cores contributed to the high activity of SERS. The well-defined and homogeneous surface morphology of DAR@Pt/Pd substrates resulted in good SERS reproducibility and stable electrochemical SERS behavior under potential excursions. The DAR@Pt and DAR@Pd substrates were used for the in situ electrochemical SERS examination during the oxidation of formic acid, from which insights into the electrooxidation of formic acid on Pt and Pd shells on Au core surfaces are given.

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Synthesis of Fe and N functionalized-mesoporous carbon: effect of Fe on surface properties and electrocatalytic activity

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Recently, heteroatom-doped carbon catalysts, due to their high stability, excellent electrocatalytic performance, and economic viability are being pioneered as suitable alternative to costly Pt-based catalysts in fuel cell. In this work, a detailed investigation is carried out on Fe and N-functionalized ordered mesoporous carbon (FeN-OMC) as ORR electrocatalyst in both alkaline and acidic media. The FeN-OMCs with different morphology are synthesized by pyrolysis of iron phthalocyanine-infiltrated corresponding SBA-15 silica templates. The as-synthesized FeN-OMC materials show excellent electrocatalytic ORR activity with nearly four electron transfer process. While the activity in alkaline media is nearly equal to or better than commercial Pt catalyst in terms of onset potential and diffusion-limited current density, it closely follows in acidic media, which is a tremendous achievement for non-precious metal catalysts developed till date. The physical presence of Fe species may be necessary in the synthesis of active heteroatom-doped carbon for high ORR activity, but may be not necessary any more for the as-prepared doped carbon to play as electrocatalyst for ORR. In this work, the electrochemical activity is discussed in terms of surface area, active species and electrical conductivity.

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발표코드: **ELEC3-1**
발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research III
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 장진호

Electrochemical performance of hybrid supercapacitor by using partially graphitic activated carbon

노광철

한국세라믹기술원 에너지효율소재팀

We used multi-structured activated carbon electrodes to fabricate hybrid supercapacitors (HSCs) showing excellent electrochemical performance. As the active material, the activated carbon coupled with Li4Ti5O12 showed a partially graphitized as well as a porous structure, and thus provided two different capacitive mechanisms: electric double layer capacitance and shallow intercalation. HSCs produced with this unique structure show excellent specific capacitances of 77 F g?1 and 62 F cm?3. Partially graphitic activated carbon has great potential for HSC applications.

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발표코드: **ELEC3-2**

발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research III

발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 장진호

Electrochemical Flow Capacitor: Design of High Energy Density Slurry Electrodes

윤하나

한국에너지기술연구원 에너지저장연구실

Large-scale and highly efficient electrical energy storage systems (ESS) that are able to quickly respond to the large and rapid fluctuations are necessary to spread the use of renewable energy sources. High energy densities of batteries are attractive, however, slow charging, limited cycle lifetimes and unsolved safety issues hinder their ESS applications. In contrast, electrochemical capacitors have a rapid response, long cycle lifetime and good safety, but they have lower energy densities than batteries. Thus, new technologies having major advantages of both batteries and electrochemical capacitors are required for grid scale energy storage applications. Electrochemical flow capacitors (EFCs) can be one of the promising alternatives for large-scale energy storage because the EFCs can independently scale their power and energy capacities, unlike conventional electrochemical capacitors with solid electrodes. Herein, we report high-performance flow capacitors using high energy density slurry electrodes.

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발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research III
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 장진호

전기화학 **transient** 법을 이용한 수퍼캐패시터의 성능 분석 연구

(Supercapacitor characterization using electrochemical transient methods)

윤성훈

중앙대학교 공과대학 융합공학부

표면에 전하가 저장되는 특성에 의해 빠른 충방전이 가능한 수퍼캐패시터(supercapacitors) 는 기존의 이차전지 (secondary batteries) 에 비해 고출력 발현이 필요한 특수한 용도로 많이 적용되고 있다. 본 연구에서는 수퍼캐패시터의 성능을 조사하기 위한 전기화학적 분석법으로서 transient 법에 기반한 방법을 제시하고자 한다. 특히 수퍼캐패시터의 기공내에서 이온의 전달 (transport) 및 전하저장을 묘사하는 transmission line model 을 이용하여 직류 및 교류 환경하에서의 주요한 transient 식(equations) 을 제시하고 이 식들이 갖는 물리적 의미를 고찰한다. 또한 실제 수퍼캐패시터의 전극에 적용하기 위해 ordered mesoporous materials (carbon, metal oxides) 을 이용하여 전극을 제작하고 전기화학 실험을 수행하여, 이론적으로 유도된 식들을 통해 기공내 이온전달 및 전하저장에 관한 특성을 비교 분석한다. 이를 통해 다공성 탄소 전극내에서의 기공 특성 (크기, 길이, connectivity) 에 따른 수퍼캐패시터의 성능과의 연계성을 제시하며, 금속산화물-탄소 나노 복합체의 수퍼캐패시터 성능 개선의 원인을 제시하고자 한다.

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발표분야: Electrochemistry as a Core Discipline in Energy Conversion and Storage Research III

발표종류: 심포지엄, 발표일시: 금 15:55, 좌장: 장진호

Operando Spectroelectrochemical Methods for Understanding Mechanism of Li-O2 Batteries

강영구

한국화학연구원 차세대전지소재연구센터

인시추(In-situ) 전기화학적분광학(spectroelectrochemical) 방법들은 이차전지의 작동원리, 안전성, 열화 메커니즘 등의 특성을 평가하는데 매우 중요한 방법으로 사용되고 있다. 특히 in-operando 방법은 전지가 작동하는 환경에서 전지 작동에 거의 영향을 주지 않으면서도 비파괴적이고, 실시간으로 분광학적인 특성 평가하여 전지소재의 화학적 변화를 측정하는 방법으로 전지의 반응 메커니즘을 이해하는 유용하게 사용될 수 있어 차세대 전지 재료 개발에 매우 중요하다.본 발표에서는 차세대 리튬 이차전지에 적용 가능한 다양한 전기화학적분광학 방법을 소개하고자 한다. 또한 전기화학적적 분광학 방법을 Li-O2 이차전지에 적용하여 전지 재료 개발에 적용한 예를 소개하고자 한다.

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발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 강석진

유기화학 강의에 거꾸로 교실 적용하기

차정호

대구대학교 과학교육학부

2014 년 3 월 20 일, 미래 교실을 찾아서라는 주제로 3 부작으로 방영된 다큐멘터리는 이후 한국 교육에 큰 파장을 일으켰다. 부산 지역의 초중학교에서 시도된 거꾸로 교실에 대한 내용은 단순히 방송에 머무르지 않고, 전국적으로 새로운 교수방법에 대한 관심과 실천으로 이어졌다. 이후 거꾸로 교실을 실행하거나 관심 있는 교사들의 네트워크가 결성되고, 재빠른 일부 지역 교육청에서는 교육혁신 사업의 주제로 채택하기도 했다. 이러한 일련의 과정을 지켜보면서, 발표자 역시 대학 교육의 현장에서 거꾸로 교실을 적용하는 데 관심이 생겼다. 처음엔 방송 내용 중에 나오는 동영상 제작 도구에 관심을 가지다가 담당 과목에 어떻게 적용할지 고민하는 단계에 이르렀다. 2014 년 2 학기부터 1 년 동안 유기화학을 강의할 기회가 주어지면서, 거꾸로 교실을 적용해 보기로 했다. 우선 강의를 위한 노트와 슬라이드를 제작하고, 이것을 활용하여 동영상을 제작했다. 동영상은 학교 강의 관리 시스템과 유튜브에 올렸고, 학생들에게 강의 전에 보고 오도록 안내하였다. 수업 중에는 강의 내용과 관련된 예제 및 연습문제를 소그룹으로 풀게 하였고, 가끔씩 개별 퀴즈를 실시하였다. 2014 년 2 학기에 유기화학(2) 강의를 만족할 만한 성과를 얻지 못하고 2015 년 1 학기에 유기화학(1) 강의를 진행하였는데, 직전 학기에 경험했던 시행착오들을 줄여가면서 다양한 방법들을 시도해 보았다. 이 과정에서 중간중간 학생들의 반응을 조사하였고, 발표자는 수업 적용과정에서 드는 생각들을 기록으로 남겼다. 이러한 경험과 자료를 바탕으로, 이 발표에서는 전공 화학 강의에 거꾸로 교실의 적용할 때 주의해야 할 점들에 대해 나누고자 한다.

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Nature-Study 사상으로부터 과학적 소양인 양성으로의 연계

박종석

경북대학교 화학교육과

우리나라 교육과정은 5 년 또는 10 년을 주기로 몇 차례 개정되어왔다. 현재 교육부는 2015 년 문이과통합형 교육과정을 마련하고 있다. 특히 최근 2007 개정, 2009 개정의 경우는 일반적 관례에 따르지 않는 매우 단기적 개정의 사례였다. 이와 같은 교육과정의 개정은 사회적, 교육적 변화에 의해 그 타당성이 담보될 수 있다. 하지만 너무 잦은 개정은 소위 ‘교육은 백년지대계’라고 하는 관점에서 비판의 대상이 될 수 있다. 지금까지의 교육과정 개정에서 세부적인 내용들은 지속적으로 바뀌어 왔지만 그것이 과학교육의 본질에 부응하는 방향인지는 의문이다. 통합과 융합을 강조하는 초등학교 수준에서도 여전히 분과적인 단원 구성이 존재하고 학생들은 교실이나 실험실에서 학습할 뿐 정작 실제 자연에서 자신이 배운 것을 찾지는 못한다. 이처럼 교육과정과 학생의 학습은 분리되어 종종 문제를 유발하곤 한다. 그러기 때문에 과학교육에서 새로운 패러다임을 기대해야 할지도 모른다.최근에 개정된 2007 개정 교육과정에서는 자유탐구, 2009 개정 교육과정에서 창의와 인성이라는 키워드가 두드러졌다. 그러나 이러한 교육과정의 변화에도 불구하고 시대를 관통하는 과학교육학적 목표는 과학지식의 습득, 탐구능력의 획득, 과학적 태도의 함양이고, 시대에 따라 의사소통, 문제해결력 등도 고려되고 있다. 그렇다면 이러한 목표들이 과학교육에서 무엇 때문에 중요시 되어야 하고 달성해야 하는가?오늘날 과학을 학교에서 마땅히 가르쳐야한다는 점에 대해서 의심하는 사람은 없다. 왜냐하면 과학은 우리가 살고 있는 자연 세계를 이해할 수 있는 지식을 제공하고, 과학적 방법을 통해 지식을 체계적으로 획득하거나 기존의 지적 자산들을 통찰할 수 있는 안목을 키우는 데 도움을 주기 때문이다(정병훈, 2014).이와 같이 과학은 우리들이 살고 있는 세계를 이해하는데 도움을 주는 도구의 역할을 한다. 하지만 학교 현장에서 과학교육은 도구인 과학, 즉 과학지식의 습득이나 탐구능력의 획득이 오히려 목적이 되고 있지는 않은가? 현실이 이와 같다면

주객이 전도된 것이 아닌가? 그렇다면 과학교육의 본질은 무엇인가?교육의 본질을 생각해보면, 교육법 1 조에 제시된 바와 같이 홍인인간의 구현이다. 교육은 인간을 대상으로 한다. 그러기 때문에 교육의 본질은 삶과 사람에 주목해야 한다. 교육의 본질은 삶다운 삶, 사람다운 사람을 떠나서는 안 된다. 대학에 “마음이 없으면 보기는 하지만 보질 못하고, 듣기는 하지만 듣질 못하고, 먹기는 하지만 그 맛을 모른다.”라고 하였다. 이와 같이 마음 즉 ‘바른 마음(正心)’이 갖춰지지 않는다면 무엇도 제대로 하지 못하게 된다(이계학, 2004). 루소 또한 교육의 목적은 기계를 만드는 것에 있지 않고 사람을 만드는 것이라고 하였으며(이용철 등, 2007), 칸트도 각 개인이 자신의 자율적 판단에 따라 성숙한 인간으로 살도록 하는 것이 교육의 가장 큰 목표라고 하였다(조관성, 2007).과학교육의 본질도 교육의 본질과 큰 차이는 없을 것이다. 과학교육에서도 인간을 교육하는 것이 과학지식이나 탐구능력의 획득보다 우선되어야 한다. 최근까지도 미국이나 우리나라에서는 과학교육에서 과학적 소양을 갖춘 인간 교육이 강조되고 있다. 하지만 과학교육에서 과학적 소양인의 양성은 강조되어 온 정도에 비하여 등한시 되고 오히려 과학적 소양에 주의를 집중하였다. 과학적 소양인은 모든 사람을 위한 과학의 주요 개념 중 하나이다. 모든 사람들이 과학적 소양을 갖춘다면 과학교육은 소기의 목표를 달성했다고 할 수 있다. 여기서 이보다 앞서 생각해 봐야 할 것은 초등과 중등을 구분하여 과학적 소양인 양성을 살펴보아야 한다. 이는 과학을 보는 시각 차이와 과학교육이 추구하는 목표의 차이에 기인한다. 이에 대해 좀 더 자세한 배경을 알아보기 위해서는 철학적으로 고찰해야 한다.우선 초등에서는 과학교육의 본질을 자연을 통한 과학의 이해에 초점을 두어야 한다. 그 철학적 배경으로 Nature-Study 의 사상을 고려해야 한다.여러 과학교육자들은 자연을 직접 경험하는 것의 중요성을 강조하고 있지만(권홍진, 김찬종, 2007; 김해경 등, 1994; 류춘렬, 2009; 배진호, 정현태, 2007; 임채성 등, 2005), 실제 수업에서 자연을 직접 경험하는 비율은 교실, 실험실에서의 수업에 비해 현저히 낮다(정완호 등, 1996; 홍정수, 장남기, 1997). 이는 “자연을 통한 과학의 이해” 보다는 “지식을 통한 과학의 이해”에 더 치중하고 있다는 것을 뒷받침한다.이와 같은 오늘날 과학교육의 현실에 비해 과학이 학교 교과목으로 처음 도입되던 19 세기 후반 초등 과학교육의 모습에서 오늘날 우리가 간과하고 있는 “자연을 통한 과학의 이해”라는 과학교육의 기본 정신을 찾을 수 있다. 이 시기 미국의 공립 초등학교에서는 Nature-Study 가 과학교육의 한 방법으로 각광받고 있었는데, 이는 어린이의 삶과 환경에서 흔히 볼 수 있는 것을 직접적으로 경험하도록 하는 운동이었다(Bailey, 1920). Nature-Study 는 사상적으로 쉘던의 사물 학습(Object Lessons), 아가시의 자연사(Natural History), 파커의 진보주의(Progressivism)에 바탕을 두고 있으며 그 명칭에서도 알 수 있듯이 자연을 학습하는 것이다. 따라서 Nature-Study 는 직접적인 경험, 자연과의 교감, 학습의 비형식성 및 자발성에 기반하여 자연을 통해 자연을 학습하는 과학교육의 한 방법으로 19 세기 후반에서 20 세기 초반까지 미국에서 유행했던 과학교육의 한 흐름이라고 하겠다.따라서 Nature-Study 는 새로운 과학교육 방법은 아니다. 그러나 “학생들이 교실에서 자연을 배우지만 정작 야외에 나가면 그것을 찾지 못한다”는 말로 자연을 통한 과학의 이해를 강조한 아가시의 격언에서 보듯이 Nature-Study 는 오늘날 과학교육에도 중요한 메시지를 준다(Kohlstedt, 2005). Nature-Study 는 초등 단계에서의 형식적인 과학 지도에 대한 반발로 발생하였다(Bailey, 1920). 오늘날의 과학교육이 자연에 대한 호기심으로 출발했던 초기의 순수성을 잃어버린 이

시점에서 Nature-Study 사상을 되짚어봄으로써 "자연을 통한 자연의 이해"라는 초등 과학교육의 대명제를 바로 세우는 것은 교육적 의의가 있다.Nature-Study 사상에 근거하면 학생들은 주변에서 쉽게 볼 수 있는 사물을 직접적으로 관찰하는 것에서부터 과학을 배우게 되고, 자연에 관심을 두게 되며 나아가 자연과 학생이 새로운 관계를 맺게 될 것이다. 이러한 Nature-Study 운동은 현재 여러 나라 과학교육에서 추구하는 과학적 소양인 육성과 일맥상통한다고 볼 수 있다.사과가 사과나무에서 떨어지는 것을 본 뉴턴의 호기심은 만유인력을 이끌어 내었고 이를 여러 차례의 실험을 통해서 확인하였으며 동시대인들에게 그 결과를 밝혔다. 이러한 일련의 과정은 과학자로서 뉴턴이 가지고 있는 과학적 소양이라고 할 수 있다. 즉, 지식의 이해와 탐구 그리고 실천 및 의사소통이라는 과정을 통해서 과학지식을 산출하고 대중에게 전파하는 역할을 수행한 것이다. 비록 위대한 과학자 뉴턴의 과학적 소양 발현은 일반에게 대중화 될 수는 없지만 모든 이를 위한 과학을 추구하는 오늘날 과학교육에서 과학적 소양인 양성이라고 하는 대전제와 연계해서 생각해 볼 필요가 있다. 과학자와 일반인의 과학적 소양 발현에 필요한 지식이나 결과물에서는 수준 차이가 있지만 그 과정은 동일한 속성을 가져야 한다. 초등 과정에서 Nature Study 사상을 통해 자연에 대한 과학의 이해가 이루어졌다면 중등 수준에서는 자연에 대한 관심이 인간과 사회에서 과학의 역할에 대한 관심으로 이어져야 할 것이다. 따라서 일반인의 과학적 소양 발현은 중등 교육 과정을 통해서 훈련되고 교육되어야 한다. 그러므로 중등 과학교육에서는 자연을 통한 과학의 이해를 바탕으로 과학적 소양인의 육성에 집중할 필요가 있다. 과학교육의 본질로서의 과학적 소양인 육성은 과학과 관련된 삶 속에서 과학지식을 바탕으로 바른 판단을 하여 사람들과의 더불어 사는 바람직한 인성을 갖춘 사람을 길러내는 것이다.근본적으로 초등과 중등을 불문하고 과학을 학교에서 가르쳐야 하는 목적은 같다. 그러나 학생의 수준이 다르고, 가르치는 교과 내용의 깊이가 다르기 때문에 이러한 점을 고려한 과학교육의 실천이 필요하다. 초등학생을 위한 과학교육의 실천은 Nature-Study 사상에 기반하고, 이로부터 교육된 중등의 학생들은 과학적 소양인으로 양성될 수 있도록 Nature-Study 사상과 과학적 소양인 양성의 연계는 오늘날 과학교육에 큰 의의를 가진다고 할 수 있다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **EDEC-3**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 강석진

산염기 개념에 대한 화학교육적 고찰

백성혜

한국교원대학교 화학교육과

중등학교부터 대학까지 다루는 산과 염기의 개념은 크게, 아레니우스, 브뢴스테드 로우리, 그리고 루이스의 정의로 요약할 수 있다. 또한 지시약의 산과 염기 개념까지 포함한다면, 초등학교의 내용도 포함할 수 있다. 그러나 각 정의가 다루는 범위와 시각이 다름에도 불구하고, 이러한 정의는 점진적 포괄모형으로 제시하는 전통이 있다. 그러나 포괄 모형은 산과 염기 개념에 대한 학생들의 이해에 어려움을 야기한다고 본다. 아레니우스의 정의가 물질로서의 산과 염기를 정의한다고 본다면, 브뢴스테드 로우리나 루이스는 과정으로서의 산과 염기를 정의하기 때문이다. 또한 아레니우스가 강산과 강염기를 대상으로 정의하였다면, 브뢴스테드 로우리는 약산과 약염기의 정의를 다루고 있고, 루이스는 보다 포괄적인 전자쌍 결합을 다루고 있다. 이 연구에서는 산염기에 관련된 각 정의가 다루는 관점의 차이가 무엇인지 살펴보고, 이러한 차이로부터 산과 염기라는 개념이 어떻게 발달하였는지 살펴봄으로써 중등학교에서 다루는 산과 염기 개념에 대한 제안을 하고자 한다.

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장소: 대구 EXCO
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전고체 전지 개발동향 및 이슈

남상철

포항산업과학연구원 ES소재연구그룹

무선 모바일(Wireless mobile) 기기의 시대가 성숙됨에 따라, 전원 장치에 대한 관심이 그 어느 때보다도 증대되고 있다. 이와 관련하여, 리튬 이온 전지는 단위 부피 당 에너지 밀도가 다른 전지 시스템에 비해 월등히 높아 현재 전자 기기 등에 널리 사용되고 있으며, 소형 전지의 형태에서 탈피하여, 자동차 및 에너지 저장 장치로 그 응용 범위를 넓혀가고 있다. 그러나, 일반적으로 알려진 리튬 이온 전지는 기본적으로 액체 전해질을 사용하고 있기 때문에, 폭발 또는 발화와 관련된 안전성의 문제가 지속적으로 발생되고 있다. 이를 해결하는 방법 중 하나로, 연료(fuel)에 해당되는 유기 용매(액체 전해질)을 고체 전해질로 바꾸어주는 방법이 있다. 이처럼 고체 전해질을 사용할 경우, 1) 폭발 또는 발화에 대한 주요 원인이 되는 유기 용매(액체 전해질)를 사용하지 않음으로써, 안전성 문제에 대한 근본적인 해결책이 될 수 있고, 2) 고체 전해질의 전위창이 넓으므로, 고전압 양극 활물질을 사용하거나, 금속 리튬을 음극 활물질로 사용할 수 있어, 액체 전해질을 사용하는 리튬 이온 전지에 비하여 이론적으로 2 내지 3 배 가량 에너지 밀도를 증대시킬 수 있다. 또한, 3) 제조공정 상으로도 LiB 기체의 제거 공정을 생략할 수 있으며, 이에 따라 공정 수율을 향상시킬 수 있을 뿐만 아니라, 공정의 단순화를 통해 원가를 절감시킬 수 있다. 본 발표에서는 최근 활발히 연구되고 있는 전고체 전지의 개발동향, 고체전해질, 이러한 전고체 전지연구에 있어서의 이슈에 대해 논의하고자 한다.

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장소: 대구 EXCO
발표코드: **ENVR1-2**
발표분야: Next Generation Energy Storage Systems
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이재영

스마트 미터 및 무정전시스템 전원용 수퍼커패시터의 개발 동향 및 시장동향

김한주

퓨리켐 관리

최근 에너지 수요가 증가하면서, 무정전전원장치 및 스마트그리드용 스마트 미터용 전원에 대한 신제품 개발요구가 많아지고 있다. 본 발표에서는 이러한 스마트미터 및 무정전전원장치의 순간출력보정 전원인 수퍼커패시터의 개발동향에 대해서 논의하고자 한다. 한국을 비롯하여, 중국, 미국, 일본의 개발동향 및 응용시장에 대한 분석을 통해서 향후 국내 수퍼커패시터 제조업체가 세계를 상대로 경쟁할수 있는 고전압제품(기존 2.7V 에서 3.3V 이상으로 확대) 개발 및 적용 시스템에서 요구되는 성능을 달성하기 위한 개발전략등을 발표하고, 향후 시장전망에 대해서 발표할 예정이다. 또한, 수송용 보조에너지 저장장치로써, 수퍼커패시터의 역할과 기존 납축전지와 하이브리드로 패키징하여 기존 배터리의 성능을 향상시킬수 있는 보조전원 특성에 대해서도 부가적으로 설명할 예정이다.

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발표코드: **ENVR1-3**
발표분야: Next Generation Energy Storage Systems
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 이재영

Enhancement of cycle performance of lithium sulfur battery *via* Vitamin C-treated graphene oxides based cathode

김진원

광주과학기술원(GIST) 환경공학부

Lithium sulfur battery (Li-SB) serve several advantages such as very high energy density, low-cost, and environmental-friendliness. However, it suffers from serious degradation of reversible capacity due to the dissolution of the reaction intermediates, lithium polysulfides, into the electrolyte. To solve the limitation, there are many study using graphene-based materials due to their high mechanical strength and electrical conductivity. Compared to graphene, oxygen functional groups on the surface of graphene oxides (GO) enhancing reaction with lithium polysulfide. Here, we investigated the enhancement of cycle performance under high current density by dual-layered cathode using vitamin C-treated GO active material. Vitamin C (L-ascorbic acid) makes GO high electrical conductivity as well as formation of sulfur nanoparticles on the surface of GO. We have observed that Vitamin C-treated GO and sulfur nanoparticle composites shows a smaller drop of capacity under high current density. Furthermore, the mechanistic origin of the improvement of reversibility, can be explained by the stabilization of sulfur in the lithium polysulfide intermediates by the oxygen functional groups of GO to prevent further dissolution and increase of initial capacity by Vitamin C-treated GO.

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발표분야: Next Generation Energy Storage Systems
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이재영

Impact of synthesis methods on the chemical, optoelectrical, electrochemical properties of graphene oxides and its derivatives

강영호[*] 김용재[1]

전남대학교 물리교육과 [1]계명대학교 화학과

Preparing graphene films using solution-processed graphene oxides is a mass production compatible graphene synthesis route. Graphene films had shown potentials as a functional electrode for various applications such as transparent electrodes for organic optoelectronics and energy-storing porous electrodes for supercapacitors. Among several available synthesis methods for graphene oxides, the modified Hummers' method is a major synthesis method adopted by many researchers. For fully fledged applications, tight control of the synthesized properties of graphene oxide is needed. However, understanding of the effects of the synthesis parameters is insufficient, hindering the advance of the applications of graphene oxides. Here, we present our study results on the effects of the various synthesis parameters in the modified Hummers' method on the properties of the graphene oxides. Focusing on the transparent electrode and the supercapacitor electrode applications, the properties of graphene electrodes were investigated using UV-visible spectroscopy, Hall measurements, atomic force microscopy, X-ray photoelectron spectroscopy, and cyclic voltammetry. Our results reveal that increasing the oxidization parameters such as the reaction time or the dosage of oxidant improves morphological and optoelectrical properties of the graphene thin films prepared by a thermal reduction of graphene oxide films. On the other hand, for the supercapacitor electrodes applications, the synthesis parameter improvements had little role in the performance, instead, the thermal reduction condition that involves thermal shocking effect was found to have a bigger role.

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발표분야: Fuel Cell Based Energy Conversion Systems
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 김형준

유무기 하이브리드 소재의 연료전지 촉매 응용 (Organic-Inorganic Hybrid Materials for Fuel Cell Applications)

정남기

충남대학교 에너지과학기술대학원

고분자 전해질 연료전지에서 환원극 촉매의 느린 산소 환원 반응과 낮은 전기화학적 안정성은 반드시 극복해야 할 중요한 이슈이다. 고가의 백금 촉매 사용량을 저감하면서 동시에 산소 환원 반응 활성을 극대화하기 위해 백금 기반의 합금촉매를 이용하고 있지만, 합금 촉매가 갖는 높은 촉매 활성에도 불구하고 공기 또는 산성 전해질에 노출되었을 때 표면 전이금속이 쉽게 산화물을 형성하거나 높은 전압영역에서 빠르게 녹아나기 때문에 내구성 문제가 여전히 남아있다. 한편, 인산형 및 알칼리 연료전지에서는, 각 전해질 내에 존재하는 인산 및 OH^- 이온 등의 spectator 이온들이 백금 표면에 강하게 흡착하여 활성 사이트를 가로 막아 산소 분자의 흡착을 방해함으로써 산소 환원 반응 활성을 저해하는 주요 요인이 된다. 특히, 크기가 매우 큰 인산 이온은 같은 양의 흡착에 의해서도 상대적으로 훨씬 많은 백금 활성 사이트를 막아 버리기 때문에 다른 연료전지 유형에 비해 매우 낮은 촉매 성능을 나타내게 된다. 본 연구에서는, 이렇게 다양한 연료전지 유형 안에서 나타나고 있는 근본적인 합금 촉매의 성능/내구성 문제와 spectator 이온 흡착에 의한 촉매 활성 감소 문제를 해결하기 위해, 다양한 성질을 갖는 유기분자를 촉매 나노 입자 표면에 기능화 시킴으로써 고성능/고안정성을 갖는 유무기 하이브리드 연료전지 촉매를 개발하였다.

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발표분야: Fuel Cell Based Energy Conversion Systems
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 김형준

Iodine-treated heteroatom-doped carbon: Surface properties and electrocatalytic activity

유종성* **SINGHKIRANPAL[1]** **송민영**

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

We report a noble technique to synthesize highly conductive and microporous N and S-doped carbon from polyaniline (PANI) via a simple template-free hydrothermal method followed by carbonization in presence of iodine. Iodine treatment removes large amount of attached oxygen and other heteroatoms, and as a consequence increases the carbon content. Thus, the iodine treatment decreases catalytically active heteroatom doping, which is unfavourable for oxygen reduction reaction (ORR), but at the same time, significantly increases the electrical conductivity, which is beneficial for ORR. In particular, iodine-treated carbonized PANI (CPANI) shows exceptionally high conductivity, about 3 times that of untreated CPANI. Iodine treatment is also found to enhance the micropore surface area of the PANI during carbonization without using any activating agent or hard template. Electrocatalytic study indicates that the activity of the iodine-treated sample is found to be much better than that of untreated sample. This remarkable upsurge in activity is mainly attributed to the high increase in conductivity and surface area of the iodine-treated sample.

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발표분야: Fuel Cell Based Energy Conversion Systems
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김형준

Pt-based nanocatalyst design for fuel cell applications

유성종

한국과학기술연구원(KIST) 연료전지센터

Recent advanced in Pt-based nanocatalysts and support materials with multi-structures for proton electrolyte membrane fuel cell (PEMFC) are reviewed. Discussions are focused on their structures and compositions, which considerably affect the electronic structures and catalytic activities of fuel cell catalysts. The nanocatalyst category includes metal alloys (including shape-controlled alloy nanoparticles), core-shells, and hollow structures. In addition, as the support materials, various carbons (carbon blacks, carbon nanotubes, carbon nanofibers, and graphenes) and metal oxides are extensively explored. We describe the catalysts and support materials mainly for the oxygen reduction reaction (ORR) since the high ORR activity is one of the most important factors to enhance the PEMFC efficiency. Based on the recent progress in catalysis and fuel cell technologies for decades, we suggest promising future works for PEMFC commercialization.

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발표분야: Fuel Cell Based Energy Conversion Systems
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 김형준

Carbon based catalysts containing transition metal-nitrogen moieties for efficient oxygen reduction reaction

조은애

한국과학기술원(KAIST) 신소재공학과

Recent major effort in fuel cells for automotive applications has been exploring cheap and active non-precious metal catalyst for the oxygen reduction reaction (ORR). Since Jasinski reported macrocyclic Co-phthalocyanine as an ORR electrocatalyst, non-precious metal catalysts containing transition metal-N_x moieties (M-N-C) have attracted continuing interest because these catalysts consist of earth-abundant substances. Recent studies revealed that the M-N-C catalysts have potential to replace platinum (Pt) catalyst due to their high ORR activity and low cost. To achieve high ORR activity, work on M-N-C catalysts has mainly focused on optimization of the synthesis process considering various precursor mixture. Although the ORR activity of the M-N-C catalyst strongly depends on the precursor selection, a large surface area is always a prerequisite for a high reaction volume. From this perspective, a nanostructure is a very attractive morphology to attain a high surface area. Herein we report two types of nanostructured M-N-C catalyst for ORR using facile synthesis route; 1) electrospun cobalt-carbon nanofiber (Co-CNF), and 2) mechanically activated iron-nitrogen-sulfur doped-graphene (Fe-N-S-graphene). These two catalysts have 1-dimensinal and very porous nanostrucure, respectively, and exhibits high ORR activity and stability in alkaline media compared with the commercial Pt/C catalyst. The high ORR activity is attributed from increase in ORR active sites. We focused on structural characteristics being associated with the ORR active sites such as doped N, S, graphitic carbon structure and surface area. By investigating the correlation between the structural variation and ORR activity, we aim to elucidate the ORR active sites of the Co-CNF and Fe-N-S-graphene catalyst for designing highly active NPMCs to replace Pt catalyst.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **KCS1-1**

발표분야: 화학물질 안전 심포지엄

발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 이익모

화학물질 등록 및 평가 등에 관한 법률 개요 및 기업 대응 방안

유문선

한국화학융합시험연구원

2015.1.1.일부로 화평법(화학물질의 등록 및 평가에 관한 법률)이 시행되었다. 화평법은 국내에서 유통되는 화학물질의 위해성으로부터 국민 건강과 환경을 보호하는 한편, 화학물질의 등록과 평가를 의무화하는 국제 추세에 대응하기 위한 법률이다. 신규 화학물질 또는 연간 1 톤 이상 기존 화학물질을 제조・수입・판매하는 자는 화학물질의 용도 및 그 양 등을 매년 환경부장관에게 보고하여야 한다. 또 해당 화학물질을 등록할 때 제조・수입 물질의 용도나 특성, 유해성 등에 대한 자료도 제출해야 한다. 화학물질의 연간 제조 또는 수입량이 10 톤 이상인 경우에는, 단계적으로 화학물질의 위해성에 관한 자료도를 새롭게 제출하여야 한다.

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발표코드: **KCS1-2**
발표분야: 화학물질 안전 심포지엄
발표종류: 심포지엄, 발표일시: 수 15:30, 좌장: 이익모

화학물질관리법 주요내용 및 기업의 준비사항 - 중소기업의 장외영향평가, 위해관리계획서를 중심으로

천영우

인하대학교 환경·안전융합전공

화학사고가 빈발하고 화학사고로 인한 피해의 규모가 점점 커짐에 따라 이에 대응하기 위해 전 세계적으로 화학물질 관련 규제의 범위와 강도가 지속적으로 확대되고 있다. 우리나라 역시 구미 불산 사고를 계기로 기존의 유해화학물질관리법을 개정하여, 화학물질관리법과 화학물질 등록 및 평가 등에 관한 법률을 제정함으로써 화학물질 관련 규제를 강화하고 있다. 2015 년 1 월 1 일부터 시행된 화학물질관리법에서는 대상 업종과 대상 물질을 확대하고, 장외영향평가제도와 위해관리계획서제도를 신설하여 사업장내의 사고관리 외에 사업장 외부의 주변 환경 및 주민에 영향을 끼치는 부분까지 관리하도록 하고 있다.
장외영향평가제도와 위해관리계획서제도는 화학산업계 대부분의 기업이 규제 대상이다. 하지만 규제 관련 정보 및 전문 인력 부족, 자금여건 등으로 많은 기업들, 특히 중소기업들이 대응에 어려움을 겪고 있다. 이에 중소기업의 입장에서 화학물질관리법의 주요 내용들을 살펴보고 중소기업의 장외영향평가제도, 위해관리계획서제도 대응 사례를 통해 중소기업의 대응능력 강화방안을 제안하고자한다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS1-3**
발표분야: 화학물질 안전 심포지엄
발표종류: 심포지엄, 발표일시: 수 16:00, 좌장: 이익모

장외영향평가와 위해관리계획서 작성과 취급시설관리 과정에서 사업장이 자주 하는 오류 사례 분석과 대응방안

윤준헌

화학물질안전원 사고예방심사과

화학물질관리법이 시행되면서 유해화학물질과 관련된 시설을 운영할 때 취급시설의 안전관리가 중요해 졌다. 취급시설을 설치하기 전에 위험성을 평가하기 위해 장외영향평가서를 작성해야 하며, 사고대비물질을 취급할 때는 비상상황이 발생하였을 때 효과적인 대응을 위해 위해관리계획서를 만들어야 한다. 또한 화학사고 발생 가능성을 줄이기 위해 화학물질 취급시설의 설치 및 관리에 대한 내용이 매우 강화되어 사업장에서는 자체점검, 설치검사, 정기검사, 수시검사, 안전진단을 수행하여야 한다. 유해화학물질 취급시설을 설치하기 전에 평가받아야 하는 장외영향평가서와 비상대응계획 수립을 위해 영업허가를 받기 전에 제출해야 하는 위해관리계획은 화학물질안전원에서 적합통보를 받아야 후속작업을 진행 할 수 있다. 따라서 사업장의 계획대로 차질이 없는 사업추진을 위해서는 평가가 지연되지 않는 것이 중요하다. 그러나 제출된 평가서를 평가하는 과정에서 보면 많은 사업장이 한 번에 평가가 끝나지 않고 보완요청을 받고 있다. 사업장에 따라 다른 부분도 있지만 보완이 요청되는 내용의 많은 부분은 대부분 사업장에서 비슷하게 반복적으로 생기는 오류이다. 또한 취급시설을 설치하고 운영할 때 화학물질관리법에서 바뀐 설치기준을 준수하는 과정에서 법과 관련규정을 해석하여 적용하는 데 어려움을 겪는 사업장이 많다. 이번 심포지엄에서는 화학물질안전원에서 장외영향평가서와 위해관리계획을 평가하는 과정에서 많이 나온 오류 사례를 유형별로 분석하여 보완 방향에 대해 제시하였다. 또한 취급시설의 설치와 운영과정에서 제기된 법해석의 주요쟁점에 대한 방침과 개선방향을 제시함으로써 사업장에서 화학물질관리법을 효과적으로 이행하는데 활용할 수 있도록 하고자 한다.

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장소: 대구 EXCO
발표코드: **KCS1-4**
발표분야: 화학물질 안전 심포지엄
발표종류: 심포지엄, 발표일시: 수 16:30, 좌장: 이익모

기업에서의 화학물질관리법 이행 및 현안

양진

SK인천석유화학

소중한 생명과 환경에 피해를 주는 크고 작은 화학사고가 최근 국내외에서 일어나고 있어 이에 대한 국민적 관심이 그 어느 때보다 높다. 정부도 여러 법률(8 개 부처 15 개 관련법)을 제정하여 화학물질로 인한 국민건강 및 환경 상의 위해·위험을 사전에 예방하려는 노력을 하고 있으나 정작 이를 이행하여야 할 일부 사업장에서는 관련 법률을 잘 모르거나 설령 알더라도 어려운 경영환경 하에서 자기주도적으로 법에 따라 화학물질을 관리하기가 어려운 실정이다.

또한 유해·위험물질 취급량과 대상기준에 따라 2019 년까지 순차적으로 적용되는 화학물질관리법을 위반 시 과태료나 행정처분 등 불이익으로 인해 해당 사업장은 경영악화의 악순환에 처하게 될 수도 있다. 그러므로 법 제정이나 관리강화 더불어 자력으로 위해·위험의 통제가 어려운 소규모 사업장까지 법을 제대로 이해하고 이행하도록 이끌어 주는 활동도 병행되어야 한다.

이러한 현실을 감안하여 화학물질관리법 1 차년도 이행 사업장인 SK 인천석유화학(주)이 화학물질의 통계조사 및 정보공개, 유해화학물질의 안전관리, 유해화학물질 영업자 및 화학사고의 대비·대응 등 화학물질관리법에서 요구하는 사업장이 이행하여야 할 내용과 이를 이행함에 있어 느낀 현안을 정리하여 소개함으로써 입법에 따른 제도에 대한 다른 관련 사업장들의 이해를 증진시켜 화학물질관리법이 각 사업장에서 자기주도적이면서 자율적으로 이행되도록 돕고자 한다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS2-1**
발표분야: [튜토리얼] Photochemistry Tutorial for OLED Applications: Energy- and Electron-Transfer Processes in Excited States
발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 한민수

Photochemistry Tutorial for OLED Applications: Energy- and Electron-Transfer Processes in Excited States

윤웅찬

부산대학교 화학과

Organic light-emitting diodes (OLED) are emerging as the leading technology for the new generation of full color flat displays and solid-state lighting sources. Early OLED devices utilized fluorescence from singlet excitons which are generated in a small portion of ca. 25% in a statistically-controlled way in the process of electrical excitation. In recent times emphasis has been placed on the identification of new highly phosphorescent materials and devices due to their ability to utilized both singlet and triplet excitons, and to allow high luminescent efficiency of OLED up to ca. 100%. In the utilizing both singlet and triplet excitons to achieve the high OLED efficiency, electronic energy transfer processes play key roles. For deeper understanding on the principles underlying the electronic excitation energy transfer between two chromophores, energy transfer mechanisms including radiative- and nonradiative-mechanism of Forster long range type and Dexter type are going to be introduced in details with emphasis on the factors controlling their rate constants. In this tutorial will be discussed utility of thermally activated delayed fluorescence which has been emphasized in more recently as a way to achieve high efficient deep- blue OLEDs .

Along with electronic energy-transfer processes, electron-transfer processes are among central issues in the area of excited state chemistry and material chemistry for opto-electronic materials like light emitting (LE) and photovoltaic (PV) materials. For understanding electron transfer processes in the excited states, (1) exciplex formations and their decay to ion radical pairs through electron transfer processes, (2) factors controlling the efficiencies and rate constants of electron transfer processes in solution related to Weller's equations, (3) Marcus theory of electron transfer related to the normal region and 'inverted region' of

electron transfer, and (4) its application to rigid electron transport systems, photosynthetic system and electronic devices will be also discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **KCS3-1**

발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry

발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 최철호

김광수 교수님의 국내 양자계산화학 분야에 대한 공헌

이진용

성균관대학교 화학과

김광수 교수님은 국내 양자계산화학 분야의 1 세대로서 가장 활발한 연구활동을 해오신 분 중의 한 분으로 한국의 양자 계산화학 발전에 큰 공헌을 하셨다. 본 발표에서는 지난 27 여년 동안 연구해 오신 연구분야와 주요한 연구성과 들을 소개하고자 한다. 또한 후진 양성에 대한 성과도 소개하고자 한다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **KCS3-2**

발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry

발표종류: 심포지엄, 발표일시: 수 15:10, 좌장: 최철호

(국문) 한국에서의 계산양자화학의 과거, 현재, 미래

(영문) Past, Present, and Future of Computational Quantum Chemistry: Korea vs World

김광수

울산과학기술대학교(UNIST) 화학과

I will address how computational quantum chemistry has evolved in Korea. Then, I will discuss its future.

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발표코드: **KCS3-3**
발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry
발표종류: 심포지엄, 발표일시: 수 15:30, 좌장: 최철호

양자화학 분야에서 이윤섭 교수님의 공헌 (Contributions of Professor Yoon Sup Lee to Quantum Chemistry in Korea)

백경구

강릉원주대학교 화학과

국내 양자화학 분야의 발전에 기여한 이윤섭 교수님의 업적을 기리기 위하여, 지금까지 수행한 주요 연구들의 내용과 의미를 간략하게 정리하여 소개하고, 지금까지 제자들을 양성하여 배출한 성과들을 소개한다.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS3-4**
발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry
발표종류: 심포지엄, 발표일시: 수 15:40, 좌장: 최철호

Computational Quantum Chemistry Including Effect of Relativity

이윤섭

한국과학기술원(KAIST) 화학과

Effect of relativity is treated at various levels in many quantum chemical packages. General strategies available in popular packages will be described from the computational point of view and the historical perspective of my personal involvement. The emphasis will be on the treatment of spin-orbit interactions which may be considered as part of relativistic effects typically ignored in electronic structure calculations of molecules in the ground state. Effect of relativity needs to be included in any quantitative calculations, and can be of importance for molecules containing heavy (4th to 6th row) or superheavy (7th row) elements. We have been working on ab initio molecular orbital methods that take spin-orbit terms into account utilizing two-component relativistic effective core potentials. Progress and future perspective of our approach and other relativistic methods in general will be presented.

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발표코드: **KCS3-5**
발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry
발표종류: 심포지엄, 발표일시: 수 16:10, 좌장: 이진용

Shaping fluorescence by protein shapes in GFP

이영민

포항공과대학교(POSTECH) 화학과

The green fluorescent protein (GFP) with great utilities in many different fields is also an interesting but challenging target from a physical chemist’s point of view. It can also baffle theoreticians as its understanding often requires adopting expensive high level quantum chemical methods. Here, we will discuss the fluorescence modulation in GFP system based on dynamics simulations with a quantum chemically constructed potential energy surface. By computationally modulating the electrostatic interactions between the chromophore phenoxy oxygen and its nearby residues, we demonstrate that the emission can shift to the blue or to the red side in a very predictable manner. We will also see that the yellow fluorescent protein (YFP), with a tyrosine residue replacing threonine in the direct vicinity of the chromophore, involves a chromophore conformational change and a new ?-stacking interaction, which in turn generate red shifts to send the fluorescence into the yellow region. With the series of demonstrations, we show that the analytical approaches such as ours can provide solid rationales on different responses of the fluorescent protein.

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일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **KCS3-6**

발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry

발표종류: 심포지엄, 발표일시: 수 16:30, 좌장: 이진용

Many-body expansion in solids

정유성

한국과학기술원(KAIST) EEWS 대학원

The many-body expansion technique is applied to the configuration problem in solids via its connection to the cluster expansion. The oscillation of N-body interaction energies is suppressed by a nonempirical weighting scheme, thus its convergence behaviour is significantly enhanced. Further cost reduction is achieved through the separation of configuration and relaxation energies. The presented approach, as a result, can efficiently perform an exhaustive search in the configuration space.

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일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS3-7**
발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry
발표종류: 심포지엄, 발표일시: 수 16:50, 좌장: 백경구

Quantum Chemistry for Electronic and Green-Energy Applications

장윤희

광주과학기술원(GIST) 신소재공학

With a combination of density functional theory calculations, force field development and molecular dynamics simulations, we try to understand the working principles of various organic materials used for memory, transistor, sensor, solar cell, and CO2 capture and try to design high-performance low-cost materials for electronics and green-energy applications. We will discuss on the essential role of quantum chemistry in these examples.

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장소: 대구 EXCO
발표코드: **KCS3-8**
발표분야: Quantum Chemistry: An Essential Tool for Modern Chemistry
발표종류: 심포지엄, 발표일시: 수 17:10, 좌장: 백경구

Quantum Chemical Molecular Dynamics in GAMESS for Condensed Phase Chemical Phenomena

최철호

경북대학교 화학과

A new way of quantum mechanical molecular dynamics study has been recently developed by integrating QM methods and Effective Fragment Potentials(EFP) as well as classical force fields(MM) for condensed phase dynamics. The applicability of the hybrid QM/EFP to the simulation of chemical reaction in aqueous solution has been successfully examined, where it was demonstrated that the QM/EFP-MD yields accurate free energy change and barrier associated with the zwitterion to neutral tautomerization of glycine in aqueous solution. The same approach has been also utilized for various solution dynamics including NaCl association/dissociation, hydrophobic association of methanol dimer and anharmonic vibrational properties in aqueous solutions, etc. A REMD (Replica-Exchange MD) version of our method has also been established using GDDI(Group Distributed Data Interface) technology. We are also extending our method to the nonadiabatic dynamics. In this talk, we introduce our hybrid Quantum Mechanical Molecular Dynamics techniques as implemented in GAMESS.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS4A-1**
발표분야: 신진연구자 학술포럼 I
발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 이은지

Toward Cellular Uptake: Poly(disulfide)s and Pseudo Amphiphiles

<u>방은경</u>* 김진범[1] 금교창[2,*]

한국과학기술연구원(KIST) 뇌의약연구단 [1]한국과학기술연구원(KIST) [2]한국과학기술연구원(KIST) 케모인포메틱스연구센터

The substrate-initiated cell penetrating poly(disulfide)s, dynamic polymers with disulfide repeats in their main chain, were reported. The disulfide bond is a dynamic covalent bond, which can be easily cleaved and reformed, but stronger than the non-covalent interactions present in supramolecular polymers. The most powerful advantage of poly(disulfide)s as carriers is that they are degradable by reductive depolymerization in the presence of glutathione in cells. Upon this step, the biomolecules, conjugated with poly(disulfide)s, can be easily released and the cytotoxicity can be minimized. Here, we report the story of poly(disulfide)s from synthesis to their cellular uptake. The activities of dynamic polyion-counterion complexes in lipid bilayer membranes have been studied for their scientific utilities as transmembrane transporters / carriers, voltage gates, and sensors. As a siRNA transporter, a pseudo amphiphile, which have a membrane-philic part and a phosphate-philic part, were designed by modifying conventional structure of cationic lipids. Inspired by phosphate ion chemosensors, the hydrophobic lipid part was maintained and the phosphate recognizing group displaces the cationic head group. The pseudo amphiphiles nicely interact with the phosphate backbone of siRNAs. Their strong interaction prevents degradation of siRNAs in the presence of RNases and the amphiphiles effectively deliver siRNAs into cells, down-regulating the target gene. The optimal condition for delivery was screened and the size and zeta potential of complexes were also measured.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS4A-2**
발표분야: 신진연구자 학술포럼 I
발표종류: 심포지엄, 발표일시: 수 15:30, 좌장: 이은지

A Dual Functional Layer to Synthesize Nanopatterned Polymer Brushes

김명웅

인하대학교 화학과

Polymer brushes are comprised of polymer chains tethered to the substrate via a terminal group, and are used in a diverse range of applications which require permanent surface modification. Polymer brushes are typically synthesized by either “grafting-to” or “grafting-from” methods, for example, thermally promoted grafting of hydroxyl terminated polymer onto a surface or surface-initiated polymerization to grow polymer chains from a surface. Herein, we describe a highly versatile “grafting-from” approach to grow polymer brushes from a range of substrates with high grafting density by using a single component random copolymer, which contains crosslinkable units to form a stable film and initiator units for surface-initiated atom transfer radical polymerization (SI-ATRP). The chemistry of the random copolymer was further modified to implement a bottom-up approach to fabricate nanopatterned polymer brushes. By assembling a block copolymer on top of the coating, nanopatterned brushes were grown after selective removal of one domain from block copolymer template. The ease of synthesis, chemical tunability, homogeneous surface, stability and applicability to a wide range of substrates makes this a versatile approach to create functionalized interfaces.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **KCS4A-3**
발표분야: 신진연구자 학술포럼 I
발표종류: 심포지엄, 발표일시: 수 16:00, 좌장: 장우동

Single Molecule Confocal Fluorescence Lifetime Correlation Spectroscopy for Accurate Nanoparticle Size Determination

천봉환

IBS CMSD & 고려대학교 화학과

For characterization of individual nanoparticles (NPs) and molecules, electron microscopies such as scanning electron and transmission electron microscopy and scanning probe microscopies such as atomic force microscopy and scanning tunneling microscopy have been employed for structural analysis at the nanometer and sub-nanometer spatial resolution. A variety of analytical spectroscopy tools such as X-ray photoelectron spectroscopy, secondary ion mass spectroscopy, and nuclear magnetic resonance have also been instrumental to assess NP chemical compositions and structural details. However, the sensitivity of these techniques is limited to ensemble-averaged measurements, and samples need to be immobilized on a substrate or in a thin film for the measurement. On the other hand, optical measurements such as dynamic light scattering and fluorescence correlation spectroscopy allow for the non- invasive assessment of the physico-chemical properties of single molecules and NPs in solution.We report on an experimental procedure in confocal single molecule fluorescence lifetime correlation spectroscopy (FLCS) to determine the range of excitation power and molecule concentration in solution under which the application of an unmodified model autocorrelation function is justified. This procedure enables fitting of the autocorrelation to an accurate model to measure diffusion length and diffusion time of single molecules in solution. This procedure determines a set of experimental parameters with which the Stoke-Einstein equation accurately measures the hydrodynamic radii of spherical nanoparticles, enabling the determination of the particle size range for which the hydrodynamic radius by the S-E equation measures the real particle radius.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **KCS4A-4**
발표분야: 신진연구자 학술포럼 I
발표종류: 심포지엄, 발표일시: 수 16:30, 좌장: 장우동

Direct demonstration of ergodicity in a supercooled liquid via single molecule experiments

팽기욱

성균관대학교 화학과

Despite decades of intensive study, a full theory of the glass transition is lacking; so too is a full understanding of the causal relationship between the onset of non-exponential relaxations in glass-forming liquids in the supercooled regime and the glass transition. Consistent with such relaxations, experiments have suggested the presence of dynamic heterogeneity, where ? over a given time ? molecular mobility in a given region may differ by orders of magnitude from that in another region, potentially just nanometers away. While some experiments have sought to quantify the size of these regions, others have sought to quantify their persistence in time, as supercooled liquids are assumed to be ergodic, requiring that over long times all dynamic environments are sampled. Here, single-molecule fluorescence measurements using a probe similar in size and mobility to the host o-terphenyl unambiguously reveal exponential relaxations distributed in time and space and directly demonstrate ergodicity of the system down to the glass transition temperature. In the temperature range probed, at least 200 times the structural relaxation time of the host is required to recover ensemble-averaged relaxation at every spatial region in the system.

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장소: 대구 EXCO
발표코드: **KCS4B-1**
발표분야: 신진연구자 학술포럼 II
발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 주상용

Allotropic transformation of sp2-carbon

정현영

경남과학기술대학교 에너지공학과

The presentation will focus on inter-allotropic transformations/hybridizations of specific types that appear uniformly across large-area carbon networks, using moderate alternating voltage pulses. By controlling the pulse-magnitude, small-diameter single-walled carbon nanotubes can be transformed predominantly into larger diameter single-walled carbon nanotubes, multi-walled carbon nanotubes of different morphologies, multi-layered graphene nanoribbons, or structures with sp3-bonds. This re-engineering of carbon bonds evolves! via a coalescence-induced reconfiguration of sp2-hybridizion, terminates with negligible introduction of defects, and demonstrates remarkable reproducibility. This reflects a potential step forward for large-scale engineering of nanocarbon allotropes and their junctions.

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발표분야: 신진연구자 학술포럼 II
발표종류: 심포지엄, 발표일시: 수 15:30, 좌장: 주상용

Plasmonic Nanomaterials for High Resolution Optical Imaging and Efficient Photocatalyst

임동권

고려대학교 KU-KIST 융합대학원

In this talk, I will discuss the synthetic strategies for two different types of unique plasmonic nanomaterials and their interesting and useful applications in the field of bioimaging (i.e., high resolution live cell Raman imaging [1] and amplified photoacoustic imaging [2]) and photocatalyst.[3] The recently reported Au-NNPs (intra-nanogap gold nanoparticles) showed its great potential as a highly sensitive Raman probe for SERS-based biodetection and bioimaging applications because of straightforward, scalable synthetic method and excellent optical properties of Au-NNPs.[4] The DNA-based wet chemical synthetic method could be further manipulated to obtain controlled intra-nanogap distance and unique shell structures which can overcome the current limitations of Au-NNP nanostructure. The hybrid plasmonic nanomaterials composed of graphene and gold nanoparticle showed great potentials in various applications such as enhanced photothermal effect [5], enhanced photoacoustic amplitude [2] and efficient visible light induced photocatalytic reaction for r-GO synthesis and solar fuel applications. The talk will focus on the detailed synthetic method of the nanomaterials investigated, background and meaning of applications. References 1.J. W. Kang., P. So., R. Dasari., and D.-K. Lim* High Resolution Live Cell Raman Imaging Using Subcellular Organelle-Targeting SERS-Sensitive Gold Nanoparticles with Highly Narrow Intra-Nanogap. Nano Letters, 15 (3), 1766-1772 (2015). 2.H. Moon, D. Kumar, H. Kim, C. Sim, J.-H. Chang, J.-M. Kim, H. Kim,* and D.-K. Lim* Amplified Photoacoustic Performance and Enhanced Photothermal Stability of Reduced Graphene Oxide Coated Gold Nanorods for Sensitive Photoacoustic Imaging, ACS Nano 9(3) 2711-2719 (2015). 3.D. Kumar, S. Kaur and D.-K. Lim* Plasmon-assisted and visible-light induced graphene oxide reduction and efficient fluorescence quenching, Chemical Communications 50, 13481-13484 (2014). 4.D.-K. Lim, K.-S. Jeon, J.-H. Hwang, H. Kim, S. Kwon, Y. D. Suh* and J.-M. Nam,* Highly uniform and reproducible surface-enhanced Raman scattering

from DNA-tailorable nanoparticles with hollow 1-nm interior gap. Nature Nanotechnology, 6, 452-460, (2011). 5.D.-K. Lim., A. Barhoumi., R. G. Wylie., G. Reznor., R. Langer., and D. Kohane, Enhanced Photothermal Effect of Plasmonic Nanoparticles Coated with Reduced Graphene Oxide. Nano Letters 13, 4075-4079 (2013).

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장소: 대구 EXCO
발표코드: **KCS4B-3**
발표분야: 신진연구자 학술포럼 II
발표종류: 심포지엄, 발표일시: 수 16:00, 좌장: 장성연

Lateral interactions between organic molecules on solid surfaces

송봉근

충남대학교 화학과

The development of nanotechnologies comprised of nanoscale materials is burgeoning in various fields, in addition to semiconductor devices and heterogeneous catalysts for which the industrial materials are already in nanoscale. Nanomaterials often show completely different properties compared to their bulk, dominated by surfaces or interfaces. Given the importance of these interfaces, study of organic molecules directly attached to solid surfaces is a topic of increasing interest. By creating interfaces between inorganic and organic functionalities, we may be able to tune the properties related to the surfaces with the versatility and tailorability of organic molecules. A deep understanding on the behavior of the molecules on the surfaces is also necessary to gain control over performance of the heterogeneous catalysts. In this talk, fundamental aspects of the adsorption and desorption of organic molecules on semiconductor and metal surfaces will be presented. In many cases, the strongest interaction that drives the adsorption of organic molecules on the surfaces is local bond formation between the molecules and the surface, such as C-dative bonding of isocyanides on Ge(100) or bidentate bridging of acetate on Au(110). However, weaker lateral interactions between the adsorbates or between adsorbates and the surface are also present, and sometimes they significantly affect the behavior of the molecules. Lateral interactions are observed in diverse aspects depending on the system, such as variations of adsorbate structure, aggregation into islands or scattering into isolated species, and coverage-dependent change in surface reaction mechanism. A combination of experimental techniques in addition to theoretical methods was helpful in elucidation of the surface processes.

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발표분야: 신진연구자 학술포럼 II
발표종류: 심포지엄, 발표일시: 수 16:30, 좌장: 장성연

Functional Organic/Inorganic Nanomaterials and Beyond

KIM JI WON

연세대학교 글로벌융합공학부

Designing materials as we desire is one of the most fascinating research area, and some of the most useful areas for developing new materials are their medical- and energy-related applications. In order to design materials such that they have functions and properties as we desire, it is critical to understand how the smallest unit that composes materials ? molecules ? changes the properties of material by their composition and structure. I would like to focus on developing organic/inorganic nanomaterials for (1) medical-related applications to understand, control, and modify the mechanism inside the cells, and (2) energy-related applications such as catalysts for organic reactions, electric/magnetic switches, and sensors for chemicals. Furthermore, based on the current knowledge, it is extremely important that we seek for next steps to design more efficient and functional materials either by combining various existing properties or by discovering novel properties.

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발표분야: Recent Trends in Drug Discovery Based on Chemistry
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 이태호

Generation of Chemistry-Based Drug Candidate and Successful Translation to Clinical Development and Global Partnering

서귀현

한미약품(주) 연구센터

Many biopharmaceutical companies are endeavoring to translate promising scientific breakthroughs into novel treatments for different severe diseases. However, it is so challenging and complex that it makes harder to reach to expected therapeutic achievement ensuring commercial success. Recently, Hanmi had successfully out-licensed mutant EGFR selective inhibitor HM61713 and BTK selective inhibitor HM71224 to two global pharmaceutical companies in USA and Europe with enormous deal values, respectively. Currently, these two molecules are developed as promising drug candidates in the fields of non-small cell lung cancer (NSCLC) and autoimmune disease through the collaboration with license partners.

This presentation would briefly introduce how medicinal chemists at Hanmi recognize the right targets of the corresponding diseases such as lung cancer and autoimmune disease and how hit and lead molecules are designed and optimized in order to generate the final drug candidates that effectively modulate the disease targets, along with the explanation of the pharmacological and clinical outcomes of the candidates.

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발표분야: Recent Trends in Drug Discovery Based on Chemistry
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 이태호

신약개발 - 레고켐 바이오사이언스

김용주

(주)레고켐바이오사이언스 신약연구소

㈜레고켐 바이오사이언스는 의약 화학을 기반으로 하여, 설립된 신약개발 Bio-Venture 이다. 창업 후, 9 년 동안 항생제, 항암제, 항응혈제 분야에서 5 개 이상의 Drug Candidates 를 발굴하여, 비임상, 임상 단계에 진입 시켰으며, 최근 5 년 동안 의약화학을 기반으로 ADC(Antibody-Drug Conjugate) 분야에 진출하여, 기반 기술인 새로운 Linker 기술을 개발하였으며, 차세대 성장 동력을 구축하였다.신약 개발은 다양한 기술이 융합 되어야만 가능한 사업 분야이다. 레고켐 바이오사이언스의 신약개발 전략, Pipelines 및 향후 성장 전략에 대해서 소개하고자 한다.

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발표코드: **KCS5-3**

발표분야: Recent Trends in Drug Discovery Based on Chemistry

발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 이태호

RNA 저해제는 미래신약의 플랫폼이 될 것인가?

박한오

(주)바이오니아

1998 년 Fire 와 Mello 교수가 이중나선 RNA 에 의한 RNA 저해 현상을 꼬마촌충에서 발견하고, 2001 년 Tuschl 그룹에서 화학적으로 합성한 21 mer 의 이중나선 siRNA 을 이용해 동물세포에서 상보적인 mRNA 를 분해시켜 유전자발현을 조절할 수 있다고 보고한 이후, 여러 회사들이 게놈프로젝트로부터 알려진 모든 유전자에 특이적인 siRN 를 설계하여 화학적으로 합성한 genome-wide siRNA library 를 공급하게 되어, siRNA 는 PCR 이후 분자세포생물학 연구의 가장 중요한 도구로 광범위하게 이용되고 있다. 이 공로로 2006 년 Fire 과 Mello 교수가 노벨상을 수상한 후 미국의 벤처기업들을 중심으로 siRNA 를 이용하여 질병관련 유전자들의 발현을 억제하는 새로운 개념의 신약으로 개발하고자 많은 연구들이 진행되어 현재 70 여 개의 신약개발 프로젝트들이 전세계에서 진행되고 있다. 어떤 질병관련 유전자들이든지 쉽게 siRNA 를 설계하여 화학적으로 합성할 수 있어서, 지금까지 small molecule 이나 antibody 로 공략하기 어려운 타깃들도 쉽게 공략할 수 있어 난치병 치료제 개발에 새로운 플랫폼 기술로서 주목을 받고 있다. 그러나 RNA 는 혈액중에서 RNA 가수분해효소에 의해 1 분내로 분해될 뿐만 아니라, 40 개 이상의 음이온을 가지고 있어 세포투과율이 매우 낮아서, siRNA 를 치료제로 개발하기 위해서는 타깃세포 내로 잘 전달되도록 하는 많은 연구들이 진행되었다. 예로서 siRNA 분자 자체의 phoshodiester bond, ribose 를 변형시키거나 3' 이나 5' 말단에 세포투과성이 좋게 conjugate 를 붙여서 이를 해결하려는 시도들이 있었고, 다른 접근방식으로는 siRNA 를 리포좀이나 micelle 형태의 나노입자 제재로 만들어 세포에 전달효율을 높이려는 연구들이 진행되었다. 그러나 이러한 나노입자 제재들도 siRNA 자체가 가지는 세포의 innate immune stimulation 으로 인한 독성들을 해결하지 못해 임상시험에서 실패하여 off-target effect 의 부작용을 극복해야 하는 문제점을 가지고 있다.

바이오니아에서는 siRNA 의 양말 단에 각각 친수성 oligomer 와 소수성인 lipid 와 cholesterol 분자들을 화학적으로 붙여서 스스로 100 nm 이하의 나노입자로 자가조립 되는 SAMiRNA™(Self-Assembled Micelle interfering RNA)를 개발하여 혈액 내 안정성과 세포전달 효율을 높이면서 innate immune stimulation 에 의한 독성이 없는 새로운 개념의 siRNA 를 개발하였으며, 이를 이용하여 여러 난치병에 대한 치료제들을 개발해 나가고 있다. 향후, 다양한 장기의 세포로 siRNA 전달효율을 높인다면, RNA 저해제는 개인별 질환유전자 발현정보를 기반으로 난치병을 치료하는 미래의 신약으로서 새로운 시대를 열어나갈 수 있을 것이다.

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발표분야: Recent Trends in Drug Discovery Based on Chemistry

발표종류: 심포지엄, 발표일시: 금 15:55, 좌장: 이태호

신약시장 동향과 신약개발지원센터의 역할

<u>윤석균</u>

대구경북첨단의료산업진흥재단(DGMIF) 신약개발지원센터

최근 신약 시장의 동향 및 신약 개발 방향에 대하여 소개하고, 이를 기반으로 국내 신약개발은 발전 방향을 논의함과 동시에 저분자 의약품 개발을 위한 대구경북첨단의료산업진흥재단 신약개발지원센터의 역할에 대해서 소개하고자 한다.

최근의 신약 개발 방향에 따라 신약개발지원센터에서는 국내 제약 연구에 대한 수요를 지속적으로 조사 및 분석을 하고 있다. 이를 통하여 국내 신약개발의 bottleneck 이 어느 분야인지 및 집중이 필요한 분야에 대한 지원 방안을 검토하고, 어떤 방식으로 국내의료산업 관계자인 병원, 출연연구소, 벤쳐 및 제약사를 지원할 것인가도 논의해 보고자 한다. 그리고 이러한 지원을 위하여 신약개발지원센터에 갖추고 있는 장비 및 지원방식, 공동연구지원 또한 개인연구자가 필요로 하는 지원시스템 등을 소개를 하고자 한다.

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장소: 대구 EXCO
발표코드: **POLY.O-1**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 유자형

Watching entangled branched polymer in real time

지아영 **GRANICK STEVE***

기초과학연구원 첨단연성물질연구단

The importance of branching in polymer physics is universally accepted but the details are disputed. We have sculpted DNA to various degrees of branching and used single-molecule tracking to image its diffusion in real time when entangled. By ligating three identical or varying length DNA segments, we construct symmetric and asymmetric Y branches from elements of lambda-DNA with 16 um contour length, allowing for single-molecule visualization of equilibrium dynamics. Using home-written software, a full statistical distribution based on at least hundreds of trajectories is quantified with focus on discriminating arm-retraction from branch point motion. Some part of our observations is consistent with the anticipated relaxation through arm retraction mechanism but other observations do not appear to be anticipated theoretically.

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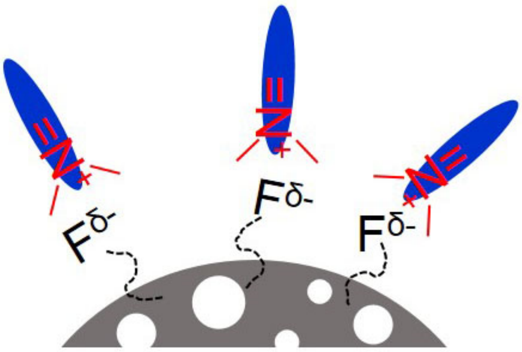
장소: 대구 EXCO
발표코드: **POLY.O-2**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 유자형

Fluorinated Covalent Organic Polymers and Their Size-selective Separation Ability of Charged Organic Molecules

변지혜 **YAVUZCAFERTAYYAR***

한국과학기술원(KAIST) EEWS대학원

The presence of organic contaminants in aquatic environment has become a great concern worldwide as a plenty of organic contaminants, i.e. pesticide, artificial dyes, and so on, are newly emerging with the increase of industrial wastewater. Due to the complexity of the pollutant system, tailoring porosity and chemical functionality of adsorbents is of critical importance to selectively remove/separate target species from water. Porous polymer networks, e.g. covalent organic polymers (COP), are recently drawn significant attention for the selective adsorption of organic pollutants for two reasons; (i) COP is designable solid of which the porosity and chemistry can be designed and controlled for the target molecules, (ii) and it is also to be stable under aqueous system. Herein, we developed a new type of fluorinated COP with high microporosity, which can be simply generated via a catalyst-free self-condensation of cheap monomer. The fluorinated COP exhibits the improved size and charge selectivity toward small-sized organic molecules, demonstrating that the combination of microporosity and fluorine functionality can achieve selective separation of charged organic molecules from water.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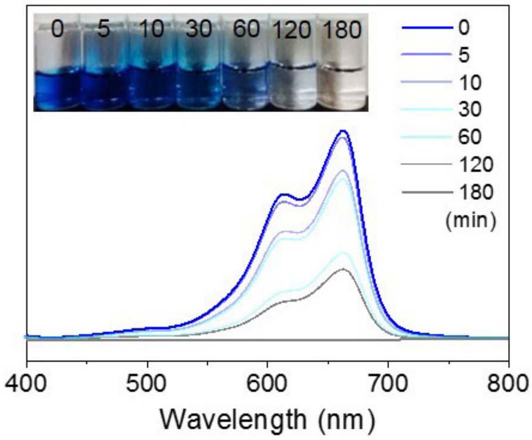
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60
120
180
(min)
400
500
600
700
800
Wavelength (nm)

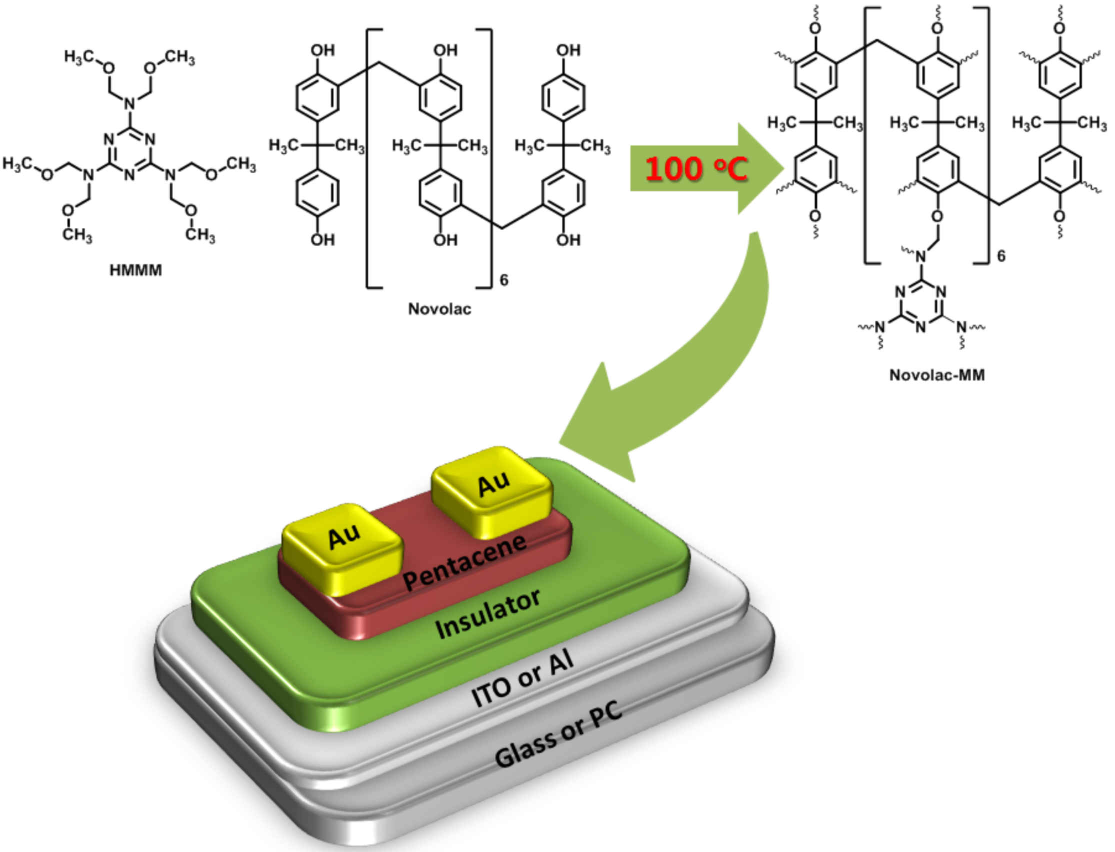
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY.O-3**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 유자형

Organic Thin-Film Transistors with Low Temperature Cross-Linked Polymers as Dielectric Layer

하종운 황도훈[*]

부산대학교 화학과

A potential gate dielectric material that can be cured and processed at low temperatures was designed and synthesized via the cross-linking of bisphenol A novolac (Novolac) and hexamethoxymethylmelamine (HMMM) in the presence of a catalytic amount of p-toluenesulfonic acid. The thin films of the prepared insulator, Novolac-MM, were completely solidified after cross-linking at 100 °C. Metal-insulator-metal (MIM) devices and pentacene-based p-type organic thin-film transistors (OTFTs) using the synthesized polymer as a dielectric layer were fabricated and compared to poly(vinylphenol)-based materials. Novolac-MM devices showed low leakage current (


HMMM
Novolac
6
100 °C
Novolac-MM
Au
Au
Pentacene
Insulator
ITO or Al
Glass or PC

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발표분야: Oral Presentation for Young Polymer Scientists

발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 유자형

Direct C-H arylation reaction for synthesis low band gap alternating polymers and small molecules and their photovoltaic performance

Gamal Mohamed 이재석[1,*]

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

The C-H arylation reaction has been used for synthesis new (DD`AD`DA`)-constituted conjugated polymers with the aid of Pd(OAc)2/Bu4NBr catalytic system. The synthesis methodology avoided the drawbacks of Stille and Suzuki coupling and obtained high yields. All of the new polymers possessed broader absorption windows with low energy band-gaps (1.34?1.64 eV), as well as low-lying HOMO energy levels. The prescreening of these polymers as an active material in bulk heterojunction solar cells was investigated and a power conversion efficiency of 2.36% was achieved. Also, series of small molecules based on the [A`(D`AD)2]architecture was developed using selective direct heteroarylation. The new small molecules bear two different acceptors and/or donors, which led to decrease the electron band gap and improve the strength of the push?pull system as well as the amount of intramolecular charge transfer from donor to acceptor units. All small molecules showed broad absorption spectra with optical band gaps, which were estimated to be in the range of 1.72?1.29 eV. The EHID(EDBTT)2:PC71BM-based solar cells reached a maximum PCE of 3.24%.

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Cross Linkable Polymeric Binders for Si anodes in Li Batteries for high performance and practical applications

MANAYATHTHEKKEYILJEENA 최후연[1] 박수진[2] 유자형[3,*]

울산과학기술대학교(UNIST) 나노생명화학공학부 [1]울산과학기술대학교(UNIST) Chemistry [2]울산과학기술대학교(UNIST) 에너지 및 화학공학부 [3]울산과학기술대학교(UNIST) 자연과학부 화학과

The electro chemical performance of Li ion battery (LIB) can be highly tuned by various factors which include morphology of anode material, nature of electrolyte and binding material, percentage of conducting materials etc. Among them, binding material have been attracted by researchers over decades, which results in the introduction of different polymeric binder, originated from nature, such as poly acrylic acid, carboxy methyl cellulose, alginic acid etc. for Si anode of LIBs. Recently several synthetic and structural modifications of these conventional polymeric binders, for example, random co polymer of polyacrylic acid with vinyl alcohol, porous scaffold of CMC, etc. has been developed by many researchers. However, the challenges of further development of Li ion rechargeable batteries still exists because of some unique property possessed by Li batteries, such as high energy density, high specific capacity and light weight to carry. Inspired from these advantages of LIBs, here in, we introduce a novel polymeric binder for Si anodes in LIB as an effort to improve the columbic efficiency and cycle durability of LIBs. We report, novel random copolymers, poly(tert-butyl acrylate-co-triethoxyvinylsilane) and Poly(acrylic acid-co-vinyl alcohol) as an efficient binders with ICE of more than 80% for LIBs. The binders form cross linking under thermal treatment, demonstrated by FT-IR, helps to minimize the pulverization of Si nano particle in the anode. In this present work we find out the optimum percentage of each monomer composition in the random co polymer by analyzing the electro-chemical-mechanical properties of series of synthesized random copolymers.

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Interfacial Film Formation Using Phenol Derivatives and Amine Polymer

왕윤선 이해신*

한국과학기술원(KAIST) 화학과

In nature, insects have an exoskeleton, which are built through catecholamine chemistry. We studied new catecholamine film at liquid/air interface by mimicking the insect cuticle formation. When the catecholamine solution exposed to air, the microfilm was formed at liquid/air interface. The film shows the folding property and self-healing property. First, the film has Janus-face; the top of the film exposed to air is hydrophobic and flatten. On the other hand, the bottom of the film faced to liquid is hydrophilic and porous. The different structure and amphiphilicity of the both sides give the folding property according to dry-wet condition. In addition, the film can beself-healing at the damaged site when catecholamine solution re-exposed to the air at liquid/air interface. The self-healing can be repeated until all catecholamines in the solution are oxidized.

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Simple preparation of 1D and branched nanostructures via in situ nanoparticlization of fully conjugated polythiophene diblock copolymers

이인환 최태림*

서울대학교 화학부

Synthesis and selfassembly of fully conjugated block copolymers based on polythiophenehave been attracted great attention, because these polymers might yield well-definedand semiconducting nanoobjects which could become stable and high performancematerials. Conventional self-assembly processes of presynthesized block copolymers generally required postsynthetic treatments such as selective solvent addition, aging, and pH change, because the synthesis of block copolymer itself did not provide sufficient driving force to assemble the polymers into the nanostructures. In addition, the generated nanostructures from conventional selfassemblyprocesses were generally fragile toward the external stimuli such as temperature change, mechanical force, and oxidation in air, thus the further post-modifications such as chemical crosslinkingwere also needed to make the nanostructures stable under external stimuli. To make the self-assemblyprocess step-economic, recently, we have reported a simple one-pot self-assemblyprocess for the formation of kinetically trapped and highly stable nanostructures, which was termed as in situ nanoparticlization of conjugated polymers (INCP). By applying this straightforward INCP strategy, unique branched nanostructures and nanocaterpillars were directly formed during the synthesis of poly(3(2-ethylhexyl)thiophene)-block-polythiophene (P3EHT-b-PT) and poly(2,5-dihexyloxy-1,4-phenylene)-block-polythiophene (PPP-b-PT),respectively. Nanostructures from P3EHTbPTwere evolved from nanosphere to nanocaterpillar to nanostar, and eventually to nanonetwork structures as increasing in length of PT. In case of PPP-b-PT, nanostructures were only evolved from nanospheres to nanocaterpillars due to the larger hydrodynamic volumn of PPP than that of P3EHT.

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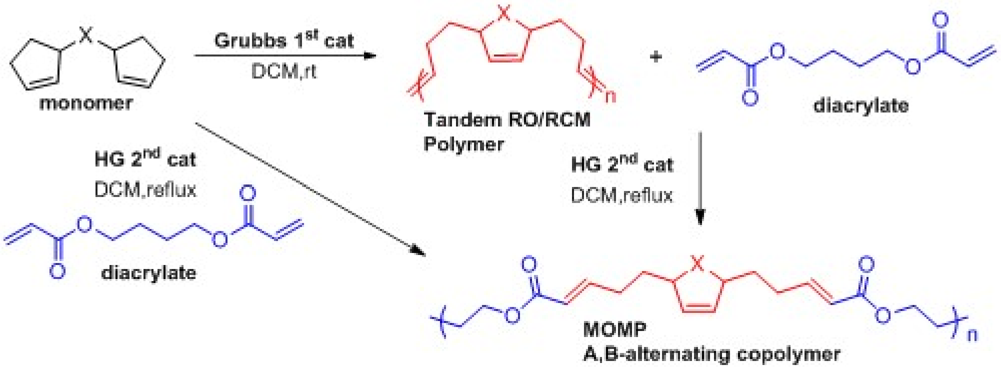
Tandem Ring-Opening/Ring-Closing Metathesis Polymerization and Multiple Olefin Metathesis Polymerization That Combines All Three Olefin Metathesis Transformations

이호근 최태림*

서울대학교 화학부

We demonstrated tandem ring-opening/ring-closing metathesis (RO/RCM) polymerization of monomers containing two cyclopentene moieties and postmodification via insertion polymerization. In this system, well-defined polymers were efficiently formed by tandem cascade RO/RCM reaction pathway. Furthermore, these polymers could be transformed to new A,B-alternating copolymers via a sequential cross metathesis reaction with a diacrylate. Additionally, we demonstrated the concept of multiple olefin metathesis polymerization in which the dicyclopentene and diacrylate monomers underwent all three olefin metathesis transformations (ring-opening, ring-closing, and cross metathesis) in one shot to produce A,B-alternating copolymer.



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발표코드: **INOR.O-1**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 분과기념강연, 발표일시: 목 09:00, 좌장: 이동환

Design and Applications of Functional Metal-Organic Frameworks

홍창섭

고려대학교 화학과

Metal-organic frameworks (MOFs) have emerged as innovative crystalline materials because a number of MOFs have exhibited surface areas much higher than those of other porous solids. Also, their structures are readily controlled by the judicial choice of appropriate metal ions and organic spacers. Such features are beneficial to seek functional materials showing proton-conducting materials and CO2 adsorption capacity. In this talk, I will introduce design and modification of MOFs via a post-synthetic method and applications on proton conductivity and CO2 capture.

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발표종류: 분과기념강연, 발표일시: 목 09:25, 좌장: 이동환

Transformation of Small Molecules at a Low Valent Nickel Center Supported by a Series of PEP Pincer-type Ligands

이윤호

한국과학기술원(KAIST) 화학과

The development of a greater understanding of the chemistry involved in the transition metal complex mediated activation of small molecules such as carbon dioxide and carbon monoxide is prompted in part by the need to develop agents for the utilization of such gases as a synthetic C1 source. Especially, we employ a series of PEP (E = N, P and Si) ligand to accommodate a nickel ion species in a tetracoordinate planar/tetrahedral environment. A particular study of such species is currently under investigation 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 hydroformylation and the Monsanto/Cativa process. In this presentation, a four coordinate (PEP)Ni-L scaffold (E = N, P or Si) where the L site is occupied by ligands such as N2, CO, CO2 and COOR will be described. The (PNP)Ni systems accommodating terminally bound CO in the three formal oxidation states (nickel(0), +1, and +2) and their reactivity toward iodoalkanes will be illustrated. The mechanistic investigations via experimental and theoretical studies will be discussed regarding the C-C bond formation at the paramagnetic nickel center. In addition, a series of CO2 adducts have been generated revealing unique binding character to a nickel center possessing a different geometry depending on the ancillary PEP ligand. With concerning the geometry and reactivity relationship, the reactivity of each Ni-CO2 adduct will be also discussed. In fact, unanticipated metal-ligand cooperation employing a (PEP)Ni scaffold will be presented in which reversible methoxy group transfer occurs between a phosphide moiety of the ligand and the nickel ion.

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발표코드: **INOR.O-3**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 홍창섭

Using Computer Models to Understand Intrinsically Irreversible, Non-Nernstian, Two-Electron Reductions of Pt(IV)-complexes

Mu-Hyun Baik

한국과학기술원(KAIST) 화학과

Computational molecular modeling has become an important tool of inquiry over the course of the last two decades. In particular, modern methods like Density Functional Theory (DFT) have allowed new perspectives on classical problems of inorganic chemistry, like redox chemistry. In this presentation I will review efforts from my research group towards utilizing DFT to better understand redox processes that are difficult to understand using classical tools of research:

Redox reactions are most conveniently studied using cyclic voltammetry (CV). To precisely determine the normal reduction potential of a redox pair, the average of the cathodic and anodic peak potentials are commonly taken. This simple and robust protocol becomes useless when the electrochemical reduction is coupled to an irreversible chemical reaction, as the corresponding anodic peak vanishes and the CV only shows a cathodic peak. Through a combination of computations and a careful shape analysis of such irreversible Faradaic response, we were able to not only extract the normal potential, but also to obtain kinetic information that is difficult to assess by other means.

This example of integrating theory and experiment in a single seamless effort highlights how we can leverage very simple techniques into a synergistic framework of investigation.

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발표코드: **INOR.O-4**

발표분야: Oral Presentation for Young Inorganic Chemists

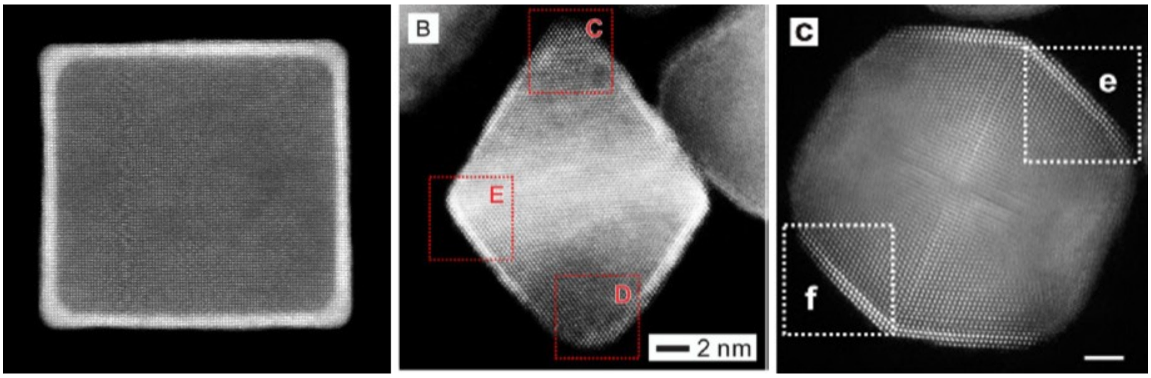
발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 홍창섭

Atomic Layer-by-Layer Deposition of Pt on Pd for Catalysts with Enhanced Activity toward Oxygen Reduction

최상일

경북대학교 화학과

Platinum is a key catalyst used for the oxygen reduction reaction (ORR) in a proton-exchange membrane fuel cell (PEMFC). Despite its great performance in ORR, its high cost and low abundance in the earth have created a major barrier for the commercialization of PEMFCs. One of the effective strategies for reducing the Pt content while retaining the activity of a Pt-based catalyst is to deposit the Pt atoms as ultrathin skins of a few atomic layers thick on nanocrystals made of another metal. During deposition, however, the Pt atoms often take an island growth mode because of a strong bonding between Pt atoms. This presentation introduces a versatile route to the conformal deposition of Pt as uniform, ultrathin shells on Pd nanocrystals. By applying different shapes of Pd nanocrystals, we determined the final shape of Pd@Pt core-shell nanocrystals. Compared to a commercial Pt/C catalyst, the Pd@Pt core?shell nanocrystals with different shapes showed enhancements in activity and durability toward the ORR. Among the various shapes, the greatest enhancement could be achieved for icosahedral Pd@Pt nanocrystals.



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발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 홍창섭

Synthesis of Nanostructured Catalytic Materials for Selective Conversion of Hydrocarbon

나경수

전남대학교 화학과

Control of chemical reaction to produce a desired product with high yield is of important issue in view of energy-saving green chemistry involving heterogeneous catalyst. Synthesis of well-defined nanostructured catalysts is one of the resolutions to achieve this goal. For example, size- or shape-controlled metal nanoparticles with high uniformity can be used for selective conversion of raw chemicals to value-added chemicals with high selectivity. In this presentation, Pt metal nanoparticles incorporated various porous materials such as hierarchically nanoporous zeolites [1,2], mesoporous aluminosilicate [3,4], and metal-organic frameworks [5,6] have been prepared. The resultant metal nanoparticles supported on various porous materials with controlled physicochemical properties are investigated in hydrocarbon conversion reaction using methylcyclopentane or n-hexane as model reactant, which can make catalytic synergies such as enhancement of catalytic activity, and change in product selectivity. Detailed results and correlation data between the catalytic phenomenon and catalytic properties will be discussed in this presentation. [1] Na, K.; Alayoglu, S.; Ye, R.; Somorjai, G. A. J. Am. Chem. Soc., 2014, 136, 17207.[2] Na, K.; Musselwhite, N.; Cai, X.; Alayoglu, S.; Somorjai, G. A. J. Phys. Chem. A, 2014, 118, 8446.[3] Musselwhite, N.; Na, K.; Alayoglu, S.; Somorjai, G. A. J. Am. Chem. Soc., 2014, 136, 16661.[4] Musselwhite, N.; Na, K.; Sabyrov, K.; Alayoglu, S.; Somorjai, G. A. J. Am. Chem. Soc., 2014, ASAP (doi: 10.1021/jacs.5b04808)[5] Na, K.; Choi, K. M.; Yaghi, O. M.; Somorjai, G. A. Nano Lett., 2014, 14, 5979.[6] Choi, K. M.; Na, K.; Somorjai, G. A.; Yaghi, O. M. J. Am. Chem. Soc., 2015, 137, 7810.

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발표코드: **PHYS.O-1**
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발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 이호재

High-performing MgO/Ni catalyst fabricated by atomic layer deposition for carbon dioxide reforming of methane reaction

김승연 김대한 정명근 한상욱 박은지 이주하 김보라 박기정 김일희 김영독*

성균관대학교 화학과

The catalytic activities of MgO-coated Ni catalysts prepared by atomic layer deposition (ALD) method with two difference shell thickness for CO_2 reforming of CH_4 (CRM) was compared with that of bare Ni catalyst. The catalytic activity and stability in the CRM reaction at 800 ^{o}C was advanced with increasing thickness of MgO shells deposited on Ni. The MgO/Ni catalyst prepared with 200-ALD MgO deposition cycles shows superior catalytic activity and the catalytic activity of MgO/Ni was fairly durable, with negligible deactivation during a 72 h CRM reaction. We suggest that the MgO shell, which is highly basic and has a strong CO_2 affinity, accelerated the reverse CO disproportionation, thereby restraining carbon deposition on the Ni surface. Moreover the 200 cycled-MgO/Ni allows particular growth of filamentous carbon on surface of catalyst, thereby reducing deactivation of the catalyst during the CRM reaction. We suggest that the fabrication of core-shell structure by ALD can progress the activity and stability of the catalysts which are operable at high temperature.

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발표코드: **PHYS.O-2**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 이호재

Carbon Dioxide Capture by Aqueous Diamine: Density Functional Theory Calculations

박소정 이진희[1] 김훈식[2] 장윤희[3,*]

광주과학기술원(GIST) 신소재공학부 [1]광주과학기술원(GIST) 신소재공학과 [2]경희대학교 화학과 [3]광주과학기술원(GIST) 신소재공학

Chemical absorption using an aqueous amine solution is currently one of the most mature technologies to capture CO_2 from post-combustion processes. Piperazine (C4H8N2; PZ), a cyclic diamine, has been used as favorable CO_2 capture properties because of fast reaction rate with CO_2, high CO_2 capacity, and high oxidative degradation resistance. Recent experimental works have shown that PZ derivatives were identified as promising solvent. To understand the CO_2 capture performance of promising cyclic diamine absorbents, we investigate their reaction with CO_2 in water using the density functional theory method (B3LYP/6-311++G**) combined with the Poisson-Boltzmann continuum-solvation model for water. We calculated to validate the reliability against the experimental pKa and then show the values calculated for cyclic diamines reproduce the experimental values. The free energy of formation calculated for a series of reaction intermediates and products explains the observed CO_2 absorption rate which involves the formation of zwitterion intermediate, rate-determining step as well as speciation during CO_2 loading. We also understand the analysis of chemical species of PZ about CO_2 absorption using calculation of in-situ IR spectrum. From this molecular level information, a guideline to improve the CO_2 loading rate and capacity of amine absorbents is provided.

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발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 이호재

Germylene-type reaction of the Ge(100) surface with tert-butyl isocyanide

송봉근[*] Jong Suk Yoo[1] Stacey F. Bent[1,*]

충남대학교 화학과 [1]Stanford University, USA

Reactions of the (100) surfaces of Ge and Si with organic molecules have been generally understood within the concept of “dimers” formed by the 2×1 surface reconstruction. For example, it was recently discovered that adsorption of tert-butyl isocyanide (TBIC) on Ge(100)-2×1 occurs through a dative bonding configuration through the isocyanide carbon atom.[1] Here, we provide an unprecedented example of germylene-type reactivity of the Ge(100) surface provoked by adsorption of a dense monolayer of TBIC. Infrared spectroscopy experiments under ultra-high vacuum conditions were conducted together with density functional theory calculations. The suggested structure of the product resembles a germa-ketenimine molecule. Overall, our study expands the knowledge on the reactivity of the Ge(100) surface that parallels that of molecular group 14 compounds.[1] B. Shong, K.T. Wong, S.F. Bent, Strong Carbon-Surface Dative Bond Formation by tert-Butyl Isocyanide on the Ge(100)-2 × 1 Surface, Journal of the American Chemical Society, 2014, 136 (16), 5848

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발표코드: **PHYS.O-4**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 목 10:05, 좌장: 이강택

Live cell imaging using Au-NNP (Nanobridged Nanogap Particles)?

서영덕[*] 남상환[1] 임동권[2,*]

한국화학연구원 나노바이오융합연구단 [1]한국화학연구원 나노바이오융합연구센터 [2]고려대학교 KU-KIST 융합대학원

Single-particle tracking Live-Cell imaging using Au-NNP(Nanobridged Nanogap Particles) will be presented. Due to a stable plasmonic amplification of Raman signal from the intra-nanogap of Au-NNP, we have a stable and strong Raman signal enough for single particle imaging of Au-NNP in live cell. Multiplex imaging by encoding different Raman dyes into this nanogap and its application will be also discussed.

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Dynamic release of bending stress in short double-stranded DNA by two types of deformation

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Bending with high curvature is one of the major mechanical properties of double-stranded DNA (dsDNA) for its biological functions. Local-melting in the middle of dsDNA (kink), which reduce the energy cost of bending, have been suggested as alternative DNA conformations in addition to the simple bending of dsDNA in the presence of high constrain force. However, the conformations of deformed dsDNA by high bending force and their dynamic characters remain unknown. Here, we report that the strong bending induces not only the kink in the middle of dsDNA but also the end-melting of dsDNA by applying single-molecule fluorescence resonance energy transfer (smFRET) to D-shaped DNA nanostructure consisted of dsDNA (30 bp) and single-stranded DNA (4 - 30 nt). We directly proved that two deformed structures of dsDNA are not permanent but dynamically interconverted each other in millisecond scales. The transition from end-melting to kink is dominated by entropy (anti-Arrhenius behavior), while the transition from kink to end-melting is dominated by enthalpy. The presence of the mismatch or permanent bubble in dsDNA accelerates the kink formation with less compressive force and the kink state becomes permanent when the size of permanent bubble is larger than three base pairs.

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Predicting retention time from molecular structure in proteomics: machine learning approach

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Liquid chromatography tandem mass spectrometry (LC-MS/MS) is slowly becoming a standard in proteomic analysis. It is quite cumbersome to identify peptides from a digested proteome. Retention time prediction is a promising approach in improving their successful identification. In this work, a Quantitative structure-retention relationships (QSRR) model for its direct prediction from the molecular structure of 185 peptides originating from 8 model proteins and two Bacillus subtilis proteomes has been developed. Genetic Algorithm (GA) was used for selection of a subset of molecular descriptors coupled to a nonlinear machine learning method: Support Vector Regression (SVR) for regression. Final GA-SVR model was thoroughly validated through 7-fold cross-validation, and Y-randomization. Robustness and stability were ensured by defining its applicability domain.

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Nocliniclal Dose Formulation : Method Validation of Mixture Dose Formulation

조원미* 김인희[1]

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Nonclinical dose formulation analysis methods are used to confirm test article concentration and homogeneity in formulations and determine formulation stability in support of regulated nonclinical studies. There is currently no regulatory guidance for nonclinical dose formulation analysis method validation or sample analysis. Regulatory guidance for the validation of analytical procedures has been developed for drug roduct/formulation testing; however, verification of the formulation concentrations falls under the framework of GLP regulations (not GMP).

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Studies on Organic Light Emitting Diode (OLED) Emitters by Ultra Performance Liquid Chromatography and Supercritical Fluid Chromatography-Mass Spectrometry

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경북대학교 화학과

Organic Light Emitting Diode (OLED) are widely used to digital display in devices such as television screens, computer monitors, portable systems such as mobile phones, handheld game consoles and personal digital assistances. Also, because of thin, light and flexible properties, OLED is drawing attention as the upcoming-generation material. For the applications, identification of side-materials in well-established OLED complexs is a very important for its purity and stability analysis. In this study, three iridium emitters and one material of photonic and optical device were identified by supercritical fluid chromatography (SFC) and reversed-phase ultra performance liquid chromatography (UPLC) coupled to electrospray ionization (ESI) Mass Spectrometry at the molecular level. SFC utilizes supercritical carbon dioxide, methanol as mobile phase and offers a faster runtime in comparison with UPLC and minimization of noise peaks in baseline for purity analysis in OLED samples. Overall, SFC- and UPLC-MS was successfully applied to OLED compounds for compositional and purity elucidation. Therfore, these results are examples of using powerful separation technique in the field of OLED and we expect that this developed technique will be involved in the actual OLED process.

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Single bubble micro extraction for analysis of chlorophenols coupled with capillary electrophoresis

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In conventional headspace (HS) extraction, analytes evaporated from a sample donor phase in a sealed vessel can be enriched to an acceptor phase often in a liquid form or a sorbent coated on a fiber. The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus an acceptor of small volume is preferred and a single acceptor drop of small volume hanging to the capillary tip has been used in HS extraction for capillary electrophoresis (CE) [1]. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME)/CE using a liquid plug inside a separation capillary as an acceptor in place of the drop [2]. Here, we present single bubble microextraction (SBME) technique coupled with CE, a simple but easy way of conducting HS extraction of a small volume sample for subsequent CE analysis. Instead of using a sealed vessel to prepare a HS, an bubble much smaller than 1 ?L was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor. Then, SBME-CE was performed using the acceptor plug remained in the capillary. Due to the small volumes of the bubble and acceptor plug, it was possible even for a small volume donor to retain a high ratio of the donor and acceptor volumes for high enrichment factors. All steps of SBME-CE were carried out automatically using a commercial CE instrument without any modification. Therefore not only the sample volume could be dramatically reduced, but also the need for a special apparatus was eliminated.

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Measurement of lipid turnover rate in HeLa cell by heavy water labeling

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Heavy water (^2H_2O) labeling is a stable isotope labeling method that has been developed to quantify *in vivo* dynamics of biomolecules such as proteins, DNAs and lipids. Change in mass isotopomer distribution by deuterium labeling enable calculation of biomolecules' turnover rates. Here we describe an experimental strategy for measuring *in vivo* lipid turnover rate in HeLa cell by ^2H_2O labeling coupled with high resolution mass spectrometry. Lipids were extracted from HeLa cell grown in 5% (mol/mol) ^2H_2O enriched media at 6 time points between 0 and 48 hours of labeling. Lipid species of glycerophospholipids, glyceryl esters and sphingolipids were identified based on *in-silico Lipidblast* library. The turnover rate of lipids in HeLa cell was determined in a range of 0.02-0.1 hr^{-1}.

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Sequential Purge and Trap Technique for Sampling of Geosmin and 2-MIB in Aqueous Samples Using Needle Trap Device (NTD)

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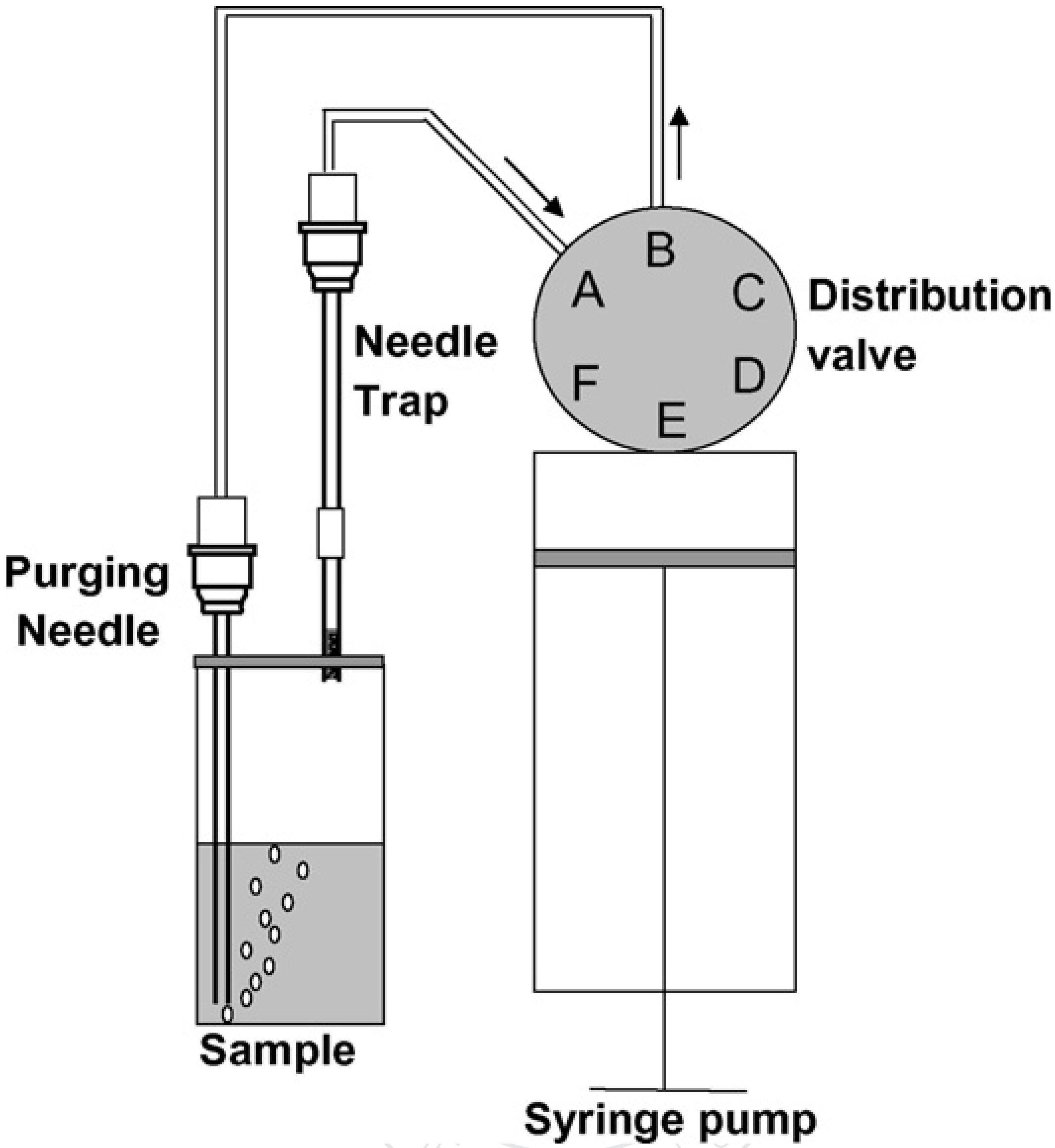
Recently, a needle trap device (NTD) was introduced to the scientific world of sample preparation. NTDs, like solid-phase microextraction (SPME) fibers, are another approach for one-step solventless sampling and sample preparation. The major advantages of NTDs as a sorbent trap technique are simplicity and convenience for sampling of VOCs from different matrixes and injection to the GC directly. Due to these reasons, they are widely used to analyze VOCs easily and efficiently in both gaseous and aqueous samples. However, fine sorbent particles packed in such a small tubing of the NTD do not make it suitable to use the conventional purge and trap technique which is one of the widely used active sampling techniques. To address this limitation, new approach called sequential purge and trap technique for NTD was reported few years ago. This technique adopted the purge and trap sampling mechanism but did not use an additional purge flow by recycling headspace air.1 We revisit this technique to sample and analyze geosmin and 2-MIB in aqueous samples. Geosmin and 2-MIB are naturally produced from blue-green algae and are known to cause earth-musty odor which are difficult to remove during tap water production process. Human noses are very sensitive to detect these compounds in ppt level (5 ng/L for 2-MIB and 30 ng/L for geosmin). In this report, we present concept of a syringe pump assisted headspace sampling technique (i.e. sequential purge and trap technique) for needle trap device again and several experimental factors to improve sampling efficiencies of geosmin and 2-MIB in aqueous samples.


Distribution valve
A
B
C
D
E
F
Needle Trap
Purging Needle
Sample
Syringe pump

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3-phase direct immersion in-tube microextraction coupled with capillary electrophoresis

최지은 고영진[1] 정두수[*]

서울대학교 화학부 [1]서울대학교 화학과

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME, LPME requires more manual maneuvers. In order to overcome such shortcomings of LPME, We developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease. Since the acceptor phase is well protected inside the capillary, ITME can be carried out under severe extraction conditions. Moreover, given that the extraction and injection processes take place simultaneously, the extraction speed and efficiency are very high. Here, we present direct immersion ITME coupled with a commercial CE instrument (DI-ITME-CE) for three-phase configuration. In three-phase DI-ITME, acidic analytes in an acidic aqueous donor solution were enriched into a basic acceptor phase through athin organic layer by the driving force of pH difference.

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Constant current mode electromembrane extraction with capillary electrophoresis for sensitive arsenic speciation

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서울대학교 화학부 [1]Lanzhou institute of chemical physics [2]서울대학교 화학부

Arsenic is an element widely distributed in the crust of the earth, causing a worldwide problem of groundwater contamination. Four arsenic compounds dimethylarsinic acid (DMA), arsenites [As(III)], mono methylarsenic acid (MMA), and arsenates [As(V)] in a unbuffered water sample were enriched by constant current mode electromembrane extraction (CC-EME) and then analyzed by off-line coupled capillary electrophoresis (CE). Under an electrical potential, $CH_3(C_8H_{17})_3N^+\ Cl^-$ (Aliquat 336) in the supported liquid membrane (SLM) acts as a carrier to mediate the transfer of anionic arsenic analytes such as DMA, MMA, and As(V) from the sample solution to an aqueous acceptor phase. Neutral As(III) was oxidized to As(V) by potassium permanganate and then enriched by CC-EME for indirect determination. Several parameters such as the electrode configuration, composition of SLM, pH of donor and acceptor phase, stirring rate, applied current, and extraction time were optimized. Under the optimal conditions, enrichment factors of 1200 to 3600 for the 4 arsenic species were obtained. The LODs for the 4 arsenic species in unbuffered water were 0.4 to 1.0 ppb As, each of which was below the WHO guideline of 10 ppb total arsenic. The established CC-EME was successfully applied for the arsenic species determination in unbuffered water with a high enrichment factor, high sensitivity, low cost and environmental friendly.

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Sensitive Arsenic Speciation with Capillary Electrophoresis

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Arsenic is naturally abundant in the crust of the earth and introduced into the aquatic system through dissolution and weathering of minerals. Chronic ingestion of arsenic in water may cause various diseases, including cancer and keratosis. The World Health Organization (WHO) has set a guideline for arsenic in drinking water at 10 ppb of total arsenic. However, arsenic toxicities vary significantly depending on the species; inorganic arsenics are known to be more toxic than organic ones. Hence the quantitation of specific arsenic species may be more meaningful than the total arsenic determination for the evaluation of the health risks from arsenic-contaminated drinking water. Capillary electrophoresis (CE) provides high performance separation suitable for the determination of arsenic species in real water samples but suffers from the low detection sensitivity. We used a counter-flow (CF) electrokinetic supercharging (EKS) technique to enhance the detection sensitivity. EKS is one of the most powerful sample stacking methods that combines field amplified sample injection (FASI) and transient isotachophoresis. For further improvements in sample enrichment and separation, CF-EKS uses a counter pressure to counterbalance the movement of the stacked sample zone during FASI, obtaining a pronounced increase in the amount of sample injected and the portion of the capillary available for electrophoresis. Four arsenic compounds were analyzed by CF-EKS to obtain 6,000 to 56,000-fold enrichments. The limits of detection (LODs) were in the range of 0.08-0.3 ppb As. For a tap water sample, LODs of 0.5-3.8 ppb As were obtained after 10-fold dilution with deionized water, significantly lower than the WHO guideline of 10 ppb total As.

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Detection of E. coli O157:H7 by ICP-MS immunoassay using metal-doped magnetic nanoparticles

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단국대학교 화학과

Enterohemorrhagic Escherichia coli O157:H7 (E. coli O157:H7) is a major food-borne pathogen causing severe disease in humans worldwide. E. coli O157:H7 is a pathogenic bacterium capable of contaminating food, causing food poisoning, bloody diarrhea, and occasionally kidney failure. For the detection, ICP-MS immunoassay employing magnetophoretic chromatography separation technique was to be used in this work. For target extraction and detection, amine-functionalized/Cs-doped multi-core magnetic nanoparticles (MNPs) were synthesized. The extraction is based on the highly bio-specific recognition interactions of antibody?antigen, i.e, antibody-conjugated MNPs captured E. coli O157:H7. The unbound excess MNPs were eliminated by magnetic separation in the presence of polyethylenglycol medium. The resultant immunoassay products were effectively extracted from sample solution by magnetic separation and then quantified by the determination of doped metal detection using Inductively Coupled Plasma Mass Spectrometer(ICP-MS). Since the proposed method reduced sample treatment time and amplify the signal, its application can be wide for various cell detection.

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Analysis of alpha-1 Antitrypsin in Serum Samples using Surface Plasmon Resonance compared to Enzyme Linked Immunoassay Sorbent Assay

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본 포스터에서는 세럼과 같은 실제 샘플에서 질병의 바이오마커로 이용되는 alpha-1 antirtypsin (AAT)를 surface plasmon resonance (SPR)로 분석하고자 하였다. 특히 알츠하이머질병과 연관있다고 알려져 있는 AAT 를 새로운 항체-압타머 어세이를 이용한 표면 샌드위치 플랫폼을 개발하여 SPR 로 정량분석하였고, 이 결과값을 enzyme linked immunoassay sorbent assay (ELISA) 실험결과값과 비교분석하였다.

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A Localized Surface Plasmon Resonance (LSPR)-based, simple, receptor-free and regeneratable Hg2+ detection system

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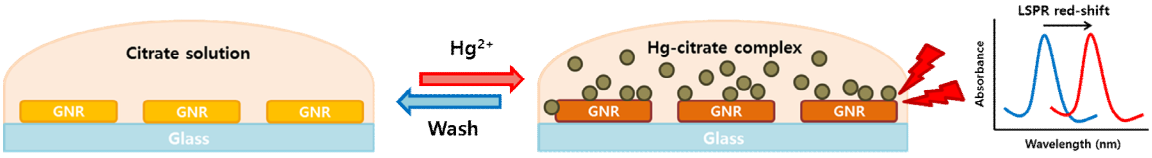
광주과학기술원(GIST) 화학과

A simple, receptor-free and regeneratable of Hg2+ sensor, which utilizes localized surface plasmon resonance (LSPR) shifts of a gold nanorod (GNR), has been developed. Precipitation induced by coordination of Hg2+ to citrate alters the local refractive index (RI) around the GNR surface on glass slide, promoting a red-shift in its LSPR absorption peak. This phenomenon is used to design a sensor that enables quantitative detection of Hg2+ in the 1 nM to 1 mM concentration range with good linearity (0.9507 correlation coefficient). A high selectivity of this sensor for Hg2+ is demonstrated by the specific LSPR red-shift of 27.67 nm promoted by this metal ion in comparison to those caused by other metal ions. In addition, the reusability of the new sensor chip is shown by its successful reuse eight-times following successive washing/precipitation steps. Lastly, the sensor displays excellent recoveries in spiking test with real water samples, such as tap water, lake and river. The simple combination of precipitation of Hg2+-citrate complex and the LSPR red-shift has led to the design of a novel sensing strategy for Hg2+ detection.



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A rapid and sensitive profiling of free fatty acids in biological samples by liquid chromatography coupled to tandem mass spectrometry with derivatization

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경희대학교 화학과 [1]경희대학교 응용화학과

Free fatty acids (FFAs) that have roles in cellular energy and signaling are critical molecules in various biological states. Due to the poor ionization efficiency of FFAs under electrospray ionization mass spectrometry (ESI-MS), it is challenging to construct a robust platform to profile various FFAs in biological samples with LC-MS. In this study, we applied trimethylsilyldiazomethane (TMSD) derivatization to improve the sensitivity of FFA profiling by increasing ionization efficiencies. Multiple reaction monitoring (MRM) was used for the selective quantification of methylated FFAs. The performance of optimized TMSD methylation was validated for a reliable FFA profiling. By using liquid chromatography (LC)-ESI-MS, the high-throughput analysis of various FFAs were successfully carried out in 5 min. In order to prove the utility of our developed method, we performed the FFA profiling of mouse brain, liver, and plasma by using LC/MS/MS with/without methylation. As a result, comparing to nonmethylation, various FFAs were successfully analyzed by using methylation derivatization. Strikingly, we can successfully identify and quantify 14, 14 and 9 FFAs from mouse liver, brain and plasma among the 29 targeted FFAs.

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High Sensitive Analytical Platform for Glycolipids Characterization from Cells to Tissues using Negative Nano-LC/MS and LC/MS/MS

황재윤 안현주*

충남대학교 분석과학기술대학원

Gangliosides are glycosphingolipids containing one or more sialic acids. They participate in diverse biological processes including cell-cell recognition and the modulation of membrane protein function. In spite of the biological importance of cell surface gangliosides, the studies for gangliosides are being delayed due to the structural complexity, amphipathic nature, and lack of sensitive analytical method. Here, we introduces a robust analytical platform for the rapid profiling and quantitation of gangliosides on cell surface using membrane enrichment method and negative ion-mode nano-LC chip based mass spectrometry. The analysis of gangliosides using high resolution mass spectrometry with a membrane enrichment method provides not only comprehensive profile on cell surface gangliosides but also confident assignment of chain length and the degree of unsaturation of ceramide. We optimized the conditions such as solvents, gradients, and sample concentration to efficiently separate ganglioside standard in negative ion-mode. For profiling of cell surface gangliosides, cell membranes were isolated and enriched by ultracentrifugation. Membranes were further separated by Folch partitioning and then fractionated by C18 SPE to extract gangliosides. Gangliosides were comprehensively profiled by negative ion mode LC/MS and the structures were elucidated by tandem MS. We successfully explored cell surface gangliosides in MCF7 breast cancer cell and obtained over 70 compositions. GM3, GM2, GM1 and GD1 were commonly observed as major gangliosides showing various ceramide portions.

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Synthesis of Ruthenium oxide coated Silicon/Carbon Nanofibers composite as anode material for lithium secondary battery

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계명대학교 화학과 [1]계명대학교 화학시스템공학과

In this study, Silicon/Carbon nanofibers (CNFs) composite was synthesized and applied as anode materials of Li secondary batteries. Silicon/CNFs was grown via chemical vapor deposition (CVD) method. The source of silicon was a silane gas blended in a non-reactive carrier gas. Ethylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 600 ℃ and maintained for 10 min to synthesize Silicon/CNFs composite. After Silicon/CNFs composite was put into the 0.01 M $RuCl_3$ solution. The sample was dried in a dryer at 80 ℃. The morphologies, compositions and crystal quality of ruthenium oxide coated Silicon/CNFs composite were characterized by SEM, EDS, TEM, XRD, Raman spectroscopy and XPS. The electrochemical characteristics of ruthenium oxide coated Silicon/CNFs composite as an anode of Li secondary batteries were investigated using three-electrode cell. The as-deposited ruthenium oxide coated Silicon/CNFs composite on Ni foam were directly employed as a 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. 1M $LiClO_4$ was employed as electrolyte and 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. Acknowledgements : 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. 2015035858).

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Detection of Co2+ using automated drop-type chemiluminescence system for monitoring of nuclear reactor

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As well-known, the Fukushima nuclear disaster is the largest nuclear disaster since the Chernobyl disaster of 1986, releasing an estimated 10 to 30% of the radiation of the Chernobyl accident. It was an energy accident, initiated primarily by the Tohoku earthquake on 11 March, 2011, and the damage caused by the tsunami produced equipment failures in boiling water reactor systems, which induced a loss-of-coolant accident followed with nuclear meltdowns and releases of radioactive materials. In this work, a monitoring sensor of Co2+ ions as a clue of the leakage from a boiling water nuclear reactor was developed and its analytical performance was studied. The sensor system was based on a drop-type chemiluminescence which showed the merits of fast analysis with ultrahigh sensitivity. In addition, it has advantages of small sample consumption and less matrix interference or environmental influence in quantitative measurement. In this work, the limit of detection for Co2+ was 41.39 ppt, obtained from calibration curve. The interference by Cu and Fe ions were studied systematically, considering chemical and electrical behavior of interfering ions.

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Quantitative Analysis of 3 Major Nutrients in Milk Powder using Near Infrared Spectroscopy and Chemometrics

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경북대학교 화학과

A well-balanced diet is a very important factor to prevent various lifestyle diseases such as obesity, diabetes and hypertension. Meeting nutritional needs is essential for growing children, especially for infants. Therefore it is necessary to develop accurate as well as precise techniques to measure nutrient content.Even though previously established methods are relatively accurate, these are time consuming and cause environmental pollution by using organic solvents and strong acid. In these regards, spectroscopic methods would be great alternatives to official methods for the quantitative analysis.Mid infrared spectroscopy provides qualitative information regarding molecular functional group from fundamental vibrations. Near Infrared Spectroscopy(NIR) uses Overtone and Combination bands associated with the fundamental vibrations seen in the Mid-IR.A fast and eco-friendly method using FT-IR and NIR has been applied to qualitative and quantitative analysis in various fields.In this study, we applied Near Infrared Spectroscopy (NIR) combined with Chemometrics to quantitative analysis of fat, protein and carbohydrates in milk powder.

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Direct electrochemistry of Glucose Oxidase Based on Chitosan-Multi walled Carbon nanotubes composite for Glucose Sensor

오인돈 정지윤 김현욱 김정희 최영봉 김혁한*

단국대학교 화학과

We simply fabricated electrode of Chitosan-Multi walled Carbon nanotubes(Chi-MWCNTs) composite for enzymatic glucose biosensor without mediator. Chi-MWCNTs(1 mg/mL) of 20 μL was loaded on the cleaned Indium-Tin Oxide(ITO) electrode, and then dried Chi-MWCNTs suspension in the oven at 35℃. Glucose Oxidase(GOx) immobilized on the Chi-MWCNTs without cross-linker or binder. GOx of 20 μL was casted on the prepared Chi-MWCNTs working electrode, and then dried at room temperature. Lastly Chi-MWCNTs/GOx composite included working electrode was rinsed with distilled water after GOx completely dried for remove the unbinding substrate.For investigation of all electrode's morphologies, scanning electron microscope(SEM) was applied. And the electrical signal was measured by cyclic voltammetry(CV) and amperometry.We confirmed no effect of interference such as ascorbic acid(AA) and uric acid(UA) on the Chi-MWCNTs/GOx composite also.In this work, fabricated electrode for detection of glucose level was shown that has advantages such as simply process of electrode fabrication, high sensitivity, low-cost, fast electron transfer and wide detection range.

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판상화약의 자가발열 분해온도

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고에너지물질인 고폭화약은 사용기간 중 많은 외부 환경에 직간접적으로 노출되고 있다. 또한 화약과 같이 산화제와 연료가 공존하는 물질들은 특정온도 이상에서는 서서히 분해반응이 일어나고, 이들 열에너지가 내부에 축적되어 대규모 폭발반응이 진행되기도 한다. 따라서 화약의 열적특성을 정확하게 해석하여 사용 중에 원하지 않는 분해반응을 예방하여야 한다.일반적인 화약들은 원통형으로 시편을 제조하여 내부온도를 측정하여 열축적 측정이 가능하나 특수목적의 판상화약은 시편형태가 판상이기 때문에 열축적 측정을 직접 하는 것이 어렵다. 본 연구에서는 소량의 시료를 이용한 DSC 실험으로부터 얻은 데이터를 이용, 이를 AKTS kinetic 프로그램에 적용하여 자가 가속분해 온도(Self Accelerating Decomposition Temperature)를 계산하여 고에너지물질의 안전한 운용안정성을 예측하였다.

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Top-down Mass Spectrometry to Monitor Thrapeutic Protein with Glycan Heterogeneity

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Biotherapeutic glycoproteins including recombinant monoclonal antibody(mAb) and Erythropoietin (EPO) are fast-growing sector in the current pharmaceutical market. They play a major role in the treatment of variety of conditions such as cancer, inflammation, auto-immune disease for mAb and anemia resulting from chronic kidney disease and inflammatory bowel disease for EPO. It is well known that glycosylation of therapeutic glycoprotein correlates with product safety, efficacy and quality. Thus it has become important to characterize its composition and molecular heterogeneity. In this study, we have developed a top-down approach using chip-based C8 nano-LC/Q-TOF MS. MS parameter was optimized such as gradient, flow rate, fragment voltage to get the best performance. The top-down approach should be preferable in the field of biopharmaceutical as it is relatively fast and more simplified sample preparation procedure. MAbs having neutral glycans and EPOs containing highly sialylated glycans are used to show the proof of concept for the method. We could directly monitor the multiple charge-state distribution and identified the presence and abundance of different glycoform with low nanogram levels of intact glycoprotein. The results can be applied to quality control evaluator and production of biotherapeutic glycoprotein. Especially method can satisfy the need for evaluating the similarity of the glycosylation profiles between biosimilar and innovator products.

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Application Research of Molecular Dynamics with Periodic Boundary Conditions for Long Alkyl Chain Aromatic Compounds by using CCS values and Ion Mobility

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경북대학교 화학과

Detailed structural characterization of compounds comprising crude oil is one of the important research topics in Petroleomics. Our previous study (Ahmed, A. et al., Anal.Chem. 86, 3300-3306, 2014) has shown the advantage of combining ion mobility mass spectrometry (IM-MS), ultrahigh-resolution mass spectrometry and theoretical collisional cross-section (CCS) calculations to increase the amount of information gained as well as to determine the molecular structures of aromatic compounds in crude oils. However, the result of previous study was limited to determine non-alkylated or short-chain alkyl aromatic compounds. In this research, we demonstrate that molecular dynamics (MD) simulation with Periodic Boundary Conditions (PBC) is a useful tool to investigate mutual relation between the theoretical CCS values from computational chemistry and experimental CCS values from ion mobility, especially for long-chain alkyl aromatic compounds in crude oil.

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Stability of Volatile organic compounds (VOCs) depending on storage temperature and duration of urine samples

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Volatile organic compounds (VOCs), ubiquitous environmental pollutants, are the organic compounds that have a high vapor pressure at room temperature. VOCs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA and cause cell mutations. Therefore, monitoring of VOCs in biological samples is very important to evaluate correlation between exposure of VOCs and human disease. However, the levels of VOCs in biological samples can vary depending on storage temperature and duration of samples because of low boiling points of VOCs. In this study, we investigated stability of 14 VOCs depending on storage temperature and duration of urine samples to establish optimal sample handling conditions. Aliquots of urine were stored at room temperature (25°C), refrigerator (4°C), or freezer (-20°C) conditions for either 1, 3, 7, 14, or 30 days. The levels of 14 VOCs in urine samples were detected by solid-phase microextraction-gas chromatograph-mass spectrometry (SPME-GC-MS). Alteration of urine samples is clearly storage temperature and duration dependent for almost all analyzed VOCs. This study provides detailed knowledge regarding stability of VOCs in urine samples and will help to ensure the reliability of laboratory test results.

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Structural identification of Nitrogen compound in Crude oils using high resolution MS/MS

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Oil is the energy source that become increasingly depleted. Therefore, it is important to find out the chemical composition of the oil and use it efficiently. There are many studies on analyzing the chemical compositions of crude oil. gas chromatography-Mass spectrophotometry (GC-MS) has been used to analyze light constituent of crude oil, but this is limited for the heavy constituents. This study shows the results of structural analysis of nitrogen compounds observed with different ionization methods, (+/-) ESI or APPI. The nitrogen composition mentioned either high molecular weight, polycondensed, or polar compounds that cannot be detected by using conventional techniques. Therefore, ultrahigh-resolution mass spectrometry (UHR-MS) is used to analyze heavy compounds. In addition, MS/MS spectra showed core structures of nitrogen compound of crude oil.

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The Analysis of TDI and TMP reactionproduct using MALDI-MS

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TDI(toluene diisocyanate)와 TMP(trimethylolpropane)반응은 urethane 결합을 이루는 폴리머반응으로 진행된다. 따라서 반응 생성물은 13 종류 이상의 시리즈 형태로 생성된다. 모든 가능성 있는 분자량을 계산을 통하여 예측하고, MALDI-MS 를 이용하여 생성된 반응혼합물을 확인하였다. 이 방법을 통하여 MALDI-MS spectrum 의 대부분을 확인하였으며, 반응조건, 시간변화에 따른 생성물의 차이를 확인 및 검증 하는 방법으로 pre-polymer 형성에 대한 reaction monitoring 을 실시 하였다. 그리고 LC-MS, IR 등의 결과를 보조적으로 이용하여 pre-polymer 생성 반응을 체계적으로 설명하였다.

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Reliable DB for High-throughput Screening of Therapeutic Antibodies Glycosylation Using LC-MS and LC-MS/MS

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충남대학교 분석과학기술대학원

Biosimilar products of monoclonal antibodies (mAbs) are one of the most fast-growing segment of the biotherapeutic market. They commonly have advantages of specificity to targeted antigens and lower safety issues in clinical trials than many other type products. As patents on clinical mAb were beginning to expire, many pharmaceutical companies have been interested in developing for biosimilars. In producing recombinant mAb, glycosylation is considered as a crucial protein quality attribute. Because it is the key factor that can affect to biological activity, as protein stability and immunogenicity, of a therapeutic glycoprotein. Additionally, recombinant antibodies being expressed from non-human mammal cell lines could have the unexpected glycosylation that introduced by host cell's original glycosylation synthesis. Thus, glycosylation with micro heterogeneity should be screened for modulating protein quality. For identifying the desired/undesired glycosylation, accurate mass was used to compositionally annotate and profile N-glycans while tandem MS using CID was employed for structure elucidation. Here, we created glycoform database for rapid identification and structural elucidation of antibody N-glycosylation based on LC-MS and LC-MS/MS analysis. RT, accurate mass, and diagnostic fragment peak were summed up to identify each glycan. Up to now, glycans from five representative mAbs including adalimumab, bevacizumab, infliximab, rituximab and trastuzumab were analyzed and total 27 glycans were incorporated to database. The glycan DB could be applied with high-throughput glycan characterization method of therapeutic antibodies produced by various cell-based expression systems in pharmaceutical industry.

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[발표취소] Time-dependent ^{31}P NMR analysis of GTP hydrolysis in paclitaxel-stabilized microtubules

백윤기* 이효원[1]

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Synthesis of silicon-coated carbon nanofibers on electroplated Co-Ni /C-fiber textiles for anode material of Li ion batteries

장건호 이상훈 이창섭*

계명대학교 화학과

In this study, carbon nanofibers(CNFs) were synthesized by thermal chemical vapor deposition(CVD) to Co-Ni electroplated on C-fiber textiles. The CNFs were coated with a SiO_2 layer by hydrolysis of Tetraethyl orthosilicate(TEOS) and Si@CNFs composite were synthesized by reduction of SiO_2@CNFs composite. SiO_2@CNFs and Si@CNFs were applied to the anode material of Li ion batteries. C-fiber textiles were oxidized with nitric acid before electroplating with Co-Ni catalysts. The oxidation process created the hydroxyl group on the C-fiber textiles, and the hydroxyl group was used as an active site for the electroplating of catalysts. After being electroplated, ethylene as a carbon source was flowed into a quartz tubular furnace heated to 700℃, and maintained for 1 h to synthesize CNFs. The CNFs were oxidized by nitric acid before being coated with silica via hydrolysis of TEOS. Coated silica layer on CNFs was reduced by inflow of H2 gas at 700℃. The characteristics of CNFs were analyzed by SEM, EDS, XPS and Raman. The SiO_2@CNFs and Si@CNFs were characterized using TEM, EDS and XPS. The as-synthesized CNFs, SiO_2@CNFs and Si@CNFs were directly employed as anode materials without any binder. The electrochemical characteristics of CNFs, SiO_2@CNFs and Si@CNFs as anodes of Li ion batteries were investigated using coin cell.

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Fabrication and Characterization of an Anode Materials for Li Secondary Batteries Based on four Carbon Materials - Si composites

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We have performed a study on the characteristics of Carbon materials -Si composites that used as an active anode materials for lithium secondary batteries. Samples employed for the battery test were commercial products of GNF, GNT, CNF and CNT. The test results of the samples were compared with the Si composites of each sample. The Si particles were ball-milled to a micron size and coated with pyrolytic carbon using by ethylene gas. Then it was finely mixed with respective two samples using ball mill. PTFE(Polytetrafluoroethylene) was used as the binder and glass fiber separator was used as the separator membrane for the composition of three electrode cell. As the electrolytes, 1M LiClO$_4$ was dissolved in a mixture of propylene carbonate(PC): ethylene carbonate(EC) in a 1:1 volume ratio. The four different Carbon materials-Si composites were evaluated as the anodic material in three electrode cells. The morphology and composition of the samples were analyzed by SEM and EDS measurements. Physicochemical properties of the samples were investigated using XRD, Raman spectroscopy and XPS. The electrochemical characteristics as an anodic material of Li secondary batteries were investigated using the galvanostatic charge?discharge and cyclic voltammetry measurements. Acknowledgements : 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. 2015035858).Acknowledgements : 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. 20151035858).

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발표분야: Oral Presentation of Young Analytical Chemists I

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Chemical behavior of non-visual on-line monitoring system in semiconductor manufacturing process

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Although semiconductor equipment industry is one of the high-profit fields integrated many state-of-art technologies, supporting material industry, its technical levels are not high as expected yet in our country. Since production efficiency and volume of chips have been improved by technical migration, the equipment control became very important for manufacturing process. So far, the efficiency control has been done by visual defect monitoring, However, it was revealed that the effect of non-visual defect on production loss is almost 30%. Therefore, a non-visual monitoring technique regarding on wafer contamination control and sample pre-treatment was developed in this work. Since the developed on-line monitoring system utilized various glassware, the chemical behavior of metal ions interested in the process was studied using ICP-MS, on the basis of lifetime of metal ions in acids.

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Combination of ring type separation and High resolution MS/MS for more information about constituents of Crude Oil compounds

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There are many studies on analyzing the chemical compositions of Crude Oil. Gas chromatography-Mass spectrophotometry (GC-MS) has been used to analyze light constituent of Crude Oil, but this is limited for the heavy constituents. The heavy constituents mentioned either high molecular weight, polycondensed, or polar compounds that cannot be detected by using conventional techniques. Latterly, Ultrahigh-resolution mass spectrometry (UHR-MS) is used to analyze heavy compounds. But UHR-MS technique has limitations. Ionization discrimination can limit the number of compounds observed by the technique. High-performance liquid chromatography (HPLC) ring-type separation is one of the methods to overcome limitations. The combined technique disclosed the aromaticity increased as the fraction number increased. The structures and distribution of heteroatom class compounds could be also explained using the combined technique. In addition, MS/MS spectra showed core structures of Crude Oil fractions.

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Cucurbit[n]uril-functionalized Water-Stable FET Sensors

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Here we present highly sensitive and selective organic field-effect transistor (FET)-based sensors with surface functionalized organic thin films. Cucurbit[n]uril (CB[n]) derivatives were used as selective molecular sensing layers on the p-channel semiconducting 5,5’-bis-(7-dodecyl-9H-fluoren-2-yl)-2,2’-bithiophene (DDFTTF) layer. For example, sensors with a CB[6] film showed highly sensitive and selective detection of acetylcholine over choline in water, while those with a CB[7] film showed highly sensitive detection of amine-containing drug molecules. This approach can be effectively applied for the development of highly sensitive and selective sensors for biogenic molecules and drugs.

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발표종류: 구두발표, 발표일시: 금 14:45, 좌장: 김병권

Identification of Lipsticks in the crime scene using analytical techniques

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경희대학교 화학과 [1]한국과학기술연구원(KIST) 특성분석센터 [2]국립과학수사연구원 화학분석과

In the crime scene, there remain many trace evidences and research that is related to trace evidence has been conducted actively to analyze the evidence more efficiently. Stain of lipstick, one of the many trace evidence, can be good evidence to find the suspect or anyone who is connected to the crime. It is necessary to make database because the components of the lipstick is slightly different depending on the kind of lipsticks. In this study, to make database for lipstick components, twenty one samples of three colors such as red, pink and orange were prepared. And we investigated the characterization of lipstick evidence using Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) and Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) and X-ray Fluorescence Analyzer (XRF). TOF-SIMS provides chemical information on surface of sample and their distribution without any treatment. ATR-FTIR is able to identify the molecular structure of lipsticks samples. And XRF is an instrument for analyzing component contained in the samples.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Pepsin immunoassay for the diagnosis of laryngopharyngeal reflux disease

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광운대학교 화학과

A number of patients who complain of laryngopharyngeal reflux disease (LPR) is on the gradual increase due to changes in climate, environment, and eating habits. LPR causes hoarseness, frequent throat clearing, bitter taste in the mouth, referred ear pain, chronic cough and even larynx cancer. However, the effective treatment of LPR is difficult because the treatment yet stay in the inhibition of gastric acid secretion as well as the symptoms persist after treatment. Therefore, appropriate treatment through accurate and rapid diagnosis is necessary. Since pepsin is proteolytic enzyme produced only in the stomach, detection techniques of pepsin in saliva is useful as a sensitive and non-invasive method for the reflux of stomach contents. Therefore, pepsin is one of the most important biomarkers to diagnose LPR. Herein, we report on a new approach to design an immunoassay based on the enzyme-linked immunosorbent assay (ELISA). Binding of antigen-antibody converts a colorless substrate to a colored product by using enzyme. Furthermore, to confirm the presence of pepsin in saliva resulting from LPR, we checked the pH of saliva through the color changes of various kinds of indicator. The general pH of saliva is about 6.7, but in the case of saliva which contains pepsin, the pH decreases. We compared the color between different pH of phosphate buffer and artificial saliva in acidic and basic condition of indicators. In this ways, we investigate the utility of colorimetric immunoassay to determine pepsin in biological samples (i.e., saliva).

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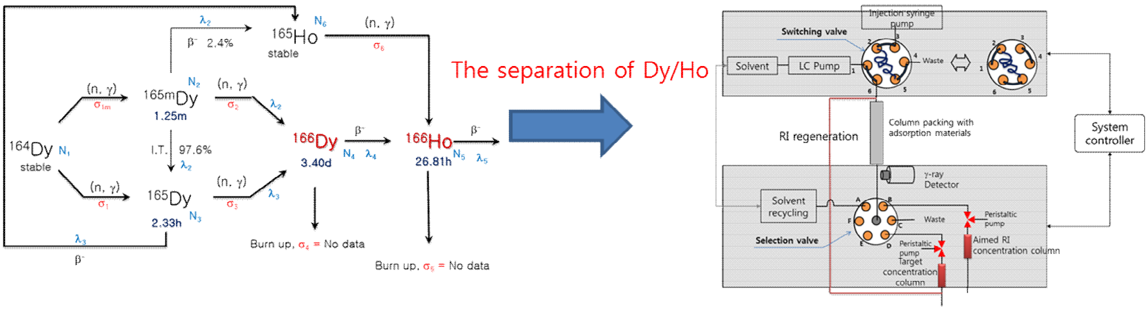
진단치료용 동위원소 생산을 위한 (n,γ)β핵종의 분리 (The separation of (n,γ)β reaction isotopes for production of theragnostic isotope)

최강혁

한국원자력연구원 동위원소이용연구부

방사성란탄족동위원소는 치료용 핵종으로 암환자의 암세포를 괴사시키는 능력이 있다. 특히, (n,γ)b 핵반응의 경우는 생성되는 모핵종과 딸핵종이 다르기 때문에 적당한 분리기술을 도입하면 비방사능(Specific Activity)이 높은 핵종을 얻을 수 있어 방사선면역체료제와 같은 방사선표적치료제 개발에 있어서 중요한 역할을 담당한다. 란탄족 동위원소의 특징은 용액상에서 +3 가이온을 가지며, 화학적인 성질이 유사하여 분리하는 방법이 쉽지 않다. 본 발표에서는 한국원자력 연구원에서 개발한 방사성동위원소의 차폐분리를 위한 분리 시스템과 방사성동위원소 취급에 있어서 작업자의 피폭을 최소화하며, 고순도, 고비방사능을 가진 동위원소의 분리 과정을 소개하고자 한다.



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발표코드: **ANAL2.O-5**

발표분야: Oral Presentation of Young Analytical Chemists II

발표종류: 구두발표, 발표일시: 금 14:54, 좌장: 김병권

Home-built solid-state NMR probes for the structural studies of biological samples like membrane proteins and the in-situ analysis of nano-materials

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한국외국어대학교 화학과

The solid-state NMR spectroscopy has been widely used for various insoluble materials like industrial polymers and biological samples. Also, solid-state NMR analysis of membrane protein on a membrane-like environments, such as bicelle and bilayer, is especially valuable for their structure and function relationship. However, most of biological proteins on lipid bilayers have high dielectric property due to containing large amounts of lipids and salts. Therefore, specific probe with high efficiency and high capacity is required to study biological samples by using solid-state NMR. Also solid-state NMR methodologies for structural study of membrane protein in bicelle could be used for the in-situ analysis of liquid crystalline materials in LCD panels and lithium and fluorine in Li ion batteries. Here, we present the development of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil for structural study of membrane protein. We also present the development of a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a solenoidal coil for analysis of industrial materials. These probes provide short and strong RF pulses, high power capability, and good RF homogeneity.

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발표종류: 구두발표, 발표일시: 금 14:57, 좌장: 김병권

Expression, purification, and NMR Structural Studies of syndecan-4 as a transmembrane protein

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한국외국어대학교 화학과

Syndecans as cell surface receptors participate in biologically important cell-cell and cell-matrix interactions and interact with numerous potential ligands including growth factors and extracellular matrix molecules. The syndecan protein family has four members. One of them, Syndecan-4 is a protein that in humans is encoded by the syndecan-4 gene. They may affect tissue development and repair and growth-factors as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4 is consisted of 25 hydrophobic amino acids and involved in formation of dimer, which is crucial for transduction of signals. Thus, we demonstrated an optimized methods for recombinant expression and purification of syndecan-4(Syd4), mutant Syd4-TM(mSyd4) and Syd4-eTC. The mSyd4 has a partially modified sequence of wtSyd4 and Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of syndecan-4.All peptides were purified by semi-preparative reversed-phase HPLC after cleaving the fusion partner with CNBr. Their biophysical properties of peptides were studied by circular dichroism (CD), mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy. CD spectra were presented that Syd4 analogues adopt a stable α-helical structure in micelle environments. Optimized structure of Syd4 analogues based on solution NMR spectroscopy and solid-state NMR spectroscopy based on 2D SAMPI4 were reinforced with Molecular Dynamics Simulation.

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발표코드: **ANAL2.O-7**

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Efficient analysis of arsenic contaminant in the ground water with capillary electrophoresis mass spectrometry

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서울대학교 화학부

In Korea, arsenic contaminants from trash yards and dead mines are becoming an issue. These contaminants dissolve in to the ground water and endanger water supplies for home, agriculture uses. We present using capillary electrophoresis and its applications to analyze arsenic compounds in the ground water with high efficiencies. Although capillary electrophoresis is suitable for aqueous sample analysis, In case of real samples, applications of capillary electrophoresis mass spectrometry with various enhancing methods still have some obstacles, such as excess amount of salt and other abundant residues. First we applied electrokinetic supercharging, consisting of transient isotachophoresis and field amplified sample injection, to overcome these obstacles. Then, we modified electrospray head unit to control flow in the capillary, which helps to conduct counter flow electrokinetic supercharging and online liquid microextraction. This poster presents the work of flow that approaches to analysis of arsenic contaminants.

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Preparation of various ground organic monolith particles as chromatographic separation media

김윤성 정원조*

인하대학교 화학과

We have recently reported a pioneering study on ground organic monolith particles as new chromatographic separation media in our laboratory. The reaction mixture was composed of methacrylic acid (MAA) as funtional monomer, Trimethylolpropane trimethacrylate (TPTM) as crosslinker, azobis-isobutyronitrile (AIBN) as initiator, polyethyleneglycol as special porogen, and toluene- Isooctane mixture as solvent. In this study, we have prepared different stationary phases by changing formulation of reaction mixture and reaction temperature in a variety of different ways. For example, xylene and n-octane were used as new solvent to increase the reaction temperature. The key idea of this approach is to make soft monoliths with large pore volumes for easy pulverizing. The variations of morphology and chromatographic separation performance of the resultant organic monolith particles will be comparatively discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Further study of PEEK encased monolith frits resulting upgraded separation performance in LC

박신영 정원조*

인하대학교 화학과

As a stream of studying for development of disposable HPLC column, our research group has been studying the technique of polymer encased monolith frits. It is very useful and novel technique owing to its reasonable price and potential of being further improved in a terms of theoretical number of plates. Thus, we have carried out some modification in the physical dimension of monolith frits encased in polymer tubing. To reduce the void volume of frit, the I.D. of poly ether ether ketone (PEEK) tubing was reduced from 500 um of the previous study to 250 um in this study. Catalyst assisted sulfornation of PEEK tubing and reaction with glycidyl methacrylate (GMA) were adopted again to improve the bonding strength between the monoltih core and the tubing inner surface. After sulfornation and anchoring of double bonds, the tubing was filled with a reaction mixture of lauryl methacryltate (LMA), ethylene glycol dimethacrylate (EDMA), initiator, and porogenic solvent. After in-situ polymerization, the tubing was thoroughly washed. Finally, it was ready to be used as frit element after cutting into thin slices. To check the frit performance comparatively, the packed columns installed with a PEEK encased frit of 250 um I.D., a PEEK encased frit of 500 um I.D., and a commercial stainless steel screen frit (1.6 mm I.D.), respectively, at the column outlet union, have been prepared. The separation efficiency with a monolith frit of 250 ㎛ I.D. showed the best results.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **ANAL2.O-10**
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A new C18 phase based on silica monolith particles showing enhanced separation efficiency in HPLC

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인하대학교 화학과

Partially or fully sub-2?m porous silica particles have proved strong feasibility as column packing material due to enhanced separation efficiency and rapid separation in liquid chromatography. Partially sub-2 ?m porous silica monolith particles of relatively uniform size have been successfully prepared by sol gel process followed by grinding and calcinations at 550˚C. The production scale has been increased twenty times in comparison to our previous study. These particles were derivatized with C18 (chlorodimethyl octadecylsilane) ligand in anhydrous toluene under reflux followed by end capping with HMDS (hexamethyl disilazane) and TMCS (trimethyl chlorosilane). The C18 bound phase was washed thoroughly and packed in a glass-lined stainless steel micro-column (1.0 mm ID and 300 mm length) using a slurry packer at a high packing pressure (18000 psi). The separation efficiencies as high as 139,000 N/m were achieved for a test mixture containing benzene and its four derivatives in 60/40 acetonitrile/ water (v/v %) with 0.1% TFA at a flow rate of 25?L/min. The separation efficiency of current stationary phase is better than that of common commercial C-18 phase. This new phase also has shown the promising possibility for fast analysis when packed in a short column.

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Investigation on Raman spectral features of lactose/PE pellets prepared with different particle sizes

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To investigate the variation of Raman spectral feature depends on particle size and its influence on accuracy of quantitative analysis, pellets composed of lactose (5-15wt%) and polyethylene (PE) were prepared, and the corresponding Raman spectra were acquired. For the preparation of pellets, the sizes of lactose were varied (below 50, 50-100, 100-200, 200-300, over 300um), while the size of polyethylene (PE) was unchanged. When the size of lactose particle was smallest, the band shape was dissimilar to those with different particle sizes. The origin for the difference is now under investigation in conjunction with the particle size as well as porosity using Monte-Carlo simulation. Finally, the lactose concentrations were determined using partial least squares (PLS) regression and the dependency of accuracy on the particle size was searched.

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발표종류: 구두발표, 발표일시: 금 15:15, 좌장: 김병권

Electrochemical detection of bisphenol A separated from molecularly imprinted polymer-solid extract phase tube

설다운 PhamKhacDuy 정회일*

한양대학교 화학과

Bisphenol A (BPA) is widely used for production of epoxy resin, polycarbonate and polyethylene. Since BPA is one of the endocrine-disruptors, its detection with simple and cost-effective scheme is greatly demanding. For this purpose, we developed a molecularly imprinted polymer (MIP) able to separate BPA in mixture samples and then a simple electrochemical detection utilizing a mechanical pencil lead as a working electrode was proposed. Since a mechanical pencil lead is cheap and easily obtainable, it could be potential for BPA detection. Initially, BPA-selective MIP was developed and its performances such as percent recovery were investigated. Then, the captured BPA was measured using a mechanical pencil lead electrode using stripping voltammetry and the resulting analytical merits such as limit of detection and response range were assessed. In addition, the same strategy was applied to detect capsaicin as a method for identify domestic and Chinese red peppers.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: Oral Presentation of Young Analytical Chemists II
발표종류: 구두발표, 발표일시: 금 15:18, 좌장: 김병권

Finding an optimal temperature able to improve accuracy for Raman spectroscopic identification of adulterated olive oils

류동현 정회일*

한양대학교 화학과

Identification of adulterated olive oils is critically demanding for its fair product value evaluation. For fast and simple identification, Raman spectroscopy could be a proper candidate since it provides rich structural information of components and the spectral acquisition is non-destructive without requiring further sample pretreatments. Since molecular vibrations of components diversely vary according to temperature, an optimal temperature able to provide enhanced spectral difference between pure and adulterated olive oils would exist. For the study, adulterated extra virgin olive oil mixed with soybean oils was initially prepared. Then, a glass vial containing a sample was initially immersed in liquid nitrogen for sufficient cooling and the vial containing the sample was quickly taken out for continuous Raman spectral collection during natural temperature elevation up to near room temperature. During the temperature elevation, 50 snapshot spectra were collected. Using spectra collected at each snapshot, the identification of adulterated olive oils was attempted and a snapshot providing most discriminant spectral feature was found. The varied spectral feature at the optimal temperature was explained.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Study on elution behavior of non-spherical gold nanoparticles in asymmetrical flow field-flow fractionation (AF4)

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Asymmetrical flow field-flow fractionation (AF4) is a diffusion-based separation technique that has been used widely for characterization of various types of colloidal particles and macromolecules. In AF4, the particles (or molecules) of different sizes migrate down the channel at different velocities due to the difference in their diffusion coefficients, yielding a size-based separation.Non-spherical particles have non-uniform diffusive (spreading) movement along the directions of the major and minor axis, while spherical particles have a uniform diffusive movement in all directions.In this study, a theory was developed on the elution behavior of non-spherical particles in AF4. In order to test the proposed theory, non-spherical gold nanoparticle (AuNR) of different aspect ratios were synthesized using the see-mediated growth method, which were coated with cetyl trimethyl ammonium bromide (CTAB) to prevent particle aggregation. The elution behavior of non-spherical particles in AF4 will be discussed based on the measured retention data of the AuNRs.

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C-terminal Modification with Putrescine for Relative Quantification by LC-MS

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Proteins are associated with many diseases such as cancer and diabetes. Recently protein quantitative analysis was diagnosed biomarker of many diseases by mass spectrometry. Protein quantification by mass spectrometry was generally used the isotope labeling. The use of typical isotope tags have developed in vivo or in vitro labeling techniques like the stable isotope labeling by amino acids in cell culture (SILAC), Isotope-coded affinity tag (ICAT) and H_2O^{18} protease technique.In this study, we have developed carboxyl modification of peptides as a method for quantitative analysis using normal putrescine (1,4-butanediamine) and heavy putrescine (1,4-butane-d8-diamine) by mass spectrometry. The carboxyl-reactive amidation reagent 1-[Bis(dimethylamino)methylene]-1H-1,2,3-triazolo[4,5-b]pyridinium 3-oxid hexafluorophosphate (HATU) is used to amidate the carboxylic acid group of the peptide angiotensin II and the tryptic digested albumin peptides to normal putrescine and heavy putrescine.As a result, amidation reaction using HATU with heavy putrescine as labeling shows 8 Da difference in comparison with original peptide which can overcome the isotope distribution overlapping. In addition, the carboxyl modified peptides increased the most abundant charge state compared to native peptides to enhanced fragmentation for electron-transfer dissociation (ETD).

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Quantitative Analysis of Perfluorinated Compounds (PFCs) in Stream of Changwon by LC-ESI-MS

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Recently, as a new environmental pollutant is increasing interest in perfluorinated compounds (PFCs). PFCs is a materials which is substituted by fluorine on the hydrogen position of the hydrocarbon chain. The high stability of the molecule because of strong covalent bonding between carbon and fluorine. Therefore, it does not react with other materials hydrolysis, photolysis, biodegradable, has a resistance to metabolic degradation. Because of these properties water-resistant, oil-resistant, surface treatment agent, surfactant was used in many industries for over 50 years. It is detected in almost all the environmental media. The purpose of this study is a quantitative analysis of PFCs in stream of Changwon using LC-ESI-MS. To obtain a calibration curve, the PFCs standards were used for quantitative analysis. The concentration distribution of the PFCs was mapped at the sixteen sampling site in stream of Changwon.

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Analysis of fluorescence-labelled starch using asymmetrical flow field-flow fractionation (AsFlFFF) with multiple detectors

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Starch is a mixture of amylose (AMY) and amylopectin (AMP). AMY molecules are essentially linear, while AMP molecules have branches with 5-6% alpha-(1,6) linkages. Usually AMY and AMP are different in physical properties such as molar mass, radius of gyration (R_g) and hydrodynamic radius (R_h). The rheological and functional properties of starch are influenced by various factors including the molecular size, molar mass distribution and the concentration ratio of AMY to AMP. It is also important to analyze proteinaceous material in starch for characterization of starch.In this study, asymmetrical flow field-flow fractionation (AsFlFFF) was employed for separation and quantitation of AMY and AMP. AsFlFFF was coupled with multiple detectors such as multi-angle light scattering (MALS) and refractive index (RI) detectors for determination of absolute molar mass, molar mass distribution, and molecular structure without the need for system calibration. And then, for analysis of proteinaceous matter in starch, starches were fluorescence-labelled, and then analyzed by AsFlFFF coupled with a fluorescence detector.

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Collection and characterization of airborne using an electrical charge-based particle collector and field-flow fractionation (FFF)

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Airborne is a particulate matter (usually having the particle size ranging 0.1~200 μm) that floats or flies in air. They are formed by either natural or artificial occurrence such as sand dust or the use of fossil fuels in power plants. They react with chemical substances, and produce compounds such as sulfate or nitrate. Frequently they contain heavy metals or toxic organic compounds. Depending on the particle size, they show different behaviors, and sometimes, affect the human health and the environment. It is thus necessary to be able to identify the cause of occurrence and to analyze the particle size and chemical composition of the airborne. For accurate analysis of airborne particles, efficient and representative sampling is required. In this study, a new airborne collector was implemented and tested. This new airborne collector employs an electrical force, and does not need a filter, allowing to avoid adsorption or modification of the particles by the filter. Also it does not require the sample concentration such as drying, washing, vortexing and centrifuging. Split flow thin cell fractionation (SF) is a continuous separation method, allowing a large-scale separation of particles into two populations of different size ranges. SF was employed to separate the collected airborne particles into two populations (one in nanometer and another in micrometer ranges). Field-flow fractionation (FFF) is a size-based separation technique that is useful for analysis of colloidal particles. Collected airborne particles were analyzed by FFF for determination of the particle size and its distribution. An inductively coupled plasma mass spectrometry (ICP-MS) was also employed for compositional analysis of the collected airborne particles.

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Preparation and characterization of lipid vesicles using dynamic light scattering and asymmetrical flow field-flow fractionation

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Vesicles are spherical shells composed of lipid bilayers that encapsulate an aqueous space. They have been used frequently as model membranes, and as nanoscale containers for drugs and other substance in the pharmaceutical and cosmetic industries. When vesicles are used for drug delivery, the stability (and the life-time) of the vesicles is directly related with their medicinal effect. Generally the stability of vesicles is related with the size and size distribution of the vesicle. Thus size characterization of vesicles is necessary for understanding of the vesicle stability. The dynamic light scattering (DLS), optical microscopy (OM), electron microscopy (EM), nuclear magnetic resonance (NMR) and nanoparticle tracking analysis (NTA) have been used for size analysis of particulate materials. Among them, DLS is simple to use, and has been widely used for measuring the particle size and its distribution. Sometimes, however, application of DLS is limited, especially when dealing with samples of complex mixtures or those of broad size distributions. Field-flow fractionation (FFF) is useful for separation and size characterization of particles having broad size distributions from a few nm up to about 100 μm. Asymmetrical flow field-flow fractionation (AsFlFFF), a member of FFF, is useful particularly for characterization of aqueous colloidal particles. In this study, nano-sized vesicles were prepared by extrusion, and then were analyzed by AsFlFFF for determination of the particle size distribution and for the stability test. Results from DLS and AsFlFFF were then compared.

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Optimization of fractionation efficiency (*FE*) and throughput (*TP*) in a large scale splitter less full-feed depletion SPLITT fractionation (FFD-SF)

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Split-flow thin cell fractionation (SPLITT fractionation, SF) is a particle separation technique that allows continuous (and thus a preparative scale) separation into two subpopulations based on the particle size and the density. In a conventional mode (conventional SF), there are two inlets and two outlets in the SF channel, which is equipped with a flow stream splitter at the inlet and the outlet of the channel, respectively. On the other hand, in the full-feed depletion mode (FFD-SF), there are only one inlet for the sample feed, and the channel is equipped with a flow stream splitter only at the outlet. In SF, there are two basic performance parameters. One is the throughput (*TP*), which was defined as the amount of sample that can be processed in a unit time period. Another is the fractionation efficiency (*FE*), which was defined as the number % of particles that have the size predicted by theory. In this study, a FFD-SF channel was developed for a large-scale fraction, which has no flow stream splitters ('splitter less FFD-SF'), and then was tested for optimum TP and FE by varying the sample concentration and the flow rates at the inlet and outlet of the channel. Polyurethane (PU) latex beads having two different size distribution (about 3 ~ 7 μm, and about 2 ~ 30 μm) were used for the test. The sample concentration was varied from 0.2 to 8 %wt/vol. The channel flow rates were varied from 70 to 160 mL/min. The fractionated particles are monitored by optical microscopy (OM). The sample recovery was determined by collecting the particles on a 0.1 μm membrane filter.

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Quantitative Analysis of Calcite in Desulfurization Gypsum Using Raman Spectroscopy

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한양대학교 화학과

According to the recent study some of gypsum board release Radon. Because a few gypsum board made by only phosphate gypsum. Phosphate gypsum has radioactive elements like U, Th. And Radon is formed as one intermediate step in the normal radioactive decay chains through which thorium and uranium slowly decay into lead. So many gypsum board manufacturer reduce amount of phosphate gypsum and increase amount of desulfurization gypsum. FGD Gypsum is a unique synthetic product derived from flue gas desulfurization (FGD) systems at electric power plantsTherefore increase demand of desulfurization gypsum analysis.In this study, It purpose that Existing analysis method of desulfurization gypsum replace new analysis method using Raman spectroscopy. Raman spectroscopy have many advantage like quick analysis, On-line analysis, nondestructive analysis. And it is possible that real time analysis.

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[발표취소] Chromo/fluorogenic detection of metal ion in sancho (zanthoxylum schinifolium) by the simple Schiff base sensor

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공주대학교 화학과 [1]극동대학교 한약발효학과

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Displacement phenomena in Serial Affinity Column Set (SACS)

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The work described here examines displacement phenomena that play a role in lectin affinity chromatography and their potential to impact reproducibility. This was achieved using Lycopersicon esculentum lectin (LEL), a lectin widely used in monitoring cancer. Four small LEL columns were coupled in series to form a single affinity chromatography system. The serial affinity column set (SACS) was then loaded with human plasma proteins. At the completion of loading, the column set was disassembled, the four columns eluted individually, the captured proteins trypsin digested, the peptides deglycosylated with PNGase F, and the parent proteins identified through mass spectral analyses. Significantly different sets of glycoproteins were selected by each column, some proteins appearing to be exclusively bound to the first column while others were bound further along in the series. Clearly sample displacement chromatography (SDC) occurs. Glycoproteins were bound at different places in the column train; identifying the presence of glycoforms of different affinity on a single glycoprotein.

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Highly sensitive SERS-based immunoassay as an early diagnostic tool in rheumatoid arthritis

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Rheumatoid arthritis is both common and chronic, with significant consequences for multiple organ systems. The key to therapeutic success lies in identifying individuals who will have severe destructive disease as early as possible, so that effective treatment can be initiated before irreversible damage occurs. Anti-cyclic citrullinated peptide (anti-CCP) antibody is well known biomarker as a particularly useful biomarker in the diagnosis of RA, with high specificity, presence early in the disease process, and ability to identify patients who are likely to have severe disease and irreversible damage.In this study, we assessed the clinical feasibility of conducting immunoassay based on surface-enhanced Raman scattering (SERS). An anti-CCP was used as a biomarker, magnetic beads conjugated with CCP were used as substrates, and the SERS nano-tags were comprised of anti-human IgG-conjugated hollow gold nanospheres (HGNs). We were able to determine the anti-CCP serum levels successfully by observing the distinctive Raman intensities corresponding to the SERS nano-tags. At high concentrations of anti-CCP (>25 U/mL), the results obtained from the SERS assay confirmed to those obtained via an ELISA-based assay. Nevertheless, quantitation via our SERS-based assay is significantly more accurate at low concentrations (

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Development of SERS imaging-based lateral flow immunosensor for rapid and sensitive detection of food toxin

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Lateral flow immunoassay (LFIA) is uncomplicated and intended assay method to detect the presence of an antigen in sample without the need for specialized or costly equipment. However, some of the problems associated with low sensitivity and limitations in quantitative analysis have made this technique less attractive. Here, we developed a surface-enhanced Raman scattering (SERS) imaging-based lateral flow immunosensor to overcome the limitation of conventional LFIA kit. In SERS imaging-based LFIA strip sensor, all the measurement principle is same with conventional LFIA strips except detection nanoprobes. The Raman-reporter labelled hollow gold nanosphere (HGN) was used as a SERS nanoprobe instead of gold nanospheres used in conventional LFIA strips. To verify the feasibility of the devised SERS imaging-based LFA strip platform, an immunoassay of staphylococcal enterotoxin B (SEB) was performed as a model reaction. The presence of SEB can be identified through the color change of the test zone. In addition, a highly precise quantitative evaluation of SEB is possible by averaging the SERS mapping signals. The sensitivity of proposed LFIA sensor was compared with contrast imaging analysis of test zone and conventional ELISA method. The LOD of the proposed LFIA sensor was estimated to be 1 pg/mL, and this low LOD value demonstrates that our SERS imaging-based LFIA immunosensor is approximately three orders of magnitude more sensitive than corresponding control methods. Accordingly, our SERS-based LFIA strip sensor shows significant potential for the rapid and sensitive detection of target markers in a simple manner.

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Wash-free immunoassay of prostate specific antigen using SERS-based microdroplet sensor

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We report a conceptually new immunoassay technique using SERS-based microdroplet sensor. Our proposed method offers a fast and sensitive assay applicable to PSA cancer marker in serum. The sensor used in this study is composed of four different compartments; the generation of microdroplets for fast PSA immunoreactions, the separation between immunocomplexes and supernant solution, the isolation of magnetic immunocomplex droplets, and the collection of SERS nano tag droplets for Raman detection. This technique allows a convenient immunoassay of PSA marker without any washing process since the magnetic immunocomplexes can be easily isolated by the droplet splitting into two smaller parts after the application of magnetic bar. Raman signals of the remaining SERS nano tags in the large droplet (supernatant solution) were measured for the quantitative evaluation of PSA marker. SERS signals for 240 droplets (8 Hz) were measured and averaged for the quantitative evaluation of PSA. The LOD, determined by our SERS-based microdroplet sensor, was estimated to be below 0.1 ng/mL for PSA cancer marker, and this value is much lower than the clinical cut-off value for the diagnosis of prostate cancer. In addition, rapid analysis with a tiny volume of sample is possible since all the process can be automatically carried out in the specially designed microdroplet channel. As a result, this SERS-based assay technique is expected to be a potential clinical tool for early diagnosis of prostate cancer.

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Highly sensitive detection of HIV-1 DNA using SERS-based lateral flow immunosensor

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We report a surface-enhanced Raman scattering (SERS)-based lateral flow assay method for the highly sensitive detection of target nucleic acids. Human immunodeficiency virus type 1 (HIV-1) DNA was used as a model analyte in this work. Here, Raman reporter (Malachite green isothiocyanate (MGITC)) and detection-DNA co-functionalized gold nanoparticles (AuNPs) were employed as SERS nano tags for targeting specific nucleic acids. In the presence of HIV-1 DNA, the sandwich type “detection DNA-conjugated SERS tag - target DNA - capture DNA” hybridization reactions occurred and the SERS tags induced strong Raman intensities on the test line. On the contrary, without HIV-1 DNA, the SERS tags could not be captured on the surface of test line, resulting in very low or no SERS intensities. With the increase of HIV-1 DNA concentration, the SERS intensities on the test line were gradually increased. The characteristic Raman scattering peak intensity of MGITC was measured for the quantitative detection of HIV-1 DNA. Under optimized conditions, the minimum detectable concentration for our SERS-based lateral flow assay was 0.5 pM, which was improved about 200-fold compared with the colorimetric detection approach or fluorescent method. This result demonstrate the potential feasibility of SERS-based lateral flow assay to detect a broad range of genetic marker for in-field or POC diagnostics.

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Ultrabright Luminescence from Au_{22} Nanocluster Protected with Rigidified Au(I)-Thiolate Shell

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연세대학교 화학과

Thiolate protected gold nanoclusters(AuNCs) have been one of the most studied materials for the past few years owing not only to their high thermodynamic and chemical stability, but also to their interesting size-specific physicochemical properties. However, the application in using their luminescent properties is still scarce because of their low quantum yield(Q.Y.; < 0.2%). In this presentation, we present the synthesis and characterization of stable, water soluble and highly luminescent AuNCs which are protected by glutathione(GS) ligands. Also a novel strategy to dramatically enhance the luminescence efficiency of gold clusters will be discussed. The key to synthesizing highly luminescent AuNCs, was to reduce the gold(III) salt slowly with sodium borohydride in the presence of ligands. To slow down the reducing reaction, the synthesis was carried out in a very dilute alkaline condition. Thus prepared cluster mixture was purified by poly-acrylamide gel electrophoresis, which isolated a distinctive red-emitting luminescent cluster with a Q.Y. of 7%. By characterizing with electrospray ionization mass spectrometry the isolated AuNCs was found to be $Au_{22}GS_{18}$. Further modification on $Au_{22}GS_{18}$ was made by ion-pairing bulky tetraoctylammonium cation to the carboxyl group at the end of the glutathione ligands, which showed a massive increase in the luminescence (Q.Y.~60%). With its ultrafine size (< 2nm), high quantum yield, low toxicity, it is expected to be a promising material in diverse fields. Furthermore, the enhancing strategy of the Au(I)-thiolate shell emission can be effectively used for detecting proteins and other biologically relevant materials that change the environment around the Au(I)-thiolate shell.

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Surface modification of medical devices using Vitamin B_6

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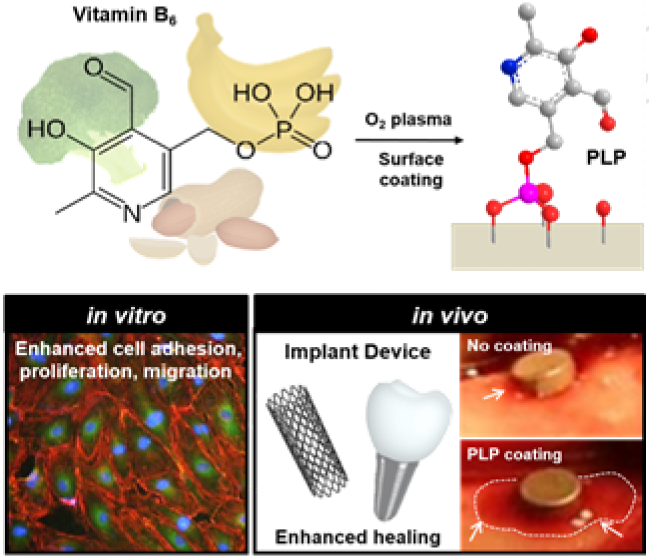
Vitamins are edible compounds registered in pharmacopoeia. In this study, we demonstrate that pyridoxal 5'-phosphate (PLP; vitamin B_6) is a multifunctional compound for surface functionalization. Vitamin B_6 can be anchored onto surfaces via the phosphate group, converting them into hydrophilic surfaces that allow for covalent tethering of molecules. We observed enhancement in endothelial cell and osteoblast proliferation, migration, and differentiation on PLP-coated surfaces as well as healing of PLP-coated dental implants in vivo.



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Platforms for Nitric Oxide Delivery

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The nitric oxide (NO) has been considered as an efficient and bio-inspired drug due to its versatile biological actions in vivo, such as apoptosis, angiogenesis, immune response, neurotransmission and cardiovascular homeostasis. Therefore, there have been continuous demands for the strategy capable of delivering NO efficiently for its practical and clinical applications. Accordingly, I rationally designed novel platforms for NO delivery including polycatecholamine-based NO-coating method and light-responsive smart NO delivery system. The polycatecholamine-based NO-coating method allows the modification of any material surfaces to store NO with appreciable storage capacity and release it in a controlled manner. The modified surfaces showed the ability to inhibit the bacterial adhesion and kill the adhered bacteria without cytotoxic effects on mammalian cells. In addition, we can develop a first strategy which can impart the light-responsiveness to an extremely unstable NO-releasing moiety under physiological conditions. This strategy was developed by exploiting a sequential reaction initiated by light. The light-induced pH-jump reagent induces the acids generation, which accelerate the degradation of the pH-sensitive CaP-coating layers on the nanoparticles. This uncapping process leads to expose a NO-releasing moiety on the surface of nanoparticles to physiological conditions, which eventually allows the NO release. These two-types of systems are expected to set the stage for the practical NO-mediated therapy.

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Development of a peptide/PDPP-based diagnostic agent and its application

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A development of a novel rapid diagnostic system attracts much attention in early diagnosis of disease. As a probes, nucleic acids such as DNA or its fragment and antibodies are used to detect a particular biomarker. Over the last couple of decades, various detection methods have been developed with a focus on convenience, rapidness, sensitivity, and reliability. These include microbiological culture, polymerase chain reaction (PCR), enzyme-linked immunosorbent assay (ELISA), and antibody-, enzyme-, and nucleic acid-based biosensors containing nanomaterials such as gold nanoparticles (GNPs), quantum dots (QDs), magnetic nanomaterials, and carbon nanotubes (CNTs); these methods employ various analytical techniques. However, several drawbacks remain such as time-consuming nature, complicated process, low sensitivity, high cost of synthesis, and limitation in diagnostic probe-storage. No techniques satisfied all the above-mentioned points for detection. Therefore, a novel ultra-sensitive and rapid strategy needs to be developed for easy detection of biomarker for a particular disease. Recently, peptides have been suggested for use as a diagnostic probes for biomarkers (chemicals, nucleic acids, metals, peptides, and proteins) instead of antibodies, enzymes, and nucleic acids. It has a great potential as novel detection probes due to their smaller size, low cost, high stability, low immunogenicity, and ease of chemical modification. Thus, peptides could be useful for adaptation in biosensor applications. Furthermore, to enhence the sensitivity, we developed a polyvalent directed peptide polymer (PDPP) and applied on detection of a various biomarker such as *Salmonella* of foodborne pathogen, beta-amyloid of Alzheimer's disease, and anthrax toxin (receptor) of Anthrax disease.

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Fabrication of Chemical Microarrays by Efficient Immobilization of Hydrazide-Linked small molecules on Epoxide-Coated Glass Surfaces

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Microarray technologies have received considerable attention owing to the fact that they serve as effective tools for high-throughput analysis of biomolecular interactions and the identification of bioactive substances that bind to biomolecules. Small molecules that regulate biological processes serve as valuable tools in studies of the functions of biomolecules, especially proteins, as well as in the development of drugs. An important component of efforts that target the discovery of bioactive molecules is high-throughput screening. Technologies that rely on the use of DNA, protein, and carbohydrate microarrays have been widely employed to accelerate the selection of lead compounds and as high-throughput analytical tools in genomic, transcriptomic, proteomic, and glycomic research. Microarray platforms enable the simultaneous assessment of a large number of samples that are available in limited quantities. Herein we describe a novel chemoselective immobilization process in which hydrazide containing compounds react with epoxides coated on glass slides. This technique has been applied to the efficient construction of chemical microarrays, which have been used to evaluate protein binding to glycans and RNA binding to peptides. In this process, hydrazide-linked small molecules that were prepared on solid supports were selectively immobilized on the epoxide-coated surface even in the presence of other nucleophilic groups, such as thiol and amine, under weak acid conditions. We believe that the chemoselective ligation reaction developed in this effort will find many applications in the preparation of bioconjugates, such as neoglycopeptides, peptide?nucleic acid conjugates, and tagged peptides.

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High Affinity Host-Guest FRET Pair for Single-Vesicle Content-Mixing Assay: Observation of Flickering Fusion Events

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Fluorescence-based single-vesicle fusion assays provide a powerful method for studying mechanisms underlying complex biological processes of SNARE (soluble N-ethylmaleimide-sensitive factor attachment protein receptor)-mediated vesicle fusion and neurotransmitter release. A crucial element of these assays is the ability of the fluorescent probe(s) to reliably detect key intermediate events of fusion pore opening and content release/mixing. Here, we report a new, reliable, and efficient single-vesicle content-mixing assay using a high affinity, fluorophore tagged host-guest pair, cucurbit[7]uril-Cy3 and adamantane-Cy5 as a fluorescence resonance energy transfer (FRET) pair. The power of these probes is demonstrated by the first successful observation of flickering dynamics of the fusion pore by in vitro assay using neuronal SNARE-reconstituted vesicles.

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Characterization of Invisible RNA State that Dynamically Couples Distant Motifs

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한국과학기술원(KAIST) 화학과 [1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA [2]Department of Biochemistry and Chemistry, Duke University School of Medicine, Durham, NC 27710, USA

There are a growing number of studies showing that regulatory ribonucleic acid (RNA) transiently forms short-lived (μs - ms lifetime) and low-populated (

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Understanding PI3K in Cancer at the Single-Molecule Level

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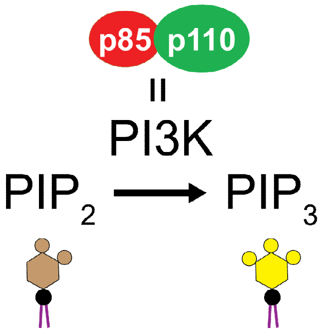
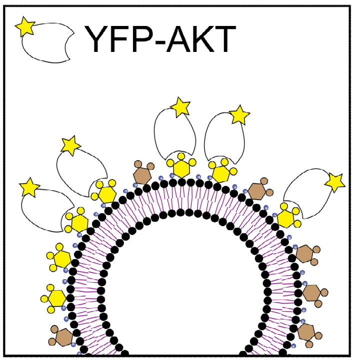
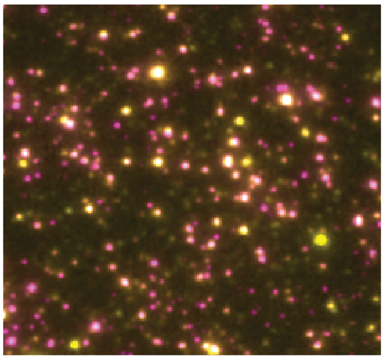
한국과학기술원(KAIST) 물리학과

PI3K-Akt signaling pathway controls cell growth, proliferation, and motility, and is frequently deregulated in many types of cancer. PI3K is a lipid kinase that converts PIP2 into PIP3 on membrane, which then recruits downstream signaling proteins such as Akt. Traditionally, the activity of PI3K has been probed indirectly by the phosphorylation of Akt. Here, we developed an assay that directly measures the activity of PI3K by single-molecule fluorescence. In this method, surface-tethered PI3K phosphorylates PIP2 on nearby vesicles, fluorescently-tagged Akt is introduced, and its binding to vesicles is imaged to quantify PI3K activity. After validating the method with fluorescent protein-tagged PI3K, we extend this assay to endogenous PI3K from breast cancer cells to understand the response of cancer cells to PI3K inhibitors. We hope this assay could be useful in screening for PI3K inhibitors or guide selection of cancer patients for PI3K-targeted therapy.







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DNA Binding Fluorescent Proteins for the Direct Visualization of Large DNA Molecules

이성현 조규봉*

서강대학교 화학과

Fluorescent proteins that also bind DNA molecules are useful reagents for a broad range of biological applications because they can be optically localized and tracked within cells, or provide versatile labels for in vitro experiments. We report a novel design for a fluorescent, DNA-binding protein (FP-DBP) that completely "paints" entire DNA molecules, whereby sequence-independent DNA binding is accomplished by linking a fluorescent protein to two small peptides (KWKWKKA) using lysine for binding to the DNA phosphates, and tryptophan for intercalating between DNA bases. Importantly, this ubiquitous binding motif enables fluorescent proteins (Kd =14.7 micro M) to confluently stain DNA molecules and such binding is reversible via pH shifts. These proteins offer useful robust advantages for single DNA molecule studies: lack of fluorophore mediated photocleavage and staining that does not perturb polymer contour lengths. Accordingly, we demonstrate confluent staining of naked DNA molecules presented within microfluidic devices, or localized within live bacterial cells.

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Discovery of Small Molecule Inhibitors of Lin28-*let-7* Interactions Through the Development of a FRET-based High-Throughput Screening

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서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

MicroRNAs (miRNAs) regulate gene expression by targeting most protein-coding transcripts. As a result, miRNAs are involved in every important cellular process in animal. Dysregulation of miRNA biogenesis is associated with many human diseases. *Let-7* miRNA family is well-known for its tumor suppression function, and it is down-regulated in many cancers. Lin28 protein is abnormally expressed in those cancer cells, and the protein binds primary and precursor *let-7* miRNAs to inhibit their maturation. In this study, a FRET-based high throughput screening system was constructed to identify inhibitors of the Lin28-*let-7* interaction with the aim of discovering novel anti-cancer agents. Unnatural amino acid mutagenesis and bioorthogonal chemistry enabled site-specific fluorescent labeling of Lin28, resulting in a highly robust and reliable Lin28-*let-7* binding assays. We identified several small molecule inhibitors of the protein-RNA interaction using the high-throupur assay. Detailed mode of action of the inhibitors will be introduced in the presentation.

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Dissecting the FK506 Biosynthetic Pathway and Generation of Novel Analogues by Pathway Engineering

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이화여자대학교 화학나노과학과

FK506, a 23-membered macrolide produced by several Streptomyces species, is an immunosuppressant widely used to prevent the rejection of transplanted organs. It also possesses various biological activities, including antifungal, anti-inflammatory, neuroprotective, and neuroregenerative activities. We have detailed the biosynthetic pathway of the unique allyl functional group of FK506 through complete sequencing, comparison to related biosynthetic gene clusters, and genetic and biochemical analyses. In addition, detailed studies elucidated the origin of the cyclohexyl ring and the two independent pathways of post-PKS modification needed to yield FK506. Based on the understanding of the biosynthetic pathways of FK506, several FK506 analogues containing altered side chains or non-natural starter units have been synthesized by mutasynthesis, where the gene producing a natural building block is disrupted allowing efficient incorporation of modified precursors, and these have shown various biological activities. Significantly, our procedure exemplifies a new combinatorial biosynthetic method to modify structurally complex molecules such as FK506 as an alternative method to chemical synthesis and to create improved therapeutic properties.

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Enantioselective Synthesis of ß-Aryl Amines via Direct Reductive Amination Catalyzed Chiral Phosphoric Acid

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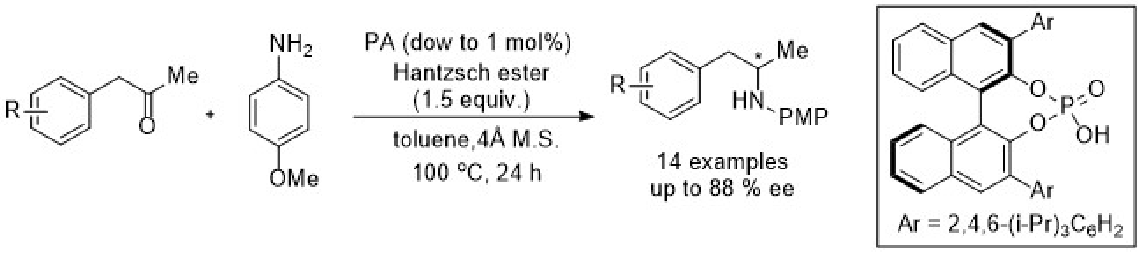
Over the past decade, chiral phosphoric acid catalysis has become one of the most rapidly growing fields in asymmetric catalysis. Among the various asymmetric reactions that involve a chiral phosphoric acid catalyst, asymmetric reduction of ketimines with organic hydride sources has become one of the most popular reactions in enantioselective phosphoric acid catalysis. Although a number of examples of the synthesis of chiral amines through chiral phosphoric acid-catalyzed asymmetric reduction of ketimines have been reported, most of the previous examples have been limited to the synthesis of chiral α-aryl amines via enantioselective reduction of ketimines derived from alkyl aryl ketones. Thus, we have developed a new method for the synthesis of chiral ß-aryl amines via chiral phosphoric acid-catalyzed asymmetric reductive amination of benzyl methyl ketones using Hantzsch ester as an organic hydride source. A variety of benzyl methyl ketone derivatives bearing various aryl groups were applicable to this protocol to afford the desired chiral ß-aryl amines in high yields and good enantioselectivity. Furthermore, the resulting chiral β-aryl amine was successfully transformed to tetrahydroisoquinoline, which is one of the key building blocks in a series of naphthylisoquinoline alkaloids. Moreover, we further attempted to apply this protocol to the synthesis of a naphthylisoquinoline moiety found in natural product.



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Synthesis of (*Z*)-α,β-Unsaturated Ketones and Arylalkyl Phosphonates using Acyl Alkenylindium and Phosphoryl Alkylindium Reagents *via* Pd-Catalyzed Cross-Coupling Reactions

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강원대학교 화학과

Cross-coupling reaction using a variety of organometallic reagents in the presence of a transition metal catalyst has been one of the most significant research subjects for the formation of C-C and C-heteroatom bonds. In particular, the Pd-catalyzed cross-coupling reaction has been widely used as a powerful tool in synthetic chemistry. To date, development of new catalysts, organometallic reagents, and electrophilic coupling partners has been continuously reported to expand the scope of cross-coupling reactions. Among them, because organoindium reagents showed advantageous properties related to their selectivity and reactivity, ease of handling and preparation, thermal stability, and low toxicity, cross-coupling reactions using organoindium reagents have also been of great interest. A synthetic method of acyl alkenylindium reagents was developed from the hydroindation reaction of allenyl ketones with indium and indium chloride in methanol under mild conditions. Their synthetic applications were demonstrated from Pd-catalyzed cross-coupling reactions with aryl bromides and iodides and alkenyl and aryl triflates for the synthesis of (Z)-α,β-unsaturated ketones. Phosphoryl alkylindium reagents are generated *in situ* from the direct insertion of indium with bromoalkyl phosphonates in the presence of CuCl, and their synthetic application to arylalkyl phosphonates is reported *via* Pd-catalyzed cross-coupling reaction with tolerance of a diversity of functional groups including ester, ketone, aldehyde, nitrile, nitro, trifluoromethyl, chloride, methoxy, hydroxy, and amino.

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Studies toward the total synthesis of pactamycin, multi-functionalized aminocyclitol natural product

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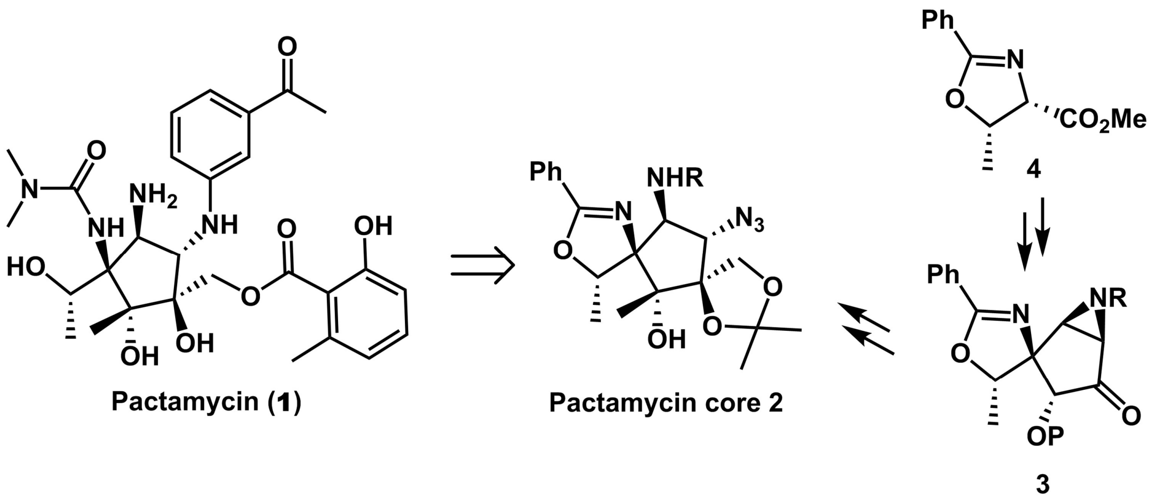
Pactamycin (1), an antitumor antibiotic produced by *Streptomyces pactum var pactum*, was isolated in 1962 and is one of the most potent cytotoxic agents *in vitro* against KB human epidermoid carcinoma cells and inhibits the synthesis of specific proteins. Pactamycin (1) has a unique multi-functionalized cyclopentane ring in which all carbons are substituted by heteroatoms. As a part of a project directed toward the total synthesis of pactamycin (1), we designed aziridine 3, potentially functionalized for further conversion into pactamycin core 2.The construction of the pactamycin carbon framework started with oxazoline 4, which was converted into azidirine 3 in 12 steps including ring-closing metathesis and stereoselective aziridine formation. Reproducible chemical methods enabling the synthesis of pactamycin core 2 containing an octa-substituted cyclopentane skeleton have been developed. Further studies toward the total synthesis of pactamycin from core 2 are now in progress and results will be disclosed.



Pactamycin (**1**)

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Rh-Catalyzed C-H Insertion Reaction of *N*-Sulfonyl-1,2,3-Triazoles with Aromatic Compounds

신서현 이필호*

강원대학교 화학과

N-Sulfonyl-1,2,3-triazoles are proven to be highly effective as precursors of α-imino rhodium carbenes. Because *in situ* generated α-imino rhodium carbenes are a kind of electrophiles, reactions of the carbenes with a wide range of nucleophiles have been examined, and a variety of heterocyclic compounds have been prepared. Besides Rh-catalyzed intermolecular arylation using α-imino rhodium carbenes is highly attractive because transition metal-catalyzed insertion reaction of carbenes to aromatic C-H bonds is one of the useful methods in organic synthesis. A synthetic route to a wide range of 2-alkoxyaryl-2-aryl enamines is developed from Rh-catalyzed alkoxyarylation of *N*-sulfonyl-4-aryl-1,2,3-triazoles with aryl ethers *via* the elimination of nitrogen molecule. In addition, 2-alkoxyaryl-2-aryl enamines are prepared *via* tandem Cu-catalyzed cycloaddition and Rh-catalyzed alkoxyarylation starting from alkynes, *N*-sulfonyl azides, and aryl ethers in one-pot. The development of Rh-catalyzed diastereoselective *N*-sulfonylaminoalkenylation of azulenes using *N*-sulfonyltriazoles is described. This procedure can be successfully applied to Rh-catalyzed diastereoselective *N*-sulfonylaminoalkenylation of azulenes starting from terminal alkynes and *N*-sulfonylazides *via* a three-component semi-one pot process.

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Synthesis of 1-Unsubstituted-*NH*-1,2,3-Triaozle by Copper Aerobic Oxidation from α-(1,2,3-Triazol-1-yl)acetophenones

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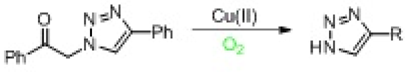
서강대학교 화학과

1-Unsubsitituted-*NH*-1,2,3-triaozle moiety is a crucial structure in the pharmaceuticals and agrochemicals. Increasing demands of 1-unsubsitituted-*NH*-NH-1,2,3-triaozle require new methods to prepare conveniently, cost-efficiently and environment-friendly even in bulk scale production. Molecular oxygen among various oxidants is considered an ideal oxidant. Therefore, copper catalyzed aerobic oxidative by C-N bond cleavage for the synthesis of 1-unsubsititued--*NH*-1,2,3-triazole provides many merits mentioned in the above. First, copper(I)-catalyzed [3+2] cycloaddtion reactions of 1-azido-acetophenono and various substituted acetylene groups gave α-(1,2,3-triazol-1-yl)acetophenones as starting materials conveniently. The title compounds could be prepared by oxidation of alpha-carbon of α-(1,2,3-Triazole-1-yl)acetophenones with molecular oxygen and copper(II) acetate catalytic amounts. This method could be useful for the preparation of target compounds with various functional groups and neutral condition in high yield.



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발표코드: **ORGN.O-6**
발표분야: Oral Presentation of Graduate Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 윤효재

Synthetic Access toward Highly Substituted Homoallylic α-Silylamines and Their Desilylative Formal [1,3]-Sigmatropic Rearrangement

정욱 박재욱* 이영호*

포항공과대학교(POSTECH) 화학과

A new synthetic strategy for highly substituted homoallylic α-silylamines possessing multiple stereocenters from silylmethyl azides was developed. A notable feature of this transformation was the formation of N-unsubstituted α-silylimine generated by ruthenium catalyst under photolytic condition. Excellent enantio- and diastereoselectivity were noted. Interestingly, the unprecedented desilylative allyl migration was discovered during purification of homoallylic α-silylamines. High level of chirality transfer from substrate to product was also observed. The synthetic utility of this rearrangement for divergent access toward homoallylic amines will be demonstrated. In addition, detailed mechanistic studies will be discussed.

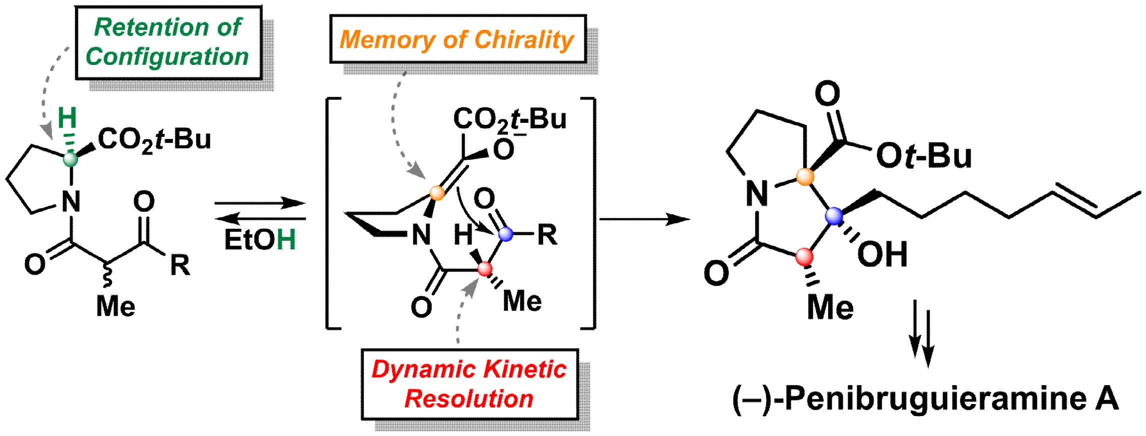
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ORGN.O-7**
발표분야: Oral Presentation of Graduate Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 윤효재

Asymmetric Total Synthesis of (—)-Penibruguieramine A Using Memory of Chirality and Dynamic Kinetic Resolution

김재현 김상희[1,*]

서울대학교 약학대학 [1]서울대학교 약학대학/약학과

(—)-Penibruguieramine A is a novel marine pyrrolizidine alkaloid, which is characterized by an unusual 1-hydroxy-2-methyl pyrrolizidin-3-one skeleton.[1] In the proposed biosynthetic pathway, the bicyclic ring system is generated by an intramolecular aldol-type reaction of proline pentaketide amide. Herein, we present the first and fully stereocontrolled total synthesis of (—)-penibruguieramine A.[2] The principles of 'memory of chirality (MOC)' and 'dynamic kinetic resolution (DKR)' were utilized to the the biomimetic aldol reaction. Our synthesis features an asymmetric construction of stereocenters with essentially complete diastereo- and enantioselectivity in the absence of external chiral sources. Noteworthy is the excellent level of memory of chirality in a protic solvent environment. A mechanistic rationalefor the excellent stereochemical outcome in a protic solvent environment is discussed . 1. Zhou, Z.-F.; Kurtan, T.; Yang, X.-H.; Mandi, A.; Geng, M.-Y.; Ye, B.-P.; Taglialatela-Scafati, O.; Guo, Y.-W. *Org. Lett.* 2014, *16*, 1390—1393. 2.Kim, J. H.; Lee S.; Kim, S. *Angew. Chem., Int. Ed.* 2015, *54*, 10875—10878.



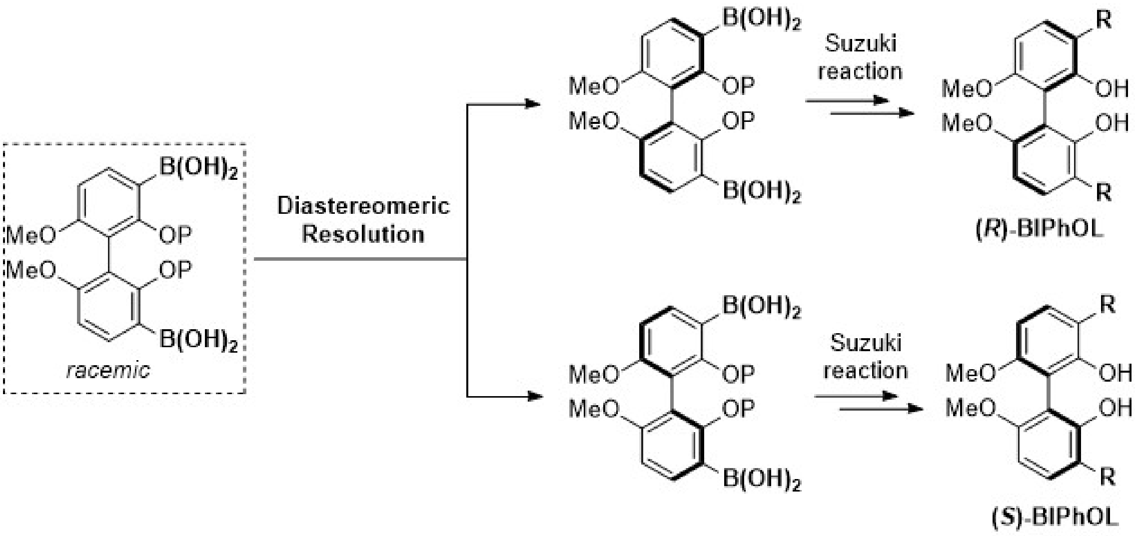
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ORGN.O-8**
발표분야: Oral Presentation of Graduate Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 10:45, 좌장: 윤효재

Asymmetric Synthesis of 3,3’-Disubstituted-6,6’-Dimethoxy-2,2’-Biphenol (BIPhOL) Derivatives via Diastereomeric Resolution Using a Boronic Acid Moiety

윤정민 천철홍*

고려대학교 화학과

Axially chiral diol compounds, such as BINOL and VAPOL, have been widely used as either chiral ligands or catalysts asymmetric synthesis. Since the reactivity and selectivity with these chiral diols in asymmetric synthesis show a strong dependence on substituents on the main framework, considerable effect has been made on the synthesis of chiral diol derivatives bearing different substituents on the periphery along the chiral axis. In addition, the dihedral angle along the chiral axis has been found to have a profound impact on the efficiency in asymmetric catalysis, in particular, in those with axially chiral diphosphine ligands. However, such an effect with axially chiral diol ligands has been far less investigated compared to axially chiral diphosphine ligands presumably due to the lack of general synthetic routes to access these axially chiral diol compounds with different substituents, except BINOL and octahydro-BINOL derivatives. In order to address this issue, we have developed an efficient method to access axially chiral diol derivatives via the diastereomeric resolution of rac-biaryl boronic acids using the boronic acid moiety as a resolving group and subsequent Suzuki-Miyaura coupling reaction of the resulting chiral-biaryl boronic acid.


B(OH)2
MeO
OP
MeO
OP
B(OH)2
racemic
Diastereomeric Resolution
Suzuki reaction
R
OH
OH
R
(R)-BIPhOL
Suzuki reaction
(S)-BIPhOL

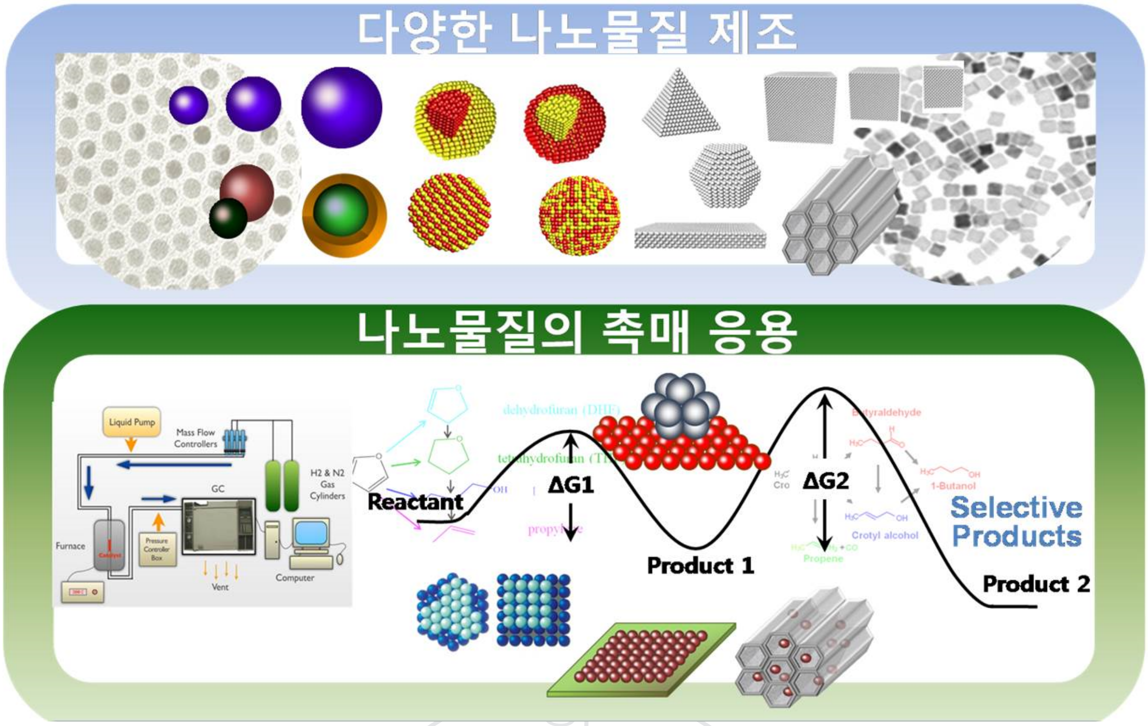
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT.O-1**
발표분야: Oral Presentation of Young Material Chemists
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김명길

Catalytic Reaction studies on Nanocatalysts

안광진

울산과학기술대학교(UNIST) 에너지 및 화학공학부

Colloidal synthesis has made great progress by controlling the size, shape, and composition of nanoparticles. An ultimate goal of industrial catalysis is to achieve the highest catalytic activity and selectivity toward only one desired product, while maintaining high stability against deactivation. Many catalytic reaction studies have been demonstrated enhancement of reaction rates and change of selectivities with the optimum nanoparticle size and shape. In addition, catalytic behaviors can also be altered at oxide-metal interfaces by creating the strong metal-support interaction. In this presentation, gas-phase heterogeneous catalytic reactions including benzene, toluene, and hexane hydrogenation and carbon monoxide oxidation, are introduced by demonstrating how the size, shape, and composition of nanoparticles and oxide-metal interfaces affect catalytic performance at the molecular level.


다양한 나노물질 제조
나노물질의 촉매 응용
Liquid Pump
Mass Flow Controllers
H2 & N2 Gas Cylinders
GC
Furnace
Pressure Controller Box
Vent
Computer
dehydrofuran (DHF)
tetrahydrofuran (THF)
propylene
Reactant
ΔG1
Product 1
ΔG2
Butyraldehyde
1-Butanol
Crotyl alcohol
Propene
Selective Products
Product 2

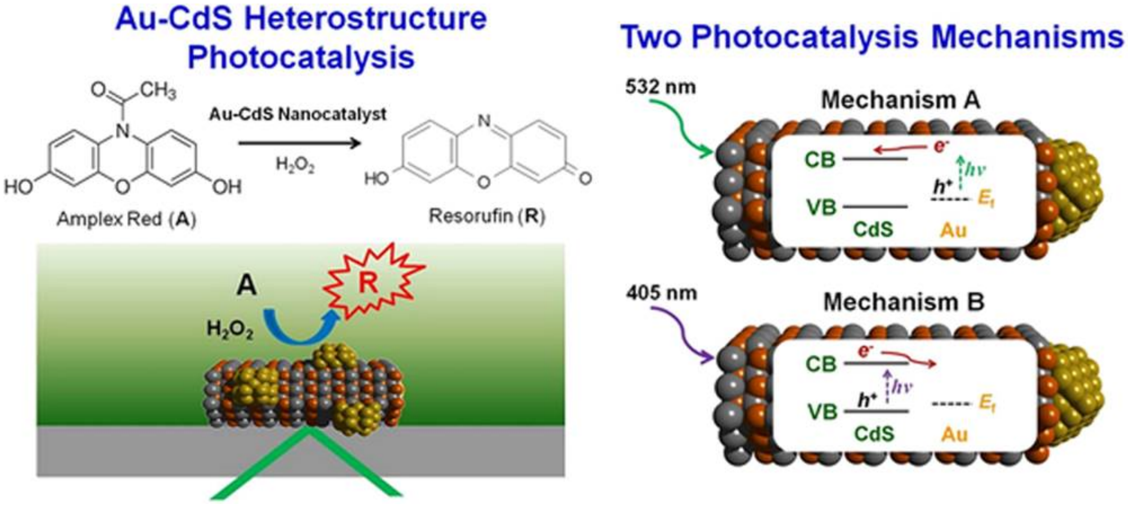
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT.O-2**
발표분야: Oral Presentation of Young Material Chemists
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 김명길

Single Molecule Nanoparticle Catalysis with Super-resolution Fluorescence Microscopy

하지원

울산대학교 화학과

Metal-semiconductor heterostructures are promising visible light photocatalysts for many chemical reactions. Here, we use high-resolution superlocalization imaging to reveal the nature and photocatalytic properties of the surface reactive sites on single Au?CdS hybrid nanocatalysts. We experimentally reveal two distinct, incident energy-dependent charge separation mechanisms that result in completely opposite photogenerated reactive sites (e- and h+) and divergent energy flows on the hybrid nanocatalysts. We find that plasmon-induced hot electrons in Au are injected into the conduction band of the CdS semiconductor nanorod. The specifically designed Au-tipped CdS heterostructures with a unique geometry (two Au nanoparticles at both ends of each CdS nanorod) provide more convincing high-resolution single-turnover mapping results and clearly prove the two charge separation mechanisms. Engineering the direction of energy flow at the nanoscale can provide an efficient way to overcome important challenges in photocatalysis, such as controlling catalytic activity and selectivity. These results bear enormous potentialimpact on the development of better visible light photocatalysts for solar-to-chemical energy conversion.


Au-CdS Heterostructure Photocatalysis
Au-CdS Nanocatalyst
H2O2
Amplex Red (A)
Resorufin (R)
A
H2O2
R
Two Photocatalysis Mechanisms
532 nm
Mechanism A
CB
VB
e-
h+
hν
Ef
CdS
Au
405 nm
Mechanism B
CB
VB
e-
h+
hν
Ef
CdS
Au

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **MAT.O-3**

발표분야: Oral Presentation of Young Material Chemists

발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 김명길

Plasmonic Nanosystems for Molecular Detection based on Localized Surface Plasmon Resonance

이승현

수원대학교 신소재공학과

Nobel metal nanoparticles have attracted a great deal of recent interest due to their unique optical properties as a result of localized surface plasmon resonances (LSPR) which produces a strong optical extinction which can be tuned throughout the visible and near-infrared wavelengths for biomedical applications. In addition, large field enhancements occur at the nanoparticle surface for applications in surface enhanced spectroscopies and enhanced photocurrent generation. The LSPR extinction peak is also very sensitive to the particles' size, shape, dispersion state and dielectric environment. we have fabricated substrates coated with these particles, and used their dielectric sensitivity to create an optical refractive index sensor based on a spectral extinction measurement and show that gold nanorods and bipyramids can be used as a label-free immunoassay for biological sensing. Since the detection mechanism is based solely on refractive index, the sensor could be used for other fields as well. Also, hybrid nanosystem with plasmonic nanoparticles and carbon nanomaterials have been employed to SERS-active substrates for environmental and nanomedicine applications. The carbon-plasmonic hybrid nanostructures demonstrate a unique technique for molecular detection and it may support to expand SERS-active substrate technology more broadly.

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **MAT.O-4**

발표분야: Oral Presentation of Young Material Chemists

발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 김명길

DNA-mediated synthesis of nanogap controlled plasmonic nanostructures

임동권

고려대학교 KU-KIST 융합대학원

The nanogap-controlled plasmonic nanostructures are useful to obtain greatly enhanced electromagnetic field in the nanogap, which is one of Raman singal enhancement mechanism. Especially the use of DNA provide a new tool to control the plasmonic nanostructures in various ways. In this talk, I will discuss the new synthetic methods for the nanogap-controlled plasmonic nanostructures, the contribution of nanogap structures in obtaining strong Raman response and the applications for high resolution live cell Raman imaging.References1. D.-K. Lim, K.-S. Jeon, J.-H. Hwang, H. Kim, S. Kwon, Y. D. Suh* and J.-M. Nam,* Highly uniform and reproducible surface-enhanced Raman scattering from DNA-tailorable nanoparticles with hollow 1-nm interior gap. Nature Nanotechnology, 6, 452-460, (2011).2. J. W. Kang, Peter T.C. So, D. Ramachandra, D.-K. Lim*, High Resolution Live Cell Raman Imaging Using Subcellular Organelle-Targeting SERS-Sensitive AuNPs with Highly Narrow Intra-Nanogap, DOI: 10.1021/nl504444w, Nano Letters (2015). 3. H. Lee, S. H. Nam, Y. J. Jung, S. Park, J.-M. Kim, Y. D. Suh* and D.-K. Lim*, DNA-mediated control of Au shell nanostructure and controlled intra-nanogap for a highly sensitive and broad plasmonic response range, DOI: 10.1039/C5TC01915J (Paper) J. Mater. Chem. C, (2015).

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **MAT.O-5**
발표분야: Oral Presentation of Young Material Chemists
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 김명길

Intriguing Charge Harvesting Features of Plasmonic Photocatalysts

Youngsoo Kim **Prashant K. Jain***

Department of Chemistry, University of Illinois at Urbana-Champaign, USA

Plasmonic noble metal nanoparticles have recently received increased attention as visible-light photocatalysts. Heterostructured plasmonic photocatalysts are composed of semiconductor and noble metal nanoparticles, such as, Au/ZnO, Au/TiO2, and have been shown to drive important chemical reactions like water splitting via absorption of visible light. However, the mechanisms for photoexcited carrier harvesting have not been clearly elucidated as these mechanisms compete with rapid energy relaxation within the metal. In our work, we accomplished a simple one-electron photochemical reaction using plasmonically excited Au nanoparticles in the absence of any semiconductor. We observed intriguing features in the reaction rate as a function of photon flux in our model system, which led us to new mechanistic insight into plasmon excitation-driven photocatalytic reactions. The results of the experiment show the photocatalytic activity of Au nanoparticles arises from electron/hole pairs generated by interband transitions, akin to that in a conventional semiconductor photocatalyst and rapid charge separation is crucial for achieving high activity. A non-linear flux regime was also found where multiple electron/hole pairs can be harvested from the metal nanoparticle which may be utilized for conducting multi-electron reactions, like the reduction of CO2 to methanol and the oxidation of water.

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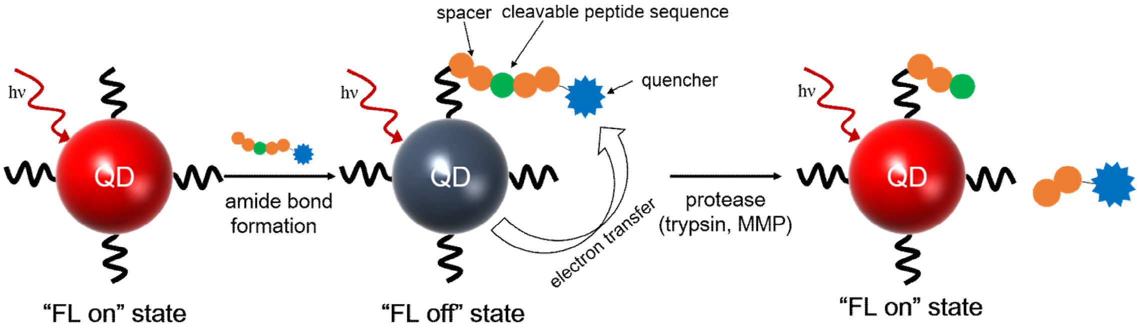
발표코드: **MAT.O-6**
발표분야: Oral Presentation of Young Material Chemists
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 김명길

Activatable NIR-II Fluorescent Quantum Dots for Cancer-microenvironment Probe

정상화 김성지*

포항공과대학교(POSTECH) 화학과

High-resolution fluorescence imaging of molecules intrinsically involved in cancer progression and metastasis would be valuable for early detection and staging of tumors. Combining the advantageous features of the second infrared (NIR-II, 1000-1400 nm) window than NIR-I window for minimal light interference from biological tissues and the design of fluorescence activation for sensitive detection of biological event, NIR-II activatable probe sensitive for cancer microenvironment, matrix metalloproteinase (MMP) was developed. At first, lead sulfide-based multishell QD structure, PbS/CdS/ZnS core/shell/shell QDs, was synthesized for highly luminescent NIR-II emitting probe for biological application The fluorescence modulation of PbS/CdS/ZnS QDs was enabled by photo-induced electron transfer from QD to methylene blue (MB) in the close proximity. For activatable probe, protease-cleavable peptide sequence, specific to MMP as cancer-related enzyme family, linked PbS/CdS/ZnS QD with fluorescence quencher of MB via covalent crosslinking. The structure of peptide sequence was modified and optimized for efficient activatable probe in the points of charged state and enzyme accessibility. Finally, ex vivo fluoresence imaging with spraying NIR-II activatable probe onto colon cancer model verified the time-dependent tumor-specific signal amplification of activatable probe.


spacer
cleavable peptide sequence
quencher
hv
QD
amide bond formation
electron transfer
protease (trypsin, MMP)
“FL on” state
“FL off” state
“FL on” state

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC.O-5**
발표분야: Oral Presentation for Young Electrochemists
발표종류: 분과기념강연, 발표일시: 목 10:00, 좌장: 김병권

Electrochemical biosensors towards point-of-care testing

양해식

부산대학교 화학과

Point-of-care testing (POCT) of biomarkers in clinical samples is of great importance for rapid and cost-effective diagnosis. Though a number of electrochemical approaches utilizing lateral-flow strips, lab-on-a-chips, and paper-based devices have been developed to this end, many of them have limitations in terms of simplicity, rapidness, cost-effectiveness and ultrasensitivity. It is extremely challenging to develop an ultrasensitive technique retaining simplicity. In this presentation, our efforts to develop simple and ultrasensitive biosensors will be introduced.

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장소: 대구 EXCO

발표코드: **ELEC.O-1**

발표분야: Oral Presentation for Young Electrochemists

발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김병권

High performance of PbSe/PbS core/shell quantum dot heterojunction solar cells: Short circuit current enhancement without loss of open circuit voltage by shell thickness control

최혜경 정소희[1,*]

과학기술연합대학원대학교(UST) 나노메카트로닉스학과 [1]한국기계연구원 나노기계연구본부

A noticeable photoconversion efficiency of colloidal quantum dot solar cell has been achieved recently, more than 9%. Still, low open circuit voltage limits further enhancement which is attributed mainly to the deep traps associated with defects from incomplete surface passivation. Here, we fabricate PbSe/PbS core/shell quantum dot-based heterojunction solar cell with precise shell thickness control. When PbS shell thickness increases, the short circuit current density increases from 6.4 to 11.8 mA/cm2 and the fill factor enhances from 30 to 49%. Contrary to expectations, the open circuit voltage remains unchanged at 0.46 V. We reveal that the core material influences on the energy levels involved in the junction in the core/shell materials confirmed by ultraviolet photoelectron spectroscopy (UPS) and UV-Vis-NIR absorption spectroscopy thereby mitigating the trade-off relationship between open circuit voltage and short circuit current density. Finally, under optimized condition, the PbSe core with 0.9-nm-thick shell yielded the power conversion efficiency of 6.5% under AM 1.5.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **ELEC.O-2**
발표분야: Oral Presentation for Young Electrochemists
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 김병권

Engineering the Electrochemical Redox Potential of Electrolytes for High-Voltage Dye-Sensitized Solar Cells

NaraYan ChanDra Deb 이재준[1,*]

건국대학교 나노기술연구센터 [1]건국대학교 응용화학과

We prepared novel electrolytes with interhalogen or pseudohalogen based multiple-redox couples for high voltage dye-sensitized solar cells (DSSCs). It is found that the interhalogen or pseudohalogen based redox systems, (I-, Br-)/I2Br- or (I-, SCN-)/I2(SCN)-, can be formed additionally in the iodine-based (I-/I3-) electrolyte by both chemically and electrochemically. The electrochemical redox potentials for these couples are more positive than that of conventional I-/I3- system, while the redox reaction involved with these ions are essentially comparable to that of I-/I3- in the conventional DSSC. The formation of these redox couples produces extra redox states at more positive potential than I-/I3- couple, which induces a shift of redox potential of the electrolyte positively in solution phase by the weight-equilibration of those redox couples. The positive shift of redox potential of the electrolyte contributes to increase the open circuit voltage (Voc) of DSSCs. The enhancement of Voc were significant regardless of sensitizing dyes, which corresponded to higher overall power conversion efficiency (?) compared to that with conventional iodine based redox couple. The degree of potential shift, so the corresponding Voc, can be controlled by adjusting the ratio of the concentrations of these redox species in the solution phase. This study is offering a very promising strategy to develop novel electrolytes of which the energy level can be controlled by introducing an additional redox species with more positive potentials without compromising the rate of regeneration of dyes.

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발표분야: Oral Presentation for Young Electrochemists
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 김병권

M@Au$_{24}$ (M=Pd, Pt) Become Au$_{25}$-like Superatom Complexes upon Electronic Charging

곽규주 김민석 이동일*

연세대학교 화학과

For the past few years, owing to unusual electronic structure with high chemical and thermodynamic stability, thiolate ligand-protected gold nanoclusters have been one of the most extensively studied nanomaterials. In particular, the exceptional stability of thiolate-protected Au$_{25}$ clusters, $[Au_{25}(SR)_{18}]^-$, arises from the closure of superatomic electron shells, leading to a noble-gas-like 8-electron configuration ($1S^2 1P^6$). Whereas the electronic properties of Au$_{25}$ clusters are rather insensitive to the change in the ligand shell, they are likely to response more sensitively to the change in core composition. In this presentation, we revealed that replacing the core Au atom with Pd or Pt results in stable $[MAu_{24}(SR)_{18}]^0$ clusters (M = Pd, Pt) having a superatomic 6-electron configuration ($1S^2 1P^4$). These clusters exhibit drastically different optical and electrochemical properties from those of the 8-electron $[Au_{25}(SR)_{18}]^-$ cluster. Voltammetric studies of $[PdAu_{24}(SR)_{18}]^0$ and $[PtAu_{24}(SR)_{18}]^0$ reveal that the HOMO-LUMO gaps of these clusters are drastically decreased to 0.32 and 0.29 eV, respectively, indicating their electronic structures are drastically altered upon doping of the foreign metal. These results were strongly supported by the density functional investigations which revealed that the MAu$_{12}$ core of the 6-electron $[MAu_{24}(SR)_{18}]^0$ clusters is slightly flattened to yield an oblate ellipsoid, accompanying the 1P orbital splitting. These clusters become 8-electron $[MAu_{24}(SR)_{18}]^{2-}$ clusters upon electronic charging, demonstrating reversible interconversion between the 6-electron and 8-electron configurations of MAu$_{24}$(SR)$_{18}$. The unique electrochemical properties observed from the stable 6-electron clusters suggest that doping of a cluster is a powerful means to fine-tune the redox properties of the cluster, which has practical implications in a variety of electrocatalytic applications.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC.O-4**
발표분야: Oral Presentation for Young Electrochemists
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 김병권

Effects of Surface Characteristics on the Charge Storage of Nitrogen-Doped Carbon Nanocoil Array

최원호 방진호[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Carbon has a unique role as an important electrode component in various energy conversion and storage applications. However, Integrating carbon nanostructures on a conductive substrate remains quite challenging, partly because it relies primarily on a high-vacuum technology such as chemical vapor deposition (CVD). To overcome the problems associated with current vacuum techniques, we demonstrate the formation of an N-doped carbon array by pyrolysis of a polymer array that was electrochemically grown on carbon fiber paper. The twisted coil-shape carbon array was investigated for use as a supercapacitor electrode. In-depth surface characterization results revealed that the microtextural properties, surface functionalities, and degree of nitrogen incorporated into the N-doped carbon array can be delicately controlled by manipulating carbonization temperatures. Furthermore, electrochemical measurements showed that subtle changes in these physical properties resulted in significant changes in the capacitive behavior of the N-doped carbon array. Pore structures and nitrogen/oxygen functional groups, which are favorable for charge storage, were formed at low carbonization temperatures. This result showed the importance of having a comprehensive understanding of how the surface characteristics of carbon affect its capacitive performance. When utilized as a substrate in a pseudocapacitive electrode material, the N-doped carbon array maximizes capacitive performance by simultaneously achieving high gravimetric and areal capacitances due to its large surface area and high electrical conductivity.

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발표코드: **KCS.O-1**
발표분야: Oral Presentation for Young International Chemists
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: David J. Churchill

Interfacial Chemistry Control for Improved Cycling Performance of High-Energy Lithium-Ion Batteries

NGUYEN DAN THIEN 송승완[1,*]

충남대학교 대학원 바이오응용화학과 [1]충남대학교 응용화학공학과

High-energy Li-ion batteries (LIB) are well-suited for electric vehicles and energy storage systems. High-energy batteries include high-capacity cathode and anode active materials and possess high cell voltage. The capacity of cathode material can increase when charging the cell to high-voltage above 4.3V vs. Li/Li^+. Conventional electrolyte consisting of $LiPF_6$ salt in ethylene carbonate based solvents however shows a limited performance on high-voltage operation due to its anodic instability. Development of new electrolyte components, which have an improved anodic stability and can form stable surface films at both cathode and anode, is needed to enable high-energy LIB. In this presentation, improved cycling performance of a high-energy LIB including silicon-carbon composite anode and layered $Li(Ni,Co,Mn)O_2$ cathode materials using various electrolyte compositions are demonstrated, and the role and importance of interfacial chemistry control are discussed.Acknowledgments This research was supported by the Korean Ministry of Trade, Industry & Energy (A0022-00725 & 10049609) and by Ministry of Education and National Research Foundation (2012026203).

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Layer-by-Layer Self-Assembled Graphene Multilayers as Pt-free Alternative Counter Electrodes in Dye-sensitized Solar Cells

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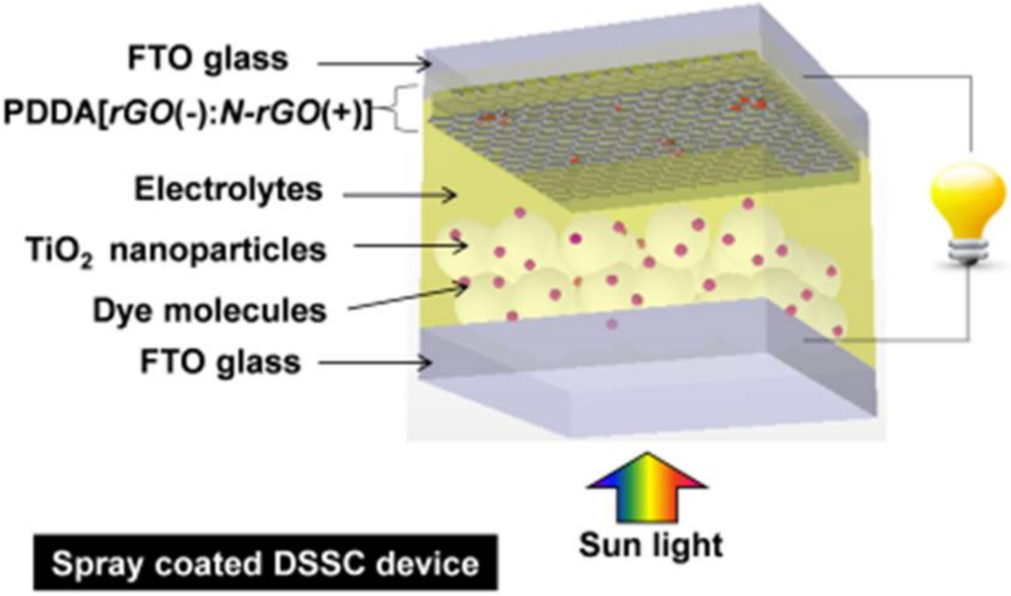
이화여자대학교 화학나노과학과

Dye Sensitized Solar Cells (DSCs) has attracted tremendous attention as a promising renewable energy technology. The major interest in DSCs is to develop platinum (Pt)-free counter electrode with feasible and eco-friendly materials for practical applications. In this regard, a low cost, charged, and large scale nitrogen-doped reduced graphene oxide [N-rGO(+)], nitrogen and sulfur dual-doped reduced graphene oxide [NS-rGO(+)], and un-doped reduced graphene oxide [rGO(-)] were applied as neat reduced graphene oxide based counter electrodes to substitute conventional Pt for DSCs. The neat rGO-based counter electrodes were developed via two types of layer-by-layer (LBL) self-assembly (SA) methods: spin coating and spray coating methods. In spin coating method, two sets of multilayer counter electrodes were fabricated on poly(diallyldimethylammonium chloride) (PDDA) coated fluorine-doped tin oxide (FTO) substrates using [GO(-)] combined with [N-GO(+)] ([rGO(-)/N-rGO(+)]n) or with [NS-GO(+)] ([rGO(-)/NS-rGO(+)]n). The DSSCs employing new types of counter electrodes exhibited ~7.0 and ~6.2% power conversion efficiency (PCE) based on ten bilayers of [rGO(-)/N-rGO(+)]10 and [rGO(-)/NS-rGO(+)]10, respectively. The DSSCs equipped with blend of one bilayer of PDDA[rGO(-):N-rGO(+)] and [rGO(-):NS-rGO(+)] prepared from spray coating showed ~ 6.4 and ~ 5.6% PCE, respectively, with ~ 56% fill factor value. This work indicates that combination of un-doped, nitrogen-doped and/or nitrogen sulfur dual-doped reduced graphene oxides can be used as a new class of electro catalysts as alternative electrodes in conventional photovoltaic devices. The Thickness of the graphene oxide multilayers were estimated by surface plasmon resonance spectroscopy (SPR). The surface coverage and morphology were analyzed by AFM and SEM spectroscopy. The doping status of reduced graphene oxide was confirmed by XPS Spectroscopy.


FTO glass
PDDA[*rGO*(-):*N-rGO*(+)]
Electrolytes
TiO_2 nanoparticles
Dye molecules
FTO glass
Sun light
Spray coated DSSC device

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Phenyl Selenium-Based Small Molecular Probes for Detection of Biological Analytes: ROS and Biothiols

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한국과학기술원(KAIST) 화학과

Organoselenium molecular probes show great promise in the detection of biological analytes such as ROS and biothiols in living biological systems. Among ROS, HOCl is a potential antimicrobial agent that plays a significant role in the human immune-defense system.[1] However, abnormal HOCl levels in living organisms can lead to diseases such as atherosclerosis, rheumatoid arthritis, lung injury, cancer, neurodegenerative disorders, and kidney and cardiovascular disease. Biothiols, such as cysteine (Cys), homocysteine (Hcy) and glutathione (GSH), play crucial roles in biological systems. GSH plays a central role in protecting the cell from oxidative damage and in maintaining biological homeostasis which plays a significant role in cell growth and function.[2] These biological species are thought to play important roles for normal physiological processes; an overproduction or deficiency of them can be indicative of cancer, neurodegenerative disease disorders such as Alzheimer’s and Parkinson’s disease, cystic fibrosis, AIDS, osteoporosis, cardiovascular disease and sickle cell anemia.[3] Hence, selective determination of these species is required for a better understanding of their role in biological systems and in early diagnosis of disease. The details of synthesis, screening, biological studies and general application of phenyl selenium-based small molecular probes will be discussed in this presentation.[4]References: 1.Hampton, M. B.; Kettle, A. J.; Winterbourn, C. C. Blood 1998, 92, 3007.2.Hyman, L. M.; Franz, K. J, Coord. Chem. Rev. 2012, 256, 2333.3.Townsend, D. M.; Tew, K. D.; Tapiero, H. Biomed. Pharmacother. 2003, 57, 145.4.Kim, Y.;‡ Mulay, S. V.;‡ Choi, M.; Yu, S. B.; Jon, S.; Churchill, D. G. Chem. Sci. 2015, (DOI: 10.1039/C5SC02090E).

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Copper-Catalyzed Direct Synthesis of 1,2,4-Oxadiazoles from Amides and Organic Nitriles

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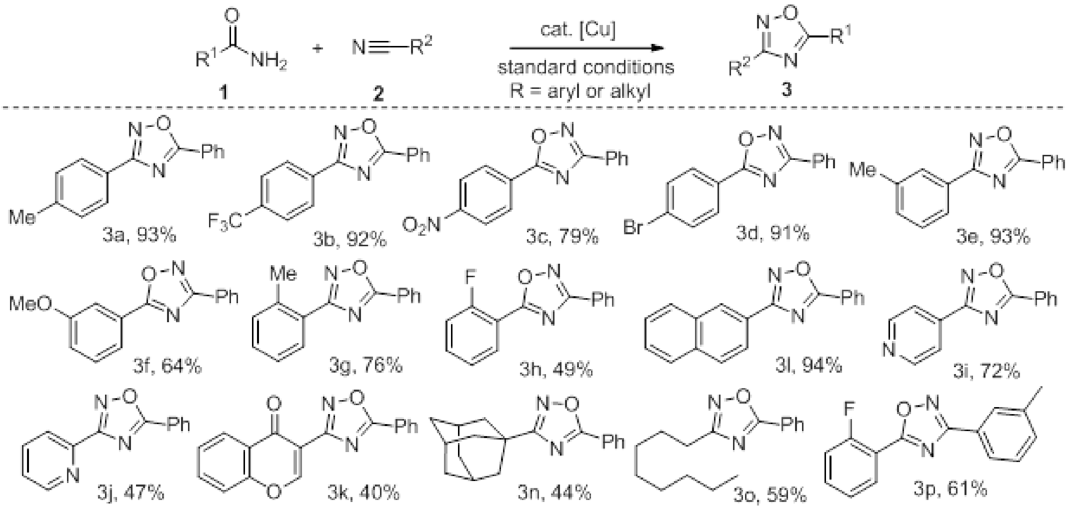
The five membered 1,2,4-Oxadiazoles are interesting heterocycles present in a variety of biologically active compounds and organic materials. The importance of these heterocycles and their derivatives exemplifies in medicinal chemistry as antidiabetic, antiinflammatory, antimicrobial, antitumor angents, immunosuppressors, neuroprotective agents as well as in material chemistry as components of polymers, liquid crystals, luminiscent, optoelectronic materials and corrosion inhibitors. Therefore, a range of methods have been explored for the synthesis of these heterocycles. Traditional methods for their synthesis typically involve the first O-acylation step of amidoximes or their precursors by activated carboxylic acid derivatives followed by intramolecular dehydration. Recently, 1,2,4-oxadiazoles were obtained from aldoxime and organic nitriles by employing ZnCl2 in the presence of stong acid PTSA. A relatively mild approch was developed by copper-catalyzed cascade annulation of amidines and methylarenes. However, most of the developed methods suffer from harsh reaction conditions such as high reaction temperature or the use of relatively unavailable starting materials. Hence, the development of efficient and simple synthetic procedure for the acquisition of 1,2,4-oxadiazoles from easily available starting materials is highly desirable. Herein, we have developed the optimized conditions for the synthesis of 1,2,4-oxadiazole from easily available amides and organic nitriles using copper catalysis.With the optimal reaction conditions, we have explored the scope and generality of this tranformation. Vaious substituted amides as well as organic nitriles were subjected under optimized reaction conditions and obtained good yields of the desired products.


R1 NH2 O
1
+
N≡—R2
2
cat. [Cu]
standard conditions
R = aryl or alkyl
N-O R1 R2 N
3
3a, 93%
3b, 92%
3c, 79%
3d, 91%
3e, 93%
3f, 64%
3g, 76%
3h, 49%
3l, 94%
3i, 72%
3j, 47%
3k, 40%
3n, 44%
3o, 59%
3p, 61%

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Discrimination of α/β-Amino Saccharide Anomers by Cucurbit[7]uril

<u>KHEDKAR JAYSHREE KESHAV</u> 장윤정[1] 김용휘[2] 이영민[1,*] 김기문[1,*]

기초과학연구원 복잡계 자기조립 연구단 [1]포항공과대학교(POSTECH) 화학과 [2]기초과학연구원 복잡계자기조립연구단

Amino saccharides (galactosamine (GalN), glucosamine (GluN) and mannosamine (MaN)) have recently been shown to bind cucurbit[7]uril (CB[7]) with excellent affinity in water and higher preference for α-anomers [Jang et al., Angew. Chem. Int. Ed., 2014, 53, 1003-1007]. Here, we present detail studies on this anomer selectivity through X-ray crystallography and computational methods. The crystal structures of GalN@CB[7] and GluN@CB[7] showed the complete encapsulation of α-GalN and α-GluN within the CB[7] cavity, respectively. The calculated structures in the gas phase using density functional theory (DFT) calculations and molecular dynamic (MD) simulations correlated well with the crystal structures. However, these gas phase calculations preferred β-anomers over α-anomers, in contrast to the experimental result in aqueous solution. Hence, we performed MD simulations with explicit water molecules on the complexes to calculate the binding free energies and consequently demonstrate the consistent preferences for α-anomers over their β-counterparts as already reported in the solution phase. Further, the similarity and dissimilarity between the crystal/gas phase features and the solution phase features are also explained. The relative solvation/desolvation free energies of amino saccharides indeed identify the effect of aqueous environment on α/β discrimination and the subsequent stabilization of α-forms. Our study suggest that the solvent contributions in non-covalent binding should be carefully considered while designing new supramolecular architects.

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Structural modifications of Nexavar central ring: Towards improved cellular anticancer potency and selective kinase profile

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과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 뇌의약연구단 [2]한국과학기술연구원(KIST) 케모인포메틱스연구센터

New 2-quinolinyl and benzothiazole-2-yl amide and urea derivatives possessing the privileged pyridylamide moiety have been designed and synthesized as anticancer sorafenib congeners. Among the synthesized derivatives, 27 compounds were selected for evaluation of their antiproliferative activity over a panel of 60 cancer cell lines at a single dose concentration of 10 uM at National Cancer Institute (NCI, USA). Eight compounds, 9b?d, 9f, 13b, 14a, 14b, and 14d showed impressive growth inhibitory results and thus were further tested at 5-dose testing mode to determine their GI50 values. The data revealed that the ureidoquinolines 9b, 9d and ureidobenzothiazole 14b are the most active derivatives with significant efficacies and superior potencies surpassing sorafenib in the majority of the tested cancer cell lines, with submicromolar or one-digit GI50 values. Kinase screening of both 9d and 13b over a panel of oncogenic kinases at single dose of 10 uM revealed their selective inhibitory activities towards both BRAFV600E and C-RAF kinases, with IC50 values in nanomolar scale.

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A Novel Ultrathin Two-Dimensional Polymer Film for Non-Volatile Memory Application

<u>RoyIndranil</u> 백강균[1] 김기문[2,*]

포항공과대학교(POSTECH) Chemistry [1]기초과학연구원 복잡계자기조립연구단 [2]포항공과대학교(POSTECH) 화학과

Ultrathin two-dimensional (2D) polymers are emerging as promising alternatives for non-volatile resistive memory devices because of their high flexibility, three dimensional-stacking capability, simple structure, transparency, easy fabrication and low cost. Until now, graphene and transition metal dichalcogenide nanosheets or their composites remain the popular pick among such ultrathin 2D materials. However, the device performance including the ON/OFF current ratio, endurance, retention time and switching voltage is far from the criteria of practical data storage technology. Therefore, design and synthesis of novel ultrathin nanomaterials as active layers for high performance non-volatile resistive memory devices is urgently required. Here, we present the facile synthesis of a solution processed 2D polymer film with a large area and uniform thickness of 2 nm on a silicon substrate. The polymer has been characterized by AFM, SEM, TEM and various other spectroscopic techniques. Interestingly, the as-synthesized polymer shows typical bipolar current-voltage (I-V) characteristics of a resistive random-access memory (RRAM) material with a high ON/OFF current ratio, long retention time and high endurance. Details of this work will be presented.

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Purine Scaffold Hsp inhibitors and theranostics

PAINADATHTHOMASAJESH LOGANATHANPALANIKUMAR[1] 박재형[2] 유자형[3,*]

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Heat shock proteins (Hsp) and their paralogs have major role in coordinating the various functions including cell proliferation, metabolism and even apoptosis. It is important to that the over expressed Hsp is crucial in cancer growth and propagation. On the other hand, mitochondria is a major organelle in cell and its dysfunction causes a variety of human disorders, including neurodegenerative and neuromuscular diseases, obesity, diabetes, ischemia reperfusion injury, cancer and inherited mitochondrial diseases. Progress in genetics and molecular biology has revealed that mitochondria play a vital role in the homeostasis of vital physiological functions, including electron transfer, apoptosis, and calcium storage. Because of this crucial role in the survival of a cell, targeting mitochondria of cancer cell will be ideal for an efficient therapeutic. The mitochondrial pool of Hsp90 and its mitochondrial paralog, TRAP1, suppresses cell death and reprograms energy metabolism in cancer cells; therefore, Hsp90 and TRAP1 have been suggested as target proteins for anticancer drug development. At the same time, the field of theranostics has emerged as an interdisciplinary research area involving chemistry, material science, biology, and medicine that combine diagnostics and therapeutics. Among various diagnosing techniques magnetic resonance imaging (MRI) provides a powerful diagnostic imaging modality, because of its non-invasiveness, high definition and precise three-dimensional positioning ability.3 Paramagnetic complexes of iron(II, III) and Gd(III) are commonly used as MRI contrast agents (CAs) to amplify the signals of MRI tomography and improve the contrast between magnetic similar but histological dissimilar tissues. Here in, we utilized purine scaffold TRAP1 inhibitors, where a TPP unit connected through a hydrophobic linker with the inhibitor was used to target mitochondria. The effect of linker length on cytotoxicity was studied with derivatives of various chain lengths and finally purine-Gd(III) complex was synthesized and studied the theranostics applications.

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Porphyrin Boxes: Rationally Designed Porous Organic Cages

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기초과학연구원 복잡계 자기조립 연구단 [1]포항공과대학교(POSTECH) 화학과 [2]기초과학연구원 복잡계자기조립연구단

Porous organic cages have attracted considerable attention in recent years owing to their potential applications including gas storage and separation. Because high structural and chemical stability and easy processability is essential for many practical applications, the quest for porous organic cages with high thermal and chemical stability has been a subject of intense research. However, to date, most of the porous organic cages have been synthesized with limited synthetic approaches, mainly based on the combination of 2-connected linear (or bent) and 3-connected triangular shaped building units. Here, we present the rational design and synthesis of large porphyrin boxes with permanent porosity and high chemical stability using well-defined and rigid 3-connected triangular and 4-connected square shaped building units. In addition, the size of cavities and windows of the organic cages can be modulated using different sized building units while maintaining the topology of the cage structures. Details of this work will be presented.

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Discovery of 2,4-diaminopyrimidines with tetrahydroisoquinolines at the 2-position of pyrimidine as ALK inhibitors

<u>AcharyRaghavendra</u> 윤정인[1] 채종학[2] 하재두[3] 황종연[4] 윤창수[5] 정희정[6] 조성윤[3] 김형래[3,*] 김필호[7,*]

한국화학연구원 의약바이오본부 [1]충남대학교 약학대학 [2]한국화학연구원 신물질연구본부/신약플랫폼기술팀 [3]한국화학연구원 난치성질환치료제연구센터 [4]한국화학연구원 신약연구본부 [5]한국화학연구원 신약연구본부 의약화학연구센터 [6]한국화학연구원 의약화학연구센터 [7]한국화학연구원 난치성질환치료제연구그룹

For the past ten years, Anaplastic Lymphoma Kinase (ALK), a receptor tyrosine kinase, has captivated tremendous interest due to its oncogenic potential and crucial role in the pathogenesis of a wide range of human cancers. To date there have been about a dozen ALK inhibitors entered into the clinical trials. Crizotinib is the first US FDA approved drug targeting ALK for the treatment of non-small cell lung cancer (NSCLC) patients. However, in the clinics crizotinib resistance was discovered due to point-mutations developed in patients treated with crizotinib. To overcome this resistance issue, second-generation ALK inhibitors have been developed and several of them are now in clinical trials, including LDK378 and CH542802. As our ongoing search for novel ALK inhibitors, we explored intensive modification at the 2-position of pyrimidine side chain in LDK378 to improve selectivity, physical property, in vitro, and in vivo efficacies. Through this effort, tetrahydroisoquinolines (THIQ) were discovered as suitable substituents for the 2-position structural fragment. Herein, we will present synthesis of THIQ analogs, and in vitro and in vivo activities of selected THIQ compounds.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Stabilized plasmid-lipid particles: Cationic liposome to encapsulate plasmid-DNA as gene delivery

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충남대학교 생화학과 [1]충남대학교 분석과학기술대학원 [2]충남대학교 자연대 생화학과

In recent studies, liposome has been used potential gene carrier in gene therapy. But liposome has several limitations of low transfection efficiency and poor cellular uptake. To overcome these limitation, we studied stabilized plasmid-lipid particle(SPLP) as enhanced gene delivery vector. SPLP is consist of lipid bilayer and encapsulated plasmid lipid, these structure have several advantage that overcome barrier of gene delivery. Generally, SPLP have a relatively low transfection than other vectors. We induced lysine residue for cell-permeability in cellular and expected increased transfection efficiency. SPLP is consist of three lipids, PEG5000-Lys7-(Palmitic acid)2, DOPE and DOTAP. DOPE was formed stabilized structure and cationic lipid DOTAP was important characteristic to encapsulate plasmid DNA. SPLP were prepared using Detergent dialysis method and confirmed particle formation by AFM and DLS. SPLPs were purified by DEAE chromatography. Cell transfection was performed using luciferase assay in HEK293 cell.

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발표분야: 고분자화학

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Solution-Processable Flexible Thin Film Transistors on Plasma Polymerized Organic Dielectrics

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광주과학기술원 신소재공학부 [1]광주과학기술원(GIST) 신소재공학부

The next generation electronic devices require mechanical flexibility, light weight, cost effective fabrication, and low power consumption. Although solution-processed thin film devices meet most of such requirements including low voltage operation, very thin organic insulating films are not typically suitable for these purposes because solution-deposited polymeric insulators contain pin-holes at low thickness (

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Synthesis of High Conductivity Polyaniline in Organic Solvents

김진구 박지웅*

광주과학기술원(GIST) 신소재공학부

We synthesized highly conductive polyaniline in organic solvents. Aniline was polymerized in the presence of organic acids and solid oxidants. Polyaniline films doped with camphorsulfonic acid exhibited average conductivity of 576 S/cm, and maximum to 637 S/cm. This method offers highly crystalline polyaniline with narrow molecular weight distribution and para-substituted aniline repeat units, providing high conductivity polymer films. We also found negative relation between polydispersity and conductivity of PANI-CSA films. These results give us some insight into what should be needed and how do we attempt for further enhancement of conductivity in polyaniline system.

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장소: 대구 EXCO
발표코드: **POLY.P-4**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Tannic Acid-Mediated Surface PEGylation for Marine Antifouling Applications

김수엽 강성민[1,*]

부경대학교 수산생물학과 [1]부경대학교 해양바이오신소재학과

The immobilization of polyethylene glycol (PEG) on surface has been of interest because of its excellent resistant to protein adsorption and marine biofouling. In this study, a facile and versatile approach to the formation of marine antifouling surface coatings was developed using TA and PEG. TA coating was carried out using iron (III) coordination chemistry, and PEG was immobilized on the TA-coated surface via hydrogen bond formation. Stainless steel and nylon were successfully modified by the approach, and the resulting substrates were used for marine antifouling application, in which diatom adhesion was significantly inhibited. We believe that this method provides an important alternative approach to the previously developed antifouling coatings for marine vessels.

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장소: 대구 EXCO
발표코드: **POLY.P-5**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Ionic thermo-responsive copolymer with multi LCST values: Easy and fast LCST-change through anion exchange

서재원 신원상*

단국대학교 나노바이오의과학

An ionic thermo-responsive copolymer with multiple lower critical solution temperatures (multi-LCSTs) has been developed and the multi-LCSTs were easily changeable according to the various counter-anion types. The multi-LCST values were achieved by introducing an ionic segment with an imidazolium moiety within the p-NIPAAm polymer chain to produce poly(NIPAAm-co-BVIm) copolymers, [p-NIBIm]+[Br]-, and changing the counter anion type to produce [p-NIBIm]+[X]- (X = Cl, AcO, HCO3, BF4, CF3SO3, PF6, SbF6). The as-prepared temperature-responsive copolymers were physicochemically characterized via 1H-NMR, FT-IR, XPS, and TGA. Their various LCST values, micelle sizes, and surface charges were determined using a UV-Vis spectrometer and a Zeta (ξ) sizer, which were fitted with temperature and stirring control. The copolymers showed a broad LCST spectrum between 39 and 52 °C. The Zeta (ξ) potential values at a pH=7 decreased from about +9.7 for [p-NIBIm]+[X]- (X = Cl ? Br) to about +2.0 mV for [p-NIBIm]+[X]- (X= PF6 ? SbF6). The micelle size (or volume) of the copolymers, [p-NIBIm]+[X]-, with different anionic species (X = Cl, Br, AcO, HCO3, BF4, PF6, SbF6, and CF3SO3) gradually increased from 181.2nm (or2.49x10-17cm-3) for [p-NIBIm]+[Br]- to 229.2nm (or5.04x10-17cm-3) for [p-NIBIm]+[CF3SO3]-, showing a clear effect of the anion on the micelle size (or volume) at a constant temperature, such as body temperature. The fact that the most important physicochemical properties for the thermo-responsive copolymers, such as the LCST value, micelle size (or volume), and surface charge, could be easy controlled only through the anion exchange suggests these are highly applicable as ionic thermo-responsive copolymers in a drug (or gene, protein) delivery system.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **POLY.P-6**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

carbazole excimer의 이론적 연구

이경언 김동욱*

경기대학교 화학과

Carbazole 은 organic electronics 에 사용되는 semiconducting material 의 중요한 구성요소로 aggregate 를 형성할 경우 그 구조에 따라서 HOMO, LUMO energy level 을 포함하는 electronic structure 가 영향을 받고 특히 excimer 형성 시 photophysical property 도 변할 수 있다. 이러한 변화가 electronic device performance 에 영향을 미칠 수 있기 때문에 carbazole aggregate 에 대한 연구는 매우 중요하다. 본 연구에서는 monomer 와 3 종류의 cofacial dimer (T-type, anti-type, syn-type)에 대해 계산하였으며 이를 통해 electronic structure 와 photophysical property 등을 살펴보았다. 바닥상태는 SOS-MP2/6-31G*로 여기상태는 SOS-CIS(D_0)/6-31G*로 최적화하였다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **POLY.P-7**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Thermal, mechanical, and morphological properties of polyol-based poly(ester amide) elastomers

오성진 손경선*

충남대학교 화학과

We developed a family of synthetic poly(ester amide)s (PEAm)s composed of polyols (mannitol or sorbitol), a diaminoalcohol, and sebacic acid to study the effect of long polyol monomers and the ester and/or amide bond content on the properties of PEAm polymer networks. These elastomers were prepared via a facile and efficient polycondensation of the three monomers, which are capable of forming ester and amide bonds, enabling the formation of crosslinked networks. The thermal and mechanical properties, swelling behaviors, and morphologies of the resulting polymers will be presented.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY.P-8**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

New chromium(III) catalysts bearing heteroscorpionate ligands : Synthesis, characterization, and ethylene polymerization behavior

최웅만 손경선*

충남대학교 화학과

We have prepared a series of new chromium(III) complexes, LCrCl3, based on tridentate ligand HC(Pz)2Py (Pz = pyrazole; Py = pyridine) and its derivatives to explore the effects of the ligand modification on the catalytic activity and selectivity in ethylene polymerization/oligomerization. The molecular structures of the new Cr(III) precatalysts were analyzed by single-crystal X-ray diffraction to confirm an unambiguous structural determination of coordination mode. Here we describe the synthesis, characterization, and the catalytic performances of the Cr(III) complexes.

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장소: 대구 EXCO

발표코드: **POLY.P-9**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Selective ethylene oligomerization with Cr complexes bearing diphosphinodiamine ligands

조서원 오성진 김윤아 손경선*

충남대학교 화학과

We have prepared a series of diphosphinodiamine(PNNP)-type ligands with bulky substituents to investigate the effects of the ligand structures on the catalytic behavior of their chromium complexes in selective ethylene oligomerization. Herein, the synthesis, characterization, and the results of selective ethylene oligomerization will be presented.

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장소: 대구 EXCO
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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Liposomes modified with Hyaluronic acid-ceramide (HA-CE) for targeted Gene delivery to CD44-positive cancer cells

Sudipta Mallick 최준식[1,*]

충남대학교 생화학 [1]충남대학교 생화학과

Hyaluronic acid-ceramide (HA-CE) modified liposomes were designed using DOTAP/DOPE for targeted delivery of therapeutic genes to the CD44-overexpressing cancer cells. Liposomes were synthesized with different molar ratios of HA-CE and most efficient formulation had been tested for further in vitro experiments. The size and zeta potential of HA-CE based liposomes was characterized by DLS. Then lipoplex prepared at different N/P ratios showed strong DNA binding affinity of liposomes for target gene delivery. Cytotoxicity of Liposome was evaluated by WST assay for different cell lines such as MDA MB 231 and NIH3T3 cells. In case of NIH3T3 cells, liposome showed negligible cytotoxicity. However CD44 positive cells; MDA MB 231 exhibited little cytotoxic effect because of higher targeting for HA-CE based liposome as compared to CD44 negative NIH3T3 cells. Then we have examined the transfection efficiency of liposome using luciferase reporter plasmid DNA. We found transfection efficiency of HA-CE based liposome was remarkably higher in case of MDA MB 231 cells as compared to NIH3T3 cells. This result was indicative for higher receptor binding endocytosis uptake of HA-CE liposomes and subsequent transfection in CD44 positive cell lines. Our finding have shown interesting prospective for tumor targeted delivery of therapeutic gene in CD44 positive cells with less cytotoxic effects.

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장소: 대구 EXCO
발표코드: **POLY.P-11**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Modified PAMAM dendrimer with short oligopeptides for early endosomal escape and enhanced gene delivery

LE THI THUY **Sudipta Mallick**[1] **최준식**[2,*]

충남대학교 Biochemistry [1]*충남대학교 생화학* [2]*충남대학교 생화학과*

Recently, non-viral vectors have become a popular research topic in the field of gene therapy. In this study, we conjugated short oligopeptides to poly(amidoamine)-generation 4 (PAMAM G4) to achieve higher transfection efficiency. Previous reports have shown that the PAMAM G4-histidine (H)-arginine (R) dendrimer enhances gene delivery by improving cell penetration and internalization mechanisms. Therefore, we synthesized PAMAM G4-H phenylalanine (F) R, PAMAM G4-FHR and PAMAM G4-FR derivatives to determine the best gene carrier with the lowest toxicity. Physicochemical studies were performed to determine mean diameters and surface charge of PAMAM derivatives/pDNA polyplexes. DNA condensation was confirmed using gel retardation assay. Cytotoxicity and transfection efficiency were analyzed using human cervical carcinoma (HeLa) and human liver carcinoma (HepG2) cells. Similar level of transfection was achieved when compared with gold standard transfection reagent PEI 25kD in both the cell lines. Therefore, our results show that these carriers are promising and may help in higher transfection with negligible cytotoxicity.

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장소: 대구 EXCO

발표코드: **POLY.P-12**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Novel Preparation and Characterization of pH-sensitive Zwitterionic Chitosan Particles

김희권

전북대학교 의학전문대학원/핵의학교실

Chitosan is a natural and biocompatible polymer which has been studied for many biomedical applications such as drug delivery. However, one of the limitations of chitosan is a property such as solubility which give weakness for drug delivery. Herein, we demonstrate that the amidation of primary amines of chitosan with succinic anhydride readily produced zwitterionic chitosan in order to increase solubility at neutral pH, and then zwitterionic chitosan particles were fabricated using a one-step aerosol method. The prepared zwitterionic chitosans were analyzed by a scanning mobility particle sizer, transmission electron microscope images, and Fourier transform infrared spectroscopy. Also the effects of UV irradiation on its surface charge were investigated, and in vitro cytotoxicity in HeLa cells was explored for biomedical purposes

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

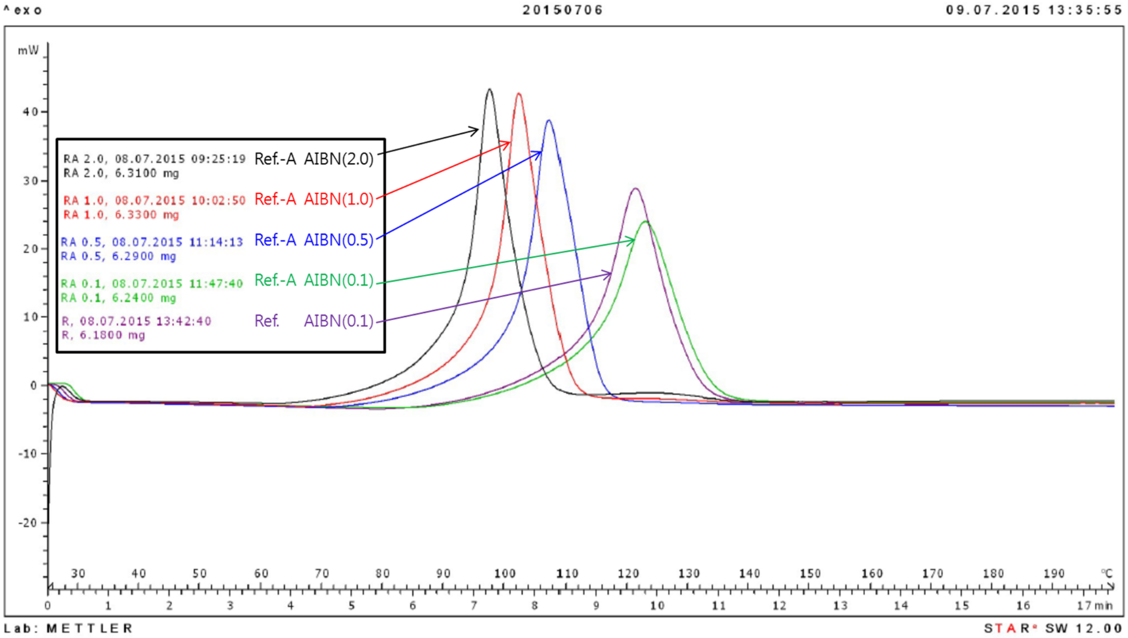
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY.P-13**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Preparation of the high functional ophthalmic polymer with initiator behavior

이민제 성아영*

대구가톨릭대학교 안경광학과

The functional hydrophilic ophthalmic lenses materials were polymerized by addition of halogen-substituted aniline. To compare polymerization degree based on the initiator, the amount of the initiator in the mixture was varied and analyzed with the DSC of METTLER TOLEDO. Also, the physical properties, such as refractive index, water content, and spectral transmittance of the copolymerized ophthalmic polymer were measured. The initiating temperature increased and the heat capacity of the hardening heat increased along with the rising additional ratio of the initiator. The copolymer with additional iodoaniline showed that the average value of refractive index increased, while water content decreased as the ratio of the additive increased. Based on the results, iodoaniline were considered to satisfy the basic requirements of hydrogel ophthalmic lenses and can be used effectively as additives for functional ophthalmic lenses. In case of the mixture containing iodoaniline, the degree of polymerization decreased compared to the basic ophthalmic lens under the same conditions. One of the methods to resolve this problem was to increase the degree of polymerization by increasing the additional amount of the initiator.(Fig. 1.)


^exo
20150706
09.07.2015 13:35:55
mW
40
30
20
10
0
-10
-20
RA 2.0, 08.07.2015 09:25:19
RA 2.0, 6.3100 mg
Ref.-A AIBN(2.0)
RA 1.0, 08.07.2015 10:02:50
RA 1.0, 6.3300 mg
Ref.-A AIBN(1.0)
RA 0.5, 08.07.2015 11:14:13
RA 0.5, 6.2900 mg
Ref.-A AIBN(0.5)
RA 0.1, 08.07.2015 11:47:40
RA 0.1, 6.2400 mg
Ref.-A AIBN(0.1)
R, 08.07.2015 13:42:40
R, 6.1800 mg
Ref. AIBN(0.1)
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 °C
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 min
Lab: METTLER
STAR° SW 12.00

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY.P-14**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Mussel-Inspired Polyglycerol: Synthesis and Versatile Surface Modification

신이슬 김병수*

울산과학기술대학교(UNIST) 화학과

The nonspecific binding of undesirable proteins, cells and microorganisms on material surfaces is one of the major problems in the biomedical fields. The nonspecific binding of these biomolecules can initiate blood coagulation, bacterial infection, inflammatory response and accumulation of organisms onto implanted materials, medical devices and underwater constructions. To inhibit these phenomena, antifouling polymers that prevent the nonspecific binding have been used as a solution. Among the various antifouling polymers, polyglycerol (PG), a promising candidate to substitute the traditional poly(ethylene glycol) (PEG), has attracted much attention with its water solubility, biocompatibility and antifouling effect. However, the immobilization of polymers onto surface requires a robust anchoring mechanism, which can be applied to various substrates. The catechol group, a key element of adhesive property of mussel renders the surface-independent binding ability and a versatile method to modification of material surfaces. In this study, we designed a new acetonide-protected catechol functionalized glycerol monomer (CAG), which was polymerized by anionic ring opening polymerization. A series of catechol functionalized polymer (PCAG) with various molecular weights and catechol contents were synthesized in a controlled manner. The acetonide protection was easily removed by acidic treatment and free catechol group was revealed. The immobilization of PCAG on various surfaces would offer the versatile surface modification method. Beyond that, the relationship between antifouling effect and its size, composition and architecture will be covered. We anticipate that this novel catechol functionalized monomer will be used in various applications in biomedical fields.

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발표코드: **POLY.P-15**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Strategy for fine-modulation of detection range in molecular beacon aptamer/conjugated polyelectrolyte bioassays by modifying the polymeric ionic density

정지은 우한영[1,*]

부산대학교 인지메카트로닉스공학과 [1]부산대학교 나노과학기술대학 나노융합공학과

The hairpin-type molecular beacon aptamer (MBA) which possesses a fluorophore and a quencher at both termini interacts with cationic conjugated polyelectrolytes (CPEs) and undergoes a conformational change to either an open chain form or a G-quadruplex depending on the presence of target (such as ATP). In the absence of a target (ATP), CPEs make MBA change their conformation to an open chain via electrostatic and hydrophobic interactions, enabling facile FRET from the CPEs to a fluorophore in MBA (turn-on state). By forming a G-quadruplex with ATP, the addition of the CPEs induces no conformational change due to the stronger interaction between the MBA and ATP, in which the resulting PL signal is strongly quenched (turn-off state). Thus, with clear turn-on/-off signal, highly sensitive and selective ATP detection is possible. Since ionic density of CPEs strongly influences their optical properties and interaction with biomolecules in aqueous media, five kinds of CPEs with different charge group per repeating unit were synthesized to control the detection range of MBA/CPEs system. Different ionic density of CPEs can control the electrostatic interaction between MBA and CPE. Finally, adjustment of ionic density (per repeat unit) of CPEs suggest an efficient way to fine-control the assay characteristics, i.e. detection range and limit of detection.

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장소: 대구 EXCO
발표코드: **POLY.P-16**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Polyethylenimine-Poly(amidoamine) Dendrimer Modified with L-Arginines as Efficient Gene Delivery Vector

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충남대학교 분석과학원 분석과학기술학과 [1]충남대학교 분석과학기술대학원 [2]충남대학교 생화학과

In this study, we synthesized polyethylenimine-polyamidoamine-arginine dendritic polymers (PPRs) as vectors for gene delivery. Four polymers, polyethylenimine-polyamidoamine generation 1 (PP1), PP2, PP1-arginine (PP1R), and PP2-arginine (PP2R), were synthesized and confirmed by 1H NMR. PPRs were shown to interact with and condense plasmid DNA effectively to form 171-179 nm polyplexes with 30-32 mV of zeta potentials at weight ratio 4:1 (polymer:plasmid DNA). Cytotoxicity of PPRs/pDNA complexes was lower than that of polyethylenimine (PEI) 25 kDa/pDNA complexes for all concentration ranges tested. In 293 cells, PP1R/pDNA complexes showed higher gene transfection efficiency than PEI 25 kDa. These results suggest that PPR could be promising dendritic gene carriers for gene therapy.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
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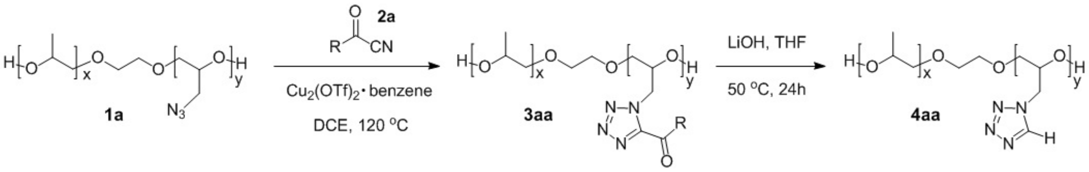
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Facile Synthesis of Glycidyl tetrazolyl Copolymers From GAP polymers

신정아 오수진* 임영권*

국방과학연구소 4-2

Tetrazole compounds have received wide attention by many chemists as energetic materials. Especially, polymers containing tetrazole compounds which are high energetic and high nitrogen contained materials are well known in energetic field as a new type of binder in propellant formulation. With this point of view, we developed a new synthetic method of tetrazole-containing polymers from glycidyl azido polymer (GAP). In the presence of catalytic amount of $Cu_2(OTf)_2$· benzene, we could obtain various tetrazole-containing copolymers from GAPs with organocyanides including electron withdrawing group (EWG) in 90 ~ 99 % conversion yields. Moreover, we carried out decarboxylation of EWG-substituted tetrazole copolymers (3aa), by treatment with LiOH, and obtained hydrogen substituted tetrazole copolymers (4aa) successfully. We believe that these polymers are good candidates for high energetic materials, pharmaceutical and material sciences.



일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **POLY.P-18**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Ion-Chelating Chain Lengths Effect of Thiophene-Based Monomers on in Situ Photo-electrochemical Polymerization

이주현 박태호[1,*]

포항공과대학교 화학공학과 [1]포항공과대학교(POSTECH) 화학공학과

We synthesized thiophene-based monomers (bis-EDOTs) with different ethylene glycol side chain (EGO) lengths (TBO3, TBO4, and TBO5) and investigated their polymerization characteristics during in Situ photo-electrochemical polymerization (PEP) at the surfaces of dye (D205)-sensitized TiO_2 nano-crystalline particles. During the PEP reaction, the thiophene-based monomers were expected to diffuse toward neighboring dyes through the growing polymer layers to enable continuous chain growth. We found that the less steric hinderance monomer (TBO3) formed a more compact polymer layer with a high degree of polymerization. Its diffusion to the active sites through the resulting growing polymer layer was, therefore, limited. We deployed layers of the polymers (PTBO3, PTBO4, and PTBO5) in iodine-free solid-state hybrid solar cells to investigate the lithium ion chelating properties of the polymers as a function of the number of oxygen atoms present in the EGOs. PTBO4 and PTBO5 were capable of chelating lithium ions, yielding a photovoltaic performance that was 142% of the performance obtained without the polymer layers (3.0 → 5.2%).

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **POLY.P-19**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Effect of Electron-Withdrawing End Groups in Non-fullerene Bithiophene Acceptors on Photovoltaic Performance

최종찬 임은희*

경기대학교 화학과

Recently, organic photovoltaic cells (OPVs) have attracted attention owing to their low cost, flexibility, and renewable energy. The OPVs showed more than 10% power conversion efficiencies (PCEs). Organic photovoltaic materials have generally designed to have polymer donor (or small molecule donor) mixed with fullerene type acceptor such as [6,6]-phenyl C61 butyric acid methyl ester. Previously fullerene type acceptors showed the high PCEs by high electron mobility and good electron affinity although weak absorption and difficult synthesis. In order to supplement fullerene`s problems, we used non-fullerene type acceptors with easy synthesis and purification.In this study, we synthesized a series of bithiophene acceptors containing the electron-withdrawing end groups. The physical, optical and electrochemical properties of the organic materials will be presented.

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Comparison of Various Core Units in Non-fullerene Small Molecule Acceptors on Photovoltaic Performance

노혜연 임은희*

경기대학교 화학과

In recent years, organic photovoltaic cells (OPVs) have attracted much attentions for renewable energy resources. They have a lot of advantages, which are low cost, flexibility, and easy synthesis. While most studies on OPVs have been conducted for electron donors to achieve power conversion efficiencies (PCEs) of 10.6%, the development of electron acceptors have been focused on fullerene derivatives that have high hole mobility and electron affinity. However, they have some drawbacks such as difficulty of synthesis and purification, and weakness of absorbance. To resolve these problem, non-fullerene acceptors have been developed and recently, high PCEs of 5.73% have been reported from polymeric materials. On the other hands, various dye units have been substituted into the small molecular acceptors as electron-withdrawing groups. Our group has also previously studied the effect of dye end groups in non-fullerene small molecule acceptors, reaching PCEs of 3.08%. In this study, we have synthesized benzene- and thiophene-based small-molecule acceptors with rhodanine dyes as electron-withdrawing groups, simultaneously transforming the conjugated core units.

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천연 수액의 특성과 분석Analysis and Characterization of Korean Lacquer

성미숙* Rong Lu[1,*] Tetsuo Miyakoshi[1,*]

가톨릭관동대학교 의과대학 생화학교실 [1]Meiji University, Department of applied chemistry

흔히 목재의 마감재로 사용되는 우리나라 천연 옻나무 수액은 채취시기에 따라 초칠, 성칠, 말칠로 구분되며 중국칠, 일본칠과 함께 Toxicodendron vernicifluum 옻나무에서 추출된다. 이 논문은 우리나라 옻의 성분, 락카아제 활성도, 건조시간, 그리고 우루시올 곁가지의 구조분석등을 하였고 동시에 중국칠, 일본칠과 비교분석하였다. 그 결과 우리나라 옻칠이 가장많은 우루시올 84.9%, 곁가지 triene 불포화도 56.1%로 측정되었다. 동일한 두께로 필림위에 도포 한 후 건조시간을 측정한 결과 중국칠, 한국칠, 그리고 일본칠 순으로 건조되었다. 또한 중국, 일본 그리고 한국 옻칠의 구조적 차이를 IR, NMR 과 GC-MS 측정 결과 같은 종이지만 환경적 차이로 약간의 구조적 차이를 볼수 있었다.Three kinds of Korean lacquer saps were analyzed including chemical composition, enzymatic activity, molecular weight distribution, unsaturated degree of side chain, and drying property. The results were compared with Chinese and Japanese lacquer saps all collected in the same month (August 2012 and 2013) to investigate similarities and differences. Compared with Chinese and Japanese, the Korean lacquer sap contains the most lipids (84.9%) and urushiol triene (56.1%) components and the second highest enzyme activity after Chinese lacquer sap. In the drying and film hardness test, Korean and Chinese film reached a stronger hardness sooner than Japanese lacquer film; in 21 days the former reached 2H and the latter only H. The results of IR, NMR, and GC-MS showed slight difference due to different growing conditions.

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Cationic polymers self-assembled from glycol chitosan conjugated polyethylenimine as an efficient gene delivery carrier

이영화 박해인 최준식*

충남대학교 생화학과

A self-assembled polymer based on nanocarrier was prepared using a modified glycol chitosan for gene delivery. We prepared glycol chitosan (GC), methyl acrylate (MA) and polyethylenimine(PEI) branched polymer (GMP) for gene therapy. The polyplexes are prepared with branched polymer and plasmid DNA (GMP/pDNA) in different weight ratios. Polyplexes diameter and surface charge were characterized by Dynamic light scattering techniques, showed positively charged nano-sized carriers. The morphology of prepared polyplex was confirmed by the atomic force microscope (AFM). Monodispersed rod shaped polyplex was observed having width in nanometer and length in micrometer scale. The gel electrophoresis and PicoGreen assay results showed complete condensation of plasmid DNA in order to form the rod shape polyplex. Compared to generally used polyethyleneimine (PEI) 25kD and PEI 800Da, GMP/pDNA nanorods showed higher transfection efficiency at each weight ratio with lower cytotoxicity, confirmed by luciferase assay and WST assay respectively, in various cell lines. Our gene delivery carriers are also efficiently taken up by cells confirmed by confocal microscope images. So, current glycol chitosan and polyethyleimine based on branched polymer can be a promising gene carrier for the effective delivery of therapeutic genes

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Preparation of Polycarbonate/Poly(acrylonitrile-butadiene-styrene)/Mesoporous Silica Composite Films and Its Rheological, Mechanical and Sound Absorption Properties

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서울과학기술대학교 의공학-바이오소재융합 협동과정 [1]서울과학기술대학교 정밀화학과

Polycarbonate (PC) and poly(acrylonitrile-co-butadiene-co-styrene (ABS) copolymer are well-known engineering plastics being used especially in electronic companies. To overcome a few disadvantage of respective polymers, the preparation of composites and blends have been investigated both in industrial and academic concerns. Here, we present the preparation of polymer composite films using PC/ABS polymers and several mesoporous materials. The mainly homogeneous composite thin films were prepared by a facile solvent casting method using modified-mesoporous silica materials and dichloromethane as a solvent. Tensile tests were performed at room temperature according to ASTM D638 using Instron 1122 universal testing machine. Rheological properties were analyzed by RMS800. The fundamental analysis for mesoporous materials were also observed; small-angle X-ray scattering (SAXS), nitrogen adsorption-desorption, nuclear magnetic resonance (NMR) and scanning electron microscope (SEM) to provide clear physical and chemical properties. As a compatibilizer and a reinforcing filler, mesoporous (organo-)silicas showed enhanced features in mechanical properties. Moreover, the composite products could be used as sound proofing materials due to the porous structure of silicas.

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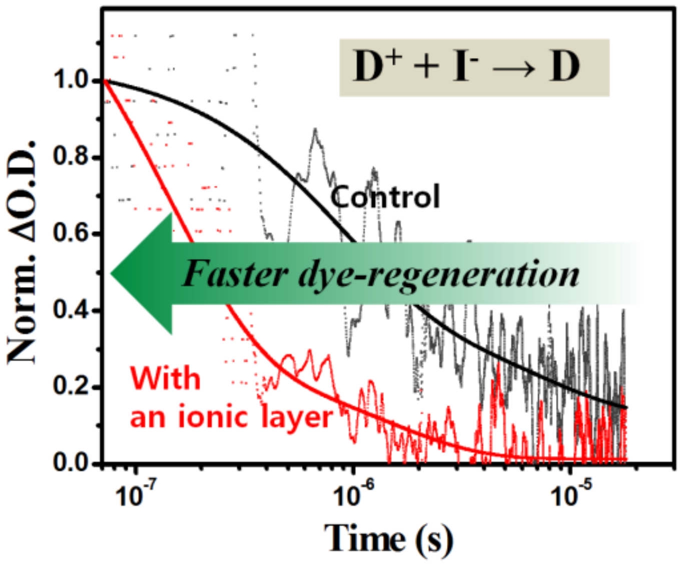
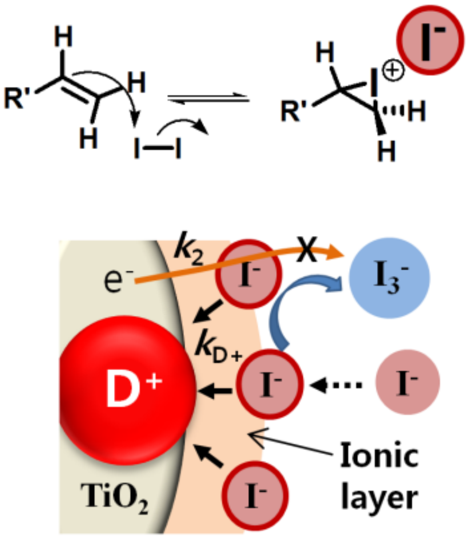
Fast cascade neutralization of oxidized sensitizers by an in situ-generated ionic I^- layer on a nanocrystalline TiO_2 electrode

김태완 박태호*

포항공과대학교(POSTECH) 화학공학과

We report a novel way to accelerate the rate of oxidized sensitizer neutralization on nanocrystalline TiO_2 electrode surfaces using a novel coadsorbent, 3,4,5-tris-butenyloxy benzoic acid (TD), having three terminal double bonds. ^{1}H NMR and contact angle measurements revealed that the terminal double bonds reacted with I_2 to form an in situ-generated ionic layer of I^- species. Transient absorption spectroscopy (TAS) and electrochemical impedance spectroscopy (EIS) studies showed that I^- species neighboring the dye molecules (D^+) accelerate the neutralization (or regeneration) rate, as well as decrease the recombination reactions of electrons with D^+ and I_3^-. Dye-sensitized solar cells treated with TD exhibit a power conversion efficiency of 10.2%, which is 22% higher due to the simultaneous improvements in J_{SC} and V_{OC}.





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Thickness Effect of Hole Transport Layer in Perovskite Hybrid Solar Cells: Performance and Reproducibility

김관우 편임옥[1] 강경호 박태호[*]

포항공과대학교(POSTECH) 화학공학과 [1]포항공과대학 화학공학과

We demonstrate the effect of hole transport layer (HTL) thickness in meso-superstructured perovskite hybrid solar cells employing $CH_3NH_3PbI_{3-x}Cl_x$ and spiro-MeOTAD. HTL is an essential component to achieve high performance perovskite photovoltaic devices, however, reports about the effect of its thickness on device performance are scarce. Herein, we systematically study the effect of spiro-OMeTAD thickness on photovoltaic properties of meso-superstructured perovskite hybrid solar cells employing $CH_3NH_3PbI_{3-x}Cl_x$ absorber. We find that there is an interplay between photovoltaic performance and reproducibility; low thickness of HTL gives best performing devices with poor reproducibility and higher thickness gives low performing devices with higher reproducibility. Finally, we achieved 15.5 % of power conversion efficiency (PCE) with 23.5 mA/cm^2 of short-circuit current (J_{SC}), 1.02 V of open-circuit voltage (V_{OC}) and 64.7 % of fill factor (FF), with 180 nm thick spiro-MeOTAD layer.

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Active Role of Liquid Crystals in Novel Planar Organic Field-Effect Transistors

서주역 김영규* 김화정

경북대학교 화학공학과

Recent advances in flexible electronics spotlight on organic electronic devices, which can be fabricated with solution processes, because of their features including ultrathin shape, lightweight, high flexibility, easiness in designing, etc. It is also expected that organic electronic devices can be manufactured by employing cost-effective 3D printing technology. Organic field-effect transistors (OFETs) are understood one of the basic organic electronic devices for various applications. However, the development of device structures has been stagnant even though various new materials have been actively synthesized. In this regard, we have recently invented novel planar OFETs that configure all electrodes on the same plane of substrates. In particular, liquid crystals (LCs) have been introduced as a gate insulator leading to LC-g-OFETs. This presentation will discuss the detailed operating mechanism of LC-g-OFETs in terms of molecular aspect and demonstrate their applications as an ultrasensitive tactile sensor.

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Fabrication of Arsenic Absorption 3D Filaments based on ABS fiber and Iron (III) Oxide

조대형 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

The arsenic contamination of groundwater is a big problem to people who live in Southeast Asia. The symptoms of arsenic(As) accumulation in human body are nausea, vomit, diarrhea, abnormal heartbeat, injuries of blood vessel, pain, variety kinds of cancers. To reduce the concentration of As, there are many solutions already exist. But the way of using 3D printer is not available yet. By using Iron(III) Oxide powder with ABS polymer, fabricating As absorbable 3d filament is successfully done and this filament show the As sensitivity. This new filament has higher As absorption ability than rusted nail which is used the most easiest way to reduce As in groundwater. Using this new filament and FDM type of 3d printer, making As absorption structure is also available. The benefit of this fabrication is that anyone can make As absorbable 3d structure easily.

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3D printable porous scaffold for dental application

김민정 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Bone scaffolds have research issues, for example, porosity, biocompatibility and mechanical strength and stability. Strategies to bone tissue engineering have focused on the use of biodegradable polymer and calcium phosphate ceramic for 3-Dimesional bone scaffold by mimicking the real structure and component of bone. In this research, first, we focused on the 3D printable pore structure for scaffold and approached by two ways in terms of the materials and 3D printing method. One is the combination of Polylactic acid(PLA) which is biodegradable polymer for biocompatibility and Poly(vinyl alcohol)(PVA), water soluble polymer. These materials were used in Fused Deposition Modeling(FDM) method. The other is Stereolithography method using Formlabs 3D printer and resin with Poly(ethylene glycol)(PEG).

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Research on Synthesis and Characterization of Water Soluble Polymer(WSP) for Optoelectronic Device

이자민 박동규*

경성대학교 화학과

We have synthesized water soluble polymer, Poly[6,6'-(fluorene-9,9-diyl)bis(trimethylhexan-1-aminium) bromide-alt-benzothiadiazole](PFDTMHAB-alt-BTD), 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 520nm (2.38 eV).

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Control of inter-molecular interaction in conducting material: Impact on Micro structure and Charge Transport

이강영 박태호*

포항공과대학교(POSTECH) 화학공학과

Conjugated organic materials enable the low-cost fabrication and application to flexible and large-area semiconductor devices that can be processed from solution at low temperatures with plastic substrates. This property makes conjugated organic material quite applicable to ubiquitous plastic electronics including flexible displays, e-paper, radio frequency identification (RFID) tags, and large-area sensors. The delicate balance of molecular design between building blocks structure and functionality can give rise to significant effects on electronic, physical, and charge transport properties of solution-process-able conjugated organic material. In this study, we synthesized a new series of highly planner conjugated organic material which were systemically controlled inter-molecular interaction. Several aspects of the effects of controlled inter molecular interaction, such as morphology and molecular orientations, provide new insights into structure-property relationships for high-performance semiconducting material having controlled inter-molecular interaction.

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Characterization of FT-IR microspectroscopy and chemical image of pH-dependent human hair

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서강대학교 화학과 [1]서강대학교 화학과,바이오계면연구소 [2]서강대학교 화학과 및 바이오융합과정

Acid rain is one of a common issue that people put up an umbrella even though drizzling because many people are afraid of the word 'acid' and their alopecia symptom. But actually acid rain does not harm to hair that much. Many researchers observed the surface of hair using scanning electron microscope and studied only change of surface cuticle layer by pH variation. The FT-IR microspectroscopy enables chemical imaging by combining the spectral and spatial information. Therefore, we can easily check chemical effects as a function of position in the cross sectioned hair. We observed FT-IR microspectroscopy for the chemical information about cuticle and cortex in damaged hair with different pH. In this research, details of damaged human hair by pH will be discussed.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Creating conductive polymer composite composed of ethyl vinyl acetate and carbon black

조애리 김희주[1,*] 백승휘[2,*] 조대형[*] 김민정[*] 권오선[*] 신관우[3,*]

서강대학교 화학과 [1]서강대학교 화학 [2]서강대학교 화학과 대학원 [3]서강대학교 화학과 및 바이오융합과정

Recently, three-dimensional (3D) printing has been emerged as an attractive technology, since it promises opening a new era of the second printing revolution following the pressing printing which was evented in Korea in 14 C. In fact the gear of technical developing progress has been already changed because the 3D printing relies on the additive manufacturing process being capable to complement to the current subtract technologies depended with pressing and milling processes for manufacture. There are already a lot of reseaches about producing functional filament going keeping track of 3D printer wave. In order to obtain functional filament which can be made from FDM type, we conducted researches mixing thermoplastic polymer with a varity of additives to give conductivity. And in creating conductive filament for 3D printing using FDM, we assumed that creating conductive glue composed by EVA(ethyl vinyl acetate) and (CB)carbon black can be a middle step in the light of creating conductive polymer composite. We tried heating and extruding out of conductive composite from mini glue gun nozzle which is similar version of extruding ABS of PLA filament from the nozzle of FDM 3d printer. The diameter of mini glue gun nozzle is 1.5mm and it is bigger than 3d printer nozzle which is generally 0.3mm. For analyzing the thermal process of extruding, thermal imaging was obtained by FLIR.

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Ink-jet Fabrication of electronics pattern on fabrics and its thermochromic response

김희주 김용준[1] 신관우[2,*] 권오선[1,*] 박종진[3]

서강대학교 화학 [1]서강대학교 화학과 [2]서강대학교 화학과 및 바이오융합과정 [3]전남대학교 고분자융합소재공학부

Flexible electronics can require delicate patterned electrodes on the flexible substrate, which are highly stretchable. Approaches to print electrodes on fabrics are often by metal-wiring, or layer-stacking. We make a micro-scale electrode patterns using by commercial ink-jet printing process. And we produce a direct fabrics display based on electrode pattern fabrics and thermochromatic dye. Fabrics based on thermochromics dye depending on critical temperature. Above critical temperature, thermochromics dye fabrics color is disappeared. We application of electrode and thermochromatic fabrics which are change the supply current, we controlled the fabrics temperature locally. With this capability, we would like to build locally changing temperature and color-varying fabrics, which make the best use of as smart camouflage fabrics.

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Synthesis of energetic polymer containing ferrocene

정지혜 신정아 정해지[1] 임영권*

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부

Tetrazoles are nitrogen-rich compounds which have high heat of formation. So they have been used as promising candidates for explosive and gas generator. Ferrocene derivatives have been widly used burning rate catalyst for propellants. We have designed polymers containing both tetrazoles and ferrocenes to obtain energetic polymers having burning rate catalyst property. So poly(glycidyl amino tetrazole-co-glycidyl ferrocenyl triazole)(PGATGFT) are synthesized by three step reactions. The structures of PGATGFTs are confirmed by IR, ^{1}H and ^{13}C NMR spectral analyses. Thermal properties of the PGATGFTs are evaluated using differential scanning calorimetry (DSC).

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Graphite 첨가에 따른 보호필름의 점착력 및 전도도 변화에 관한 연구

김경석 오지만 전진 윤아연 김성호*

순천향대학교 화학과

저 점착 Pressure sensitive adhesive(PSA)를 이용한 보호필름은 전자산업에서 매우 다양한 용도로 사용되고 있다. 본 연구에서는 보호 필름에 이용되는 저 점착 PSA 에 graphite 를 첨가하고, 점착시트를 제조 하였다. 첨가된 Graphite 의 양을 조절 해가며, 점착시트의 점착력과전도도를 측정하였다. PSA 는 아크릴계중합물을 이용하였으며, 기재는 PET 를 liner 는 저밀도 polyethylene 이 코팅된 박리지를 사용하였다. Grephie 함량변화가 점착력과 전도도에 미치는 영향을 기술 하였다.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Plasma modification of poly(2-heptadecyl-4-vinylthieno[3,4-d]thiazole) low bandgap polymer and its application in solar cells

김준헌 김인태*

광운대학교 화학과

For the first time, we here propose a green methodology to modify a low bandgap polymer for highly efficient solar cells using atmospheric pressure plasma jet or soft plasma operating on different feeding gases (air, Ar and N_2). The physical properties of the modified polymer were investigated using conductivity measurements, UV-visible spectroscopy, photoluminescence spectroscopy, X-ray photoelectron spectroscopy, cyclic voltammograms, atomic force microscopy, cathodoluminescence and confocal Raman spectroscopy. Further, we examined the variation of the work function of the polymer before and after plasma treatment using a λ-focused ion beam. Additionally, photovoltaic cells based on the plasma-modified polymer having ITO/PEDOT:PSS/PHVTT (with or without plasma modification):$PC_{71}BM$/LiF/Al configuration were fabricated and then characterized. We found that the power conversion efficiency (PCE) of the plasma-modified polymer increased dramatically as compared to the control polymer (without plasma treatment). PCE of the control polymer was found to be 4.11%, while after air, Ar and N_2 gas plasma treatment the polymer showed PCEs of 4.85%, 4.87% and 5.14% respectively. Thus, plasma treatment not only alters the surface properties, but also modifies the bulk properties (changes in HOMO and LUMO bandgap level). Hence, this work provides new dimensions to explore more about plasma and polymer chemistry.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, characterization and properties of newly synthesized polymer containing thiazole unit and 3,6-Bis(5-bromo-2-thienyl)-2,5-bis(2-hexyldecyl)-2,5-dihydro-pyrrolo[3,4-c]pyrrole-1,4-dione

차주현 김인태*

광운대학교 화학과

In polymer solar cells(PSCs), diketopyrrolopyrrole unit plays important role as main chain of polymer. So we introduce this unit to existing polymer for increasing efficiency. Hence, we synthesized hetero aromatic ring based polymer using Herrmann's catalyst. This polymer is conjugated polymer containing thiazole unit and diketopyrrolopyrrole unit in the main chain. The structure of polymer was identified by?^{1}H-NMR,?^{13}C-NMR and FT-IR spectroscopy. The molecular weight was measured using Gel Permeation Chromatography(GPC). The optical property and electric property of the polymer checked in the UV-vis spectroscopy and cyclic voltametry(CV).

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Modification in the physical properties of the newly synthesized conducting polymer with the addition of ionic liquids

조태종 김인태*

광운대학교 화학과

Ionic liquids (ILs) are a unique class of solvents, having various properties such as non-volatility, non-flammability, electrochemical stability and high conductivity. Due to unique properties, ILs present a means to realize the next generation of energy storage technology. In this experiment, we have studied the interaction between the conducting polymer and ILs. For this study we have synthesized the novel conducting polymer containing the Pyrrole and Thiophene groups. Additionally, we have used the imidazolium and ammonium family ILs, such as 1-Buthyl-3-methylimidazolium bromide ([BMIM]Br), 1-Ethyl-3-methylimidazolium bromide ([EMIM]Br), triethylammonium methanesulfonic acid (TMEAS), triethylammonium 4-aminotoluene-3-sulfonic acid (TBH) ILs. The molecular interaction studies between conductign polymer and ILs, have been carried out with UV-vis spectroscopy, FR-IR spectroscopy, Conductivity measurement and confocal Raman spectroscopy. This type of study is very useful to use polymer and ILs combination as new conducting materilas.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Functionalization of polymer side chain for biological applications

김영선 김인태*

광운대학교 화학과

In this study, our goal is to develop the polymers which have biological importance. Especially, we predict that the synthesized polymers can interaction with amino acids of protein. These polymers are conjugated polymer containing benzobisthiazole unit and aromatic rings in the main chain. The target polymers with various functional groups such as hydroxy, carboxyl acid, or ester can interact with protein surface. The optical property of the synthesized polymers can be checked in the UV-vis spectroscopy. The electric property of the polymer can be measured in the conductivity measurements.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Thiophene based conducting polymer is applied to Liquid Crystal as side chain: Synthesis and characterization

김종현 김인태*

광운대학교 화학과

Conjugated polymers have emerged as an important material for numerous applications for example, photovoltaic devices, light emitting diodes (LEDs), field effect transistors (FETs), and electrochromic devices, etc. Liquid crystal(LC) show special optical properties. In this work, we synthesized several LC polymers and observed their a optical properties and structures. The structure of the compounds was ascertained by 1H NMR, 13C NMR, and FT-IR spectroscopy. We also observed the optical properties UV/Vis absorption, photoluminescence(PL) spectroscopy for the synthesized the polymers. Through this work, we can find the possibilities of polymers for organic photovoltaic devices (OPVs).

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Naphthalene-, Anthracene-, and Pyrene-substituted Fullerene Derivatives as Electron Acceptors in Polymer-based Solar Cells

김희운 김지훈[1] 김범준[2] 윤성철[3] 황도훈*

부산대학교 화학과 [1]부산대학교 [2]한국과학기술원(KAIST) 생명화학공학과 [3]한국화학연구원 화학소재연구단

A series of aryl-substituted fullerene derivatives were prepared in which the aromatic moiety of [6,6]-phenyl C$_{61}$-butyric acid methyl ester (PC$_{61}$BM) was modified by replacing the monocyclic phenyl ring with bicyclic naphthalene (NC$_{61}$BM), tricyclic anthracene (AC$_{61}$BM), and tetracyclic pyrene (PyC$_{61}$BM). The PC$_{61}$BM derivatives were synthesized from C$_{60}$ using tosylhydrazone and were tested as electron acceptors in poly(3-hexylthiophene) (P3HT)-based organic photovoltaic cells (OPVs). The lowest unoccupied molecular orbital (LUMO) energy level of NC$_{61}$BM (-3.68 eV) was found to be slightly higher than those of PC$_{61}$BM (-3.70 eV), AC$_{61}$BM (-3.75 eV), and PyC$_{61}$BM (-3.72 eV). The electron mobility values obtained for the P3HT:PC$_{61}$BM, P3HT:NC$_{61}$BM, P3HT:AC$_{61}$BM, and P3HT:PyC$_{61}$BM blend films were 2.39 x 10^{-4}, 2.27 x 10^{-4}, 1.75 x 10^{-4}, and 2.13 x 10^{-4} cm^{2} V^{-1} s^{-1}, respectively. P3HT-based bulk-heterojunction (BHJ) solar cells were fabricated using NC$_{61}$BM, AC$_{61}$BM, and PyC$_{61}$BM as electron acceptors, and their performances were compared with that of the device fabricated using PC$_{61}$BM. The highest power conversion efficiencies (PCEs) observed for devices fabricated with PC$_{61}$BM, NC$_{61}$BM, AC$_{61}$BM, and PyC$_{61}$BM were 3.80%, 4.09%, 1.14%, and 1.95%, respectively, suggesting NC$_{61}$BM as a promising electron acceptor for OPVs.

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Syntheses of Polymeric Excipients by Controlled Radical Polymerization for the Delivery of Cisplatin Pharmacophore

이상민

가톨릭대학교 화학과

Over the past decades, biocompatible polymers have been proposed as a delivery platform to improve the aqueous solubility of small-molecule drugs, allowing for the selected delivery to disease cells. Although such delivery systems have been demonstrated to possess great potential to decrease the toxic side effects often associated with conventional chemotherapy, successes have been limited due to the lack of both targeting ability to particular disease sites and specific triggers to release the encapsulated drug under predefined biochemical condition. To overcome these challenges, we prepared a series of block-copolymers composed of poly(ethylene glycol) and poly(acrylic acid), which can be employed as a polymeric excipient to deliver cisplatin pharmacophore as a model drug. After polymerization via either nitroxide-mediated radical polymerization or atom-transfer radical polymerization, the copolymer was employed to incorporate the aqua derivative of cisplatin pharmacophore, which leads to the formation of self-assembled core-shell type nanoscale structures. The resulting nanoparticles possess the Pt(II)-encapsulating core, where the polymer chains are cross-linked via divalent metal-coordination, allowing for the enhanced structural stability.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of Polysaccharide Derivatives as a Delivery Platform for Cisplatin Pharmacophore

이상민

가톨릭대학교 화학과

Over the past decades, platinum(II)-based anti-cancer drugs have increasingly become one of the most popular therapeutic agents of great importance in clinical cancer treatments. However, such Pt^{II}-based chemotherapy has been limited mostly due to the toxic side effects and recurrent occurrence of multi-drug resistance (MDR) in cancer tissue. To overcome these limitations, various Pt^{II} agents have been encapsulated in nanoscale delivery platform, which can exhibit great potential to minimize both detrimental side effects and MDR in cancer treatments. Hence, we employed biocompatible polysaccharides such as alginic acid and chitosan modified with both poly(ethylene glycol) and malonic acid, as a delivery platform for cisplatin pharmacophore. The resulting polysaccharides exhibited the formation of monodispersed nanoparticle cross-linked with divalent Pt^{II} ions, showing great potential for nanoscale delivery platform.

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Light-responsive hydrogel beads for remotely controlled transdermal release system

김하늘 양승윤[1] 윤진환*

동아대학교 화학과 [1]부산대학교 바이오소재과학과

Here, we have prepared visible-light responsive hydrogel microbeads by spray injection of the precursor solution with alginate templating method. The hydrogel beads consisting of temperature poly(N-isopropylacrylamid--*co*-vinyl-2-pyrrolidinone) and photothermal magnetite nanoparticles (MNP) could be produced with a uniform size and shape. MNP dispersed in the hydrogel matrix can absorb light and convert photo energy into thermal energy, thereby volume shrinkage of hydrogel could be achieved. We further fabricated transdermal patch using generated hydrogel beads as drug reservoirs, achieving the on-demand release of drug triggered by visible light irradiation.

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Conjugation of histidine and arginine to cystamine core polyamidoamine(PAMAM) with high flexible γ-Amino butyric acid(GABA) for gene delivery

박혜원 송수정[1] 최준식*

충남대학교 생화학과 [1]충남대학교 분석과학기술대학원

Polyamidoamine (PAMAM) dendrimers are well known non-viral vectors for gene delivery application. Especially PAMAM conjugated with different amino acids have enhanced cell uptake ability and low cytotoxicity compared to other non-viral vectors. Moreover cystamine core PAMAM has ability to degrade inside low pH of endosome leading to the easily release of biomolecules. In present work, we designed γ-amino butyric acid (GABA), histidine, arginine modified cystamine core PAMAM. GABA has four carbon chains that plays a role as flexible linker, hence easy interaction with cell membrane. cPAMAM-GABA-HR synthesis was confirmed by H^1-NMR. We performed gel retardation assay and DNA release phenomenon of cystamine core PAMAM using DTT. We measured size of polyplex by DLS and AFM. Cytotoxicity was examined by WST assay and transfection efficiency was confirmed using luciferase reporter plasmid in HeLa cells. GFP expression was detected by fluorescence microscopy. This work can be a promising candidate of non-viral vectors in gene delivery application.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

촉진내후성 시험에 의한 도막의 광열화 특성 평가

양정원 **공영대***

동국대학교 화학과

공업도료 중 건축용 도료의 경우 지붕재 코팅 등에 사용이 되어 다양한 기후인자(열,빛,수분)에 노출되어있다. 건축용 도료는 일반적으로 Polyester-Melamine 타입의 열경화 시스템을 이용하여 소지를 코팅하는데, Polyester-Melamine 은 수분에 의한 가수분해 및 산화반응을 통해 열화되는 것으로 알려져 있다. 이러한 열화 현상은 실제로 제품의 수명에 영향을 주고, 제품수명을 예측하기 위해 기후영향을 증가시켜 장시간의 옥외 현상을 모사하는 시험장비들이 개발되어왔다. 촉진내후성 장비중 특정 UV 를 조사하여 고분자의 열화를 조사하는 QUV 장비를 이용하여, UV 조사 전후의 표면상태 및 구조를 다양한 장비를 이용하여 확인하였다. 실제로 FTIR-ATR 을 측정하면 가수분해 및 산화반응에 의한 OH;NH 및 CHn 피크의 변화를 감지할 수 있는데, 기존에 알려져 있는 작용기 이외에 C=O 및 Triazine ring 작용기 또한 변화함을 확인할 수 있었다. IR 이외에 NMR, XPS 를 이용하여 작용기 변화를 교차검증함으로써 Polyester-Melamine 열화 메커니즘에 새로운 패러다임을 제시하고자 한다. 추가로 R static 통계기법의 주성분 분석으로 스펙트럼 영향력에 따른 작용기 순서를 나열하고 변수와의 상관관계를 해석하여 POI(photooxidation Index) 계산하였으며, 이러한 평가법을 통해 열화 현상을 설명하고자 한다.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

우루시올 고분자/키토산 복합막의 제조 및 특성 분석

공성준 원종옥*

세종대학교 화학과

이온전도성 막은 배터리와 관련된 여러 분야에서 많은 응용 가능성을 갖고 있다. 이온전도성 막이 사용되는 배터리들의 효율은 막의 소재와 그 특징들에 큰 영향을 받는다. 특히 막의 가격은 배터리의 총 생산비용에서 큰 비중을 차지한다. 현재 대표적으로 상용화 되어있는 불소계 전해질 막 역시 가격이 높다는 단점을 갖고 있다. 그에 따라 고가의 전해질 막을 대체할 수 있는 저가의 고분자 전해질 막에 관한 연구가 활발히 진행되고 있다. 본 연구에서는 보다 낮은 생산 비용의 막을 만들기 위해 천연고분자인 키토산과 옻으로 알려진 우루시올을 소재로 사용하였다. NH_2 작용기를 가진 키토산은 기존의 연구들을 통해 비교적 높은 이온전도도를 나타낼 수 있는 소재로 알려져 있다. 이러한 키토산을 중심으로 막의 낮은 내구성을 향상시키기 위해 내 화학 약품성이 높은 옻을 혼합하여 막을 제조하였다. 최종적으로 키토산과 우루시올이 함께 가교되며, 이를 통해 보다 내구성이 향상된 이온전도성 막을 제조하였다. 다양한 몰 비의 우루시올 고분자/키토산 복합막을 제조하고, 완성된 막의 특성을 확인하기 위하여 IR 스펙트럼 분석과 Thermogravimetric Analyzer(TGA)를 통해 분석하였으며, Electrochemical Impedance Spectroscopy(EIS)를 측정하여 필름의 이온전도도를 확인하였다. 키토산/우루시올 (1:100) 복합막의 경우 (2.4×10^{-2} S/cm)의 이온전도도 값을 나타냈으며, 다른 비율의 경우 키토산의 함량이 증가함에 따라 이온전도도 값이 증가하는 것을 확인하였다.

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Alkaline Anion Exchange Membranes [PVA/PDDA-OH^-] 제조 및 연료전지 성능연구

조은해 원종옥*

세종대학교 화학과

최근에 사용되고 있는 Anion Exchange Membranes[AEMs]들은 값이 비싸고 유독성 재료들을 많이 사용하며, 고온의 알칼리 조건에서 불안정한 단점을 가지고 있다. Poly(Dially Dimethyl Ammonium chloride)[PDDA]는 전도성 이온 Cl^-를 포함하고 물과의 용해력이 좋은 고분자이다. 이 PDDA 를 film 제조에 용이하고 값이 싼 Poly Vinyl Alcohol[PVA]와 섞어서 만든 membrane 은 우수한 OH^-전도도와 높은 농도의 KOH 용액에서 견딜 수 있는 강한 알칼리성 안정성을 보여 앞에 말한 단점들을 보완할 수 있다. PVA 와 PDDA 를 질량 비 1:0.125, 1:0.25, 1:0.5,1:0.75, 1:1 로 섞어 petri dish 에 붓는 다음 건조시켜 만들어진 membrane 은 140℃에서 1 시간 annealing 시켜 열적 안정성을 주고, 용매가 IsoPropyl Alcohol[IPA]인 5wt% GlutarAldehyde[GA]용액에서 1 시간 cross-linking 을 시켜 화학적 안정성을 주었다. 2M 의 KOH 용액에서 PDDA 가 포함하고 있는 Cl^-을 OH^-으로 치환시켜 PVA/PDDA-OH^-인 Alkaline Anion Exchange Membranes[AAEMs]을 만들었다. 만들어진 AAEMs 로 Electrochemical Impedance Spectroscopy[EIS]를 이용하여 측정한 결과 PDDA 의 양이 많아질수록 우수한 OH^- 전도도 $2.1\text{x}10^{-2}$S/cm (1:0.75)를 보임을 확인하였다.

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비수계 VRFB에서 전기 방사법을 이용한 다공성 멤브레인의 장기 안정성 향상 연구

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바나듐 레독스 흐름전지(Vanadium redox flow battery, VRFB)는 대용량 전력저장 시스템의 하나로써 전해질을 반영구적으로 사용할 수 있기 때문에 친환경적이며, 전해질의 반영구적인 사용으로 인한 전지의 긴 수명, 또한 전기를 액체 상태인 전해질에 저장하기 때문에 용량 확장의 자유로움, 빠른 반응시간, 높은 충 방전 효율이라는 다양한 장점들로 인해 전해질, 전극, 멤브레인 등 VRFB 의 다양한 분야에 관한 관련연구가 진행되고 있다. VRFB 에서 멤브레인은 VRFB 구성 핵심 물질이며, VRFB 에 응용되는 멤브레인의 특성으로 높은 이온전도도, 낮은 이온 투과성, 그리고 우수한 화학적 안정성과 기계적 강도가 요구된다. 본 연구에서는 수계 레독스 흐름 전지보다 넓은 범위의 작동 전압과 온도를 보장하는 비수계 레독스 흐름 전지에 적합한 멤브레인의 특성을 확인하기 위하여 다공성 멤브레인(Celgard)의 장점인 낮은 전기 저항으로 높은 전류밀도의 흐름전지에서 높은 에너지효율을 확인했고 또한 멤브레인의 장기안정성을 증가시키기 위하여 전기방사법을 이용하여 다공성 멤브레인에 nano fiber 를 적층하여 개선된 성능을 발휘하는 멤브레인을 제조 하였다. 막의 성능은 VRFB single cell test 기를 사용하여 충 방전 실험을 진행하였고, 막의 안정성을 확인하기 위해 흡수도와 활물질 투과도, 전기저항, Electron Impedance Spectroscopy 를 이용하여 이온전도도 $1.3X10^{-1}$ 로 확인하였다. 결과적으로 기존의 다공성 멤브레인 보다 전기방사법을 이용한 electrospun membrane 이 막의 안정성과 약 5%의 에너지 효율이 상승하는 것을 확인 하였다.

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Hemiaminal Dynamic Covalent Network 로 인한 에폭시 접착제의 Self-healing 특성 연구

김지영 원종옥*

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에폭시 수지는 접착력과 표면 안정성에 관한 기계적 물성, 그리고 내화학성이 우수하고 경화시 수축변형이 적고 경화속도를 조절할 수 있는 특성으로 인해 접착제, 전기,전자부품, 복원 재료, 표면 코팅제, 페인트와 잉크, 제품 마감재 등으로 광범위하게 사용되고 있다. 또한 다양한 충전제를 포함할 수 있어 충전제에 따른 효과를 볼 수 있음에 따라 그 응용이 다양하다. 하지만, 응용 관점에서 볼 때, 에폭시 수지의 우수한 내구성과 안정성에도 불구하고 최대 단점인 취성으로 인해, 환경과 외력으로 인한 균열이 에폭시 수지 내부에 형성되면 더 이상 에폭시 수지의 기능을 상실하게 된다. 또한, 현재 응용되고 있는 에폭시 수지들은 자연분해가 불가능하여 환경오염과 관련된 문제점이 인식됨에 따라 에폭시 수지의 환경 친화적인 응용 방법과 에폭시 수지의 열분해 혹은 화학적 분해에 관한 연구가 요구되고 있다. 따라서 본 연구에서는 self-healing 효과를 가진 첨가제를 합성하여 이를 에폭시 접착제에 도입하여 self-healing 에폭시 접착제를 제조하고 그 특성을 확인하였다. Self-healing additive 는 Jeffamine 과 paraformaldehyde 를 이용하여 합성하였다. 에폭시 수지로는 bisphenol-A 계열의 불포화 결합을 수소화시킨 hydrogenated bisphenol-A 계인 ST-3000, 경화제로는 상온 경화가 가능한 아민계 경화제인 Isophorone-diamine(IPDA)과 Jeffamine 을 사용하고, Jeffamine 의 경우 0~50wt%, IPDA 의 경우 0~24wt% 의 self-healing additive 를 첨가하여 에폭시 접착제의 접착 성능을 확인하였다. 접착력은 인장강도를 이용하여 측정하였으며 본 시료의 인장강도와, 외력에 의해 분리시킨 후 다시 접착시킨 시료의 인장강도를 비교하여 self-healing 에폭시 접착제의 효과를 확인하였다. 본래 에폭시/D230 접착제가 갖는 5.67MPa 의 인장강도에 비해 15wt% self-healing additive 를 포함한

시료의 경우 0.28MPa 로 감소하는 것을 확인하였고, 에폭시/IPDA 접착제에서는 4.36MPa 의 인장강도에 비해 15wt% self-healing additive 를 포함한 시료의 강우 5.71MPa 로 인장강도가 유지되는 것을 확인하였다. 추가적으로 외력에 의해 분리되었다가 다시 접착된 접착제의 경우 에폭시/D230 에서는 다소 불규칙한 경향의 강도를 나타냈지만 0.1~0.71MPa, 에폭시/IPDA 에서 0.12~0.76MPa 의 인장강도를 갖는 것을 확인하였다. 결과적으로 모든 additive 농도에 대해서, 분리 된 이후의 접착 능력은 초기 접착 능력에 비해 감소하였다.

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Synthesis of some amide derivatives and polymerization by dehydration

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A series of amide derivatives were synthesized. The structure of these compounds were characterized by DIP-MS, EA, FT-IR and NMR. These compounds may be used as monomers for polymerization by dehydration of amide groups to triazine group.

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Characteristics of the imidazole-based antistatic coating applied to the optical material

김재영 노혜란*

서울과학기술대학교 안경광학과

계면활성제 형태의 저분자형 대전방지제는 각종 수지에 대한 상용성이 우수하고 가격이 저렴함은 물론 소량으로도 대전방지 효과가 우수한 장점이 있다. 본 연구에서는 양쪽성 계면활성제인 이미다졸을 이용하여 광학렌즈용 대전방지제를 제조하여 그 성능을 분석하였다. 코팅막의 내구성을 향상하기 위해서 아크릴레이트를 첨가하여 UV 광 경화를 하였다. 그 결과 습도가 30%인 환경에서 이미다졸을 포함하는 코팅을 한 후 정전기 수치가 11.8kV 에서 0.11kV 로 감소하였다. 또한, 먼지의 부착력이 감소함을 육안으로 확인할 수 있었다. 가시광선 투과도는 코팅이 없는 경우와 96%정도로 비슷하여 광학렌즈의 기능이 저하되지 않았고, 내마모성, 부착력, 내약품성, 내온수성은 양호하였다. 내구성은 2 주이상 지속되는 것으로 나타났다. 따라서, 이미다졸을 이용한 정전기방지코팅막을 광학 렌즈에 응용 가능함을 확인하였다. 이는 가시광선 투과도의 저하 없이 정전기 발생 방지가 가능하여 신체접촉이 많은 안경렌즈, 스마트폰, TV 등 다양한 광학렌즈에 적용될 수 있을 것으로 사료된다.

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Development of New Photovoltaic Conjugated Polymers Based on Di(1-benzothieno)[3,2-b:2’,3’-d]pyrrole: Benzene Ring Extension Strategy for Improving Open-circuit Voltage

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We have synthesized a series of novel di(1-benzothieno)[3,2-b:2’,3’-d]pyrrole (DBTP)-based conjugated polymers for organic photovoltaic devices. We first introduced DBTP moiety as an electron donating part in the conjugated polymer system to improve the open-circuit voltage (Voc) in photovoltaic properties. The DBTP backbone has a fused ring structure with extended benzene rings at the end of the 4H-dithieno[3,2-b:2',3'-d]pyrrole (DTP) moiety. The synthesized DBTP-based polymers effectively enhanced Voc compared to DTP-based polymers by decreasing the highest occupied molecular orbital (HOMO) energy levels of polymers without damaging other photovoltaic parameters. The alternation of DBTP and 3,6-dithien-2-yl-2,5-dialkylpyrrolo[3,4-c]pyrrole-1,4-dione (DTDPP) formed a promising donor polymer, PDBTP4, exhibiting an excellent molar absorption coefficient of 17,600 L?cm-1?mol-1 at the absorption maximum of 719 nm and a broad absorption covering 550 to 850 nm. PDBTP4:[6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) devices exhibited more than twice improved PCE of 6.80% with 0.28 V higher Voc than DTP-DTDPP polymer:PC71BM devices at the similar fabrication process. The benzene ring extension strategy is successfully working on the polymers containing strong electron donating DTP moiety. We believe that this approach can be used in other polymer systems showing poor Voc value.

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우루시올/카라기난 천연 고분자 전해질 막 제조

조경현 원종옥*

세종대학교 화학과

옻나무의 수액인 옻칠 (lacquer)은 무공해 천연 도료로 열과 산에 강하여 예로부터 긴 시간 보존이 필요한 기물에 많이 사용되어 왔다. 옻칠에 가장 많이 포함되어 있는 우루시올은 불포화 결합을 가진 알킬기 한 분자와 하이드록실기 두 분자가 치환된 벤젠고리의 구조로 옻칠에 함께 함유되어 있는 효소 라카아제 (lacase)의 작용으로 산화와 탈수를 동반한 가교 반응을 통하여 우루시올 고분자를 형성한다. 본 연구에서는 우루시올을 주 성분으로 하는 옻칠에 고분자 전해질을 도입하여 내구성과 치수 안정성이 좋은 이온 전도성 복합막을 제조하였다. 카라기난 (carrageenan)은 수용성 생분해성 고분자 전해질로 분자 내 설폰기를 가지고 있다. 세 종류의 kappa, iota, lamda 카라기난 중, 물에 녹아 단단한 겔을 형성하는 kappa 카라기난을 이온 전도성을 부여하기 위한 고분자 전해질로서 우루시올 복합막에 적용하였다. 옻칠과 카라기난 수용액을 1:0.01, 1:0.015, 1:0.02 의 비율로 블렌드하여 제조한 혼합액을 테플론 템플레이트에 캐스팅 하여 이온 교환기를 가진 천연 고분자 전해질 카라기난 (kappa-carrageenan)이 이온 전도성을 제공하고 우루시올 고분자가 지지체인 높은 내구성과 이온 전도성을 가지는 우루시올/카라기난 복합막을 제조하였다. 제조된 복합막의 내산성과 치수 안정성을 확인하고 electrochemical impedance spectroscopy 를 이용하여 복합막에 포함된 카라기난의 비율에 따른 이온 전도도의 변화를 분석하였다.

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Fabrication of Silica based Nanohybrids for Dental Composite Resin Restoratives

박은지 정일두*

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Silica nanoparticles are most often synthesized by the sol-gel process, in which alkoxysilanes are allowed to undergo hydrolysis and condensation reactions. Composite resins have been successfully used in dentistry as esthetic filling restoratives with their high mechanical strengths. However, lack of direct chemical adhesion to tooth and slow degradation made them not very useful without applying extra bonding agents. BisGMA based composite resin restoratives are known for their excellent esthetics, easy handling, improved mechanical strength, and wear resistance. In the present study, we use polymerizable silica nanoparticles with BisGMA in order to achieve a higher mechanical strength as well as durabilities.

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Single Crystalline TiO_2 Nanowires by Electrospinning

최유진 정광운[1,*]

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Single crystalline titanium dioxide (TiO_2) nanowires TiO_2 with anatase structure were fabricated by electrospinning poly(vinylpyrrolidone)/ethanol solutions mixed with hydrothermally synthesized titanium dioxide nanowires and titanium (Ⅳ) isopropoxide. 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 supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), Korea.

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Fabrication and characterization of porous, hollow, polymeric nanoparticles based on colloidal silica

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Interesting of polymer capsules are increasing in various fields, including synthetic chemistry, biotechnology, pharmaceutics, and diagnostics, catalysis. Currently, there is an increased focus on the synthesis and examination of nanoporous materials with nanostructures. Porous, hollow, and polymeric nanoparticles were prepared using colloidal silica(CS) as a template. These nanoparticles were prepared by initially coating silica with 3-methacryloxypropyltrimethoxysilane (MPS) and forming a shell by the polymerization of a mixture of styrene, methyl vinyl ketone (MVK) and divinylbenzene (DVB). After silica core was removed by etching with hydrofluoric acid, the resulting polymeric shell was then made porous by photodegrading poly(MVK) component in the nanoparticles with ultraviolet (UV) irradiation. The porous, polymeric shell was characterized by 13C NMR and FT-IR. The morphology and the size distribution was determined with FE-SEM, TEM, and DLS, respectively.

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Synthesis and Characterization of Thermoresponsive Polymeric Hollow Nanospheres

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During the last decade, polymer hollow microspheres have been interesting for their various applications, such as encapsulation for controlled release of drugs and enzymes, fillers, pigments, catalysts, and adsorption materials for sound. Currently, thermoresponsive polymer core-shell structures of nanometer dimensions have attracted great interest due to their potential applications. In this study, thermoresponsive polymeric hollow nanoparticles were synthesized from colloidal silica (CS) and poly(ethylene glycol) methyl ether-3-(triethoxysilyl)propyl isocyanate (PEGME-IPTES) as templates for hollow and a passage connecting the inside and outside of the hollow with NIPAAm. Colloidal silica was first synthesized using TEOS by sol-gel method. PEGME-IPTES was synthesized using a 3-(triethoxysilyl)propyl isocyanate (IPTES) with poly(ethylene glycol) methyl ether (PEGME) in the presence of dibutyltin dilaurate. The nanoparticles were prepared by initially coating silica with 3-methacryloxypropyltrimethoxysilane (MPS) and PEGME-IPTES, forming a shell by the polymerization of NIPAAm, then silica core and PEGME-IPTES were removed by etching with hydrofluoric acid. Thermoresponsive polymeric hollow nanoparticle was characterized by 1H NMR, 13C NMR, and FT-IR spectroscopies. The particle size of the colloidal silica was also confirmed by using DLS.

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Preparation of 4-arm PCL-b-PLA-b-PMVK Triblock Copolymer as Biodegradable Microparticles by RAFT Polymerization

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Biodegradable triblock copolymers based on 4-arm polycaprolactone (PCL) were synthesized by ring opening polymerization of PLA followed by RAFT polymerization of poly(methyl vinyl ketone)(PMVK). Microspheres based on 4-arm triblock copolymers were prepared by emulsion-evaporation method, and then photodegraded with UV irradiation to obtain porous microparticles. In order to polymerize by RAFT method, PCL-PLA based macro-CTA (chain transfer agent) was first synthesized by reacting carboxylic acid-terminated CTA with PCL-PLA, and used to synthesize triblock copolymer with methyl vinyl ketone (MVK). The morphology of the particles before and after UV irradiation were confirmed by SEM and TEM images and the release studies of paclitaxel, anti-cancer agent for female cancers from the particles were evaluated by HPLC. PCL-PLA based biodegradable microparticles will be anticipated to enhance drug release and could find potential application for biomaterials.

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Peculiar monotropic phase transition behaviors of a butterfly-shaped molecule

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A diphenylpyrimidine molecule (DPP-6C12) was synthesized by covalently attaching two tridodecyl benzoate tails (6C12) at the both sides of the diphenylpyrimidine (DPP) moiety. Peculiar phase transition behaviors of DPP-6C12 and their origins were investigated with the combined techniques of thermal, scattering, spectroscopic, and microscopic analyses. On the basis of the experimental results and analyses, it was realized that a butterfly-shaped DPP-6C12 formed three ordered phases: a plastic crystal phase (PK), a crystal phase (K), and a liquid crystal phase (Φ). This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), Korea.

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Synthesis of porous polymeric particles by γ-ray radiation

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Porous polymer particles have attracted great interests due to numerous applications in many areas of advanced materials science. This research introduces preparation of the porous polymeric particles by γ-ray radiation and solvent extraction. The sodium poly(styrene sulfonate) emulsions are formed in the hexadecane with surfactant. We chose the inverse emulsion polymerization format with surfactant to form water in oil (w/o) emulsions. So, polymeric particles have been fabricated by γ-ray induced crosslinking of polystyrene sulfonate and the pores are formed by MEK which extracts the water within the polymer particles because MEK is miscible in both organic solvents and water. The size and the morphology of the synthesized particles have been characterized by dynamic light scattering (DLS) and scanning electron microscope (SEM).

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poly(styrene-co-methacrylate) 아이오노머의 물 흡수 매커니즘

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이 연구에서는 PSMA 아이오노머의 물 흡수 매커니즘을 이해하기 위하여 아이오노머를 물에 적극적으로 노출해 파단면의 SEM 이미지와 물 흡수 거동을 분석했다. 이온기의 함량이 높을수록 초기흡수도와 최대흡수도는 커졌으며, 12.2 mol% 아이오노머에서는 초기흡수도가 양이온 종류의 영향을 받는 것으로 보였다. 양이온의 반지름이 커질수록 바륨 양이온의 아이오노머를 제외하고는 초기흡수도가 커졌다. 물이 시료에 흡수되었을 때 시료는 불투명하게 바뀌었는데 그것은 물분자가 고분자 매트릭스를 뚫고 들어갔다는 것을 의미하며 그 결과 고분자 매트릭스는 작은 밀도와 내부에 크랙을 갖게 된다. 아이오노머 고분자 사슬 사이의 간격이 넓어짐과 동시에 아이오노머 전체에 생기는 크랙은 물분자가 고분자 매트릭스 내에 존재할수 있는 충분한 공간을 제공하는 것으로 보인다.

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Octhyl Amine으로 중화된 폴리(스타이렌-co-스타이렌 술포네이트) 아이오노머의 온도 변화에 따른 상처 크기의 변화

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본 연구에서는 폴리스타이렌과 폴리(스타이렌-co-스타이렌 술포네이트) 공중합체에 octhyl amine(OA)로 중화하여 만든 아이오노머의 자가치유 효과에 대해 조사하였다.먼저 일반커터날이 장착된 350g 하중의 장치를 사용하여 시료 표면에 상처를 냈으며 상처의 크기는 시료의 종류와 상관없이 평균적으로 75-85 ㎛의 크기를 보였다.열처리 온도를 설정하기 위해 시차주사열량계를 사용하여 시료들의 Tg 를 구하였으며, 이를 바탕으로 실험 온도는 Tg, Tg±30℃, Tg+60℃의 네 구간으로 설정 하였다. 열처리 시간은 시료들의 Tg 도달 이후에 5 초, 10 초, 30 초, 1 분, 5 분, 10 분 간격으로 열처리를 하였다. 이 때 Tg 는 오븐 내부의 등온속도에 맞춰 측정된 시료의 Tg 이므로 각각의 설정된 온도범위에 따라 시료의 Tg 는 조금씩 차이가 났다. 열처리 후에 시료의 상처 크기 변화는 현미경으로 측정하였으며, 시료의 열처리 전후 인장강도를 통해 물성변화를 측정하였다.

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PAN/Pitch 혼합용액을 이용한 다공성 탄소 필름의 제조

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다공성 탄소 물질은 넓은 표면적, 전기 전도도 그리고 열 안정성 등의 우수한 특성을 가지기 때문에 전극, 필터, 화학 흡착제, 촉매 지지체 등으로 널리 사용되고 있다. 다공성 필름을 제조하기 위해서는 breath figure, 상 분리 현상 또는 혼합되지 않는 용매를 이용하는 방법 등이 있다. 본 연구에서는 N, N-dimethyl formamide (DMF)를 용매로 사용한 polyacrylonitrile (PAN)/Pitch 혼합 용액을 이용하여 스핀코팅 방법으로 다공성의 탄소 필름을 제조하였다. 이 고분자 필름은 탄화과정에서 PAN 과 Pitch 의 탄화수율 차이에 의해 다공성 구조가 발달하게 된다. 제조된 다공성 탄소 필름에서는 PAN 에 비해 Pitch 의 탄화수율이 낮기 때문에 필름 표면에 단차가 발생한다. 필름의 표면 구조는 PAN 과 Pitch 의 농도와 혼합 비율에 의해 결정된다. PAN 의 혼합 비율을 증가시킬수록 구멍의 크기와 수가 감소하고, Pitch 의 혼합 비율을 증가시킬수록 구멍의 크기와 수가 증가한다.

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Various Ways to Fabricate Porous Filaments for Fused Deposition Modeling

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3D printing technology has made it easy to produce highly customized products for personal use and sale. The Fused Deposition Modeling (FDM) technique has higher potential for product manufacturing using thermoplastic filaments like Acrylonitrile Butadiene Styrene (ABS), Polylactic acid (PLA). Many researchers are developing filaments with better mechanical properties or specific functions such as conductivity, flexibility. With the limited range of filaments commercially available, I fabricated porous filaments by various methods which can be applied in various purposes with large surface area like human bones, catalyst and so on.

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Polymers derived from PAMAM G4 dendrimer with amino acids for gene delivery

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In this study, we synthesized polymers that used PAMAM G4 dendrimer with amino acids and this polymers was applied to gene delivery. There are viral vector and non-viral vector for Gene delivery. We introduced non-viral vector which has low immune effects and cytotoxicity into gene delivery because Viral vector have high transfection and high immune problems, but Non-viral vector have low transfection efficiency. To overcome this problem, we conjugated PAMAM G4 dendrimer and amino acids. One of the many dendrimers is PAMAM dendrimer, this dendrimer was conjugated with Lys(K), Phe(F) and Arg(R) which have individual function. Lys(K) and Arg(R) are well known CPPs(Cell-penetrating peptides) and make complexes more stable, Phe(F) enhances cellular uptake efficiency. synthesized polymers was measured for size of complexes by DLS and confirmed that WST-1 assay and transfection efficiency using Hela cell line, Hep G2 cell line and HEK 293 cell line.

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Stabilized plasmid-lipid particles : introduction enzymatically cleavable oligo-peptide

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Plasmid DNA-cationic lipid complexes have a limiting transfection such as distribution by dnase and toxic side effect both in vitro and in vivo. In this research, we report the ‘stabilized plasmid-lipid particles’ (SPLP) using enzymatically cleavable oligo-peptide. Particle makes the detergent dialysis method and can be encapsulation plasmid DNA. Also, the SPLP composed of DOPE, the cationic lipid DOTAP and PEG5000-GLFG-K-C16. GFLG (Gly-Phe-Leu-Gly) sequence is known to be cleaved by enzyme Cathepsin-B and may promote endosomal escape after intracellular internalization. We purify the non-encapsulation DNA by DEAE-sepharose chromatography and measure size diameter by DLS. The encapsulation DNA is analyzed by lysis to TritionX-100 and Pico-Green assay. Furthermore, the transfection efficiency and cytotoxicity were determined by luciferase assay and MTT assay.

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3-Dimentional Network Structured Epoxy Polymer for Fixing Catalytic Carbonaceous Materials

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Carbonaceous materials present active catalytic propeties in electrochemical reaction. Carbon blacks, espacially, have many crystal edges and show more active catalytic property than highly structured carbon materials, such as graphites, graphenes, and carbon nanotubes. Carbon black powders cannot retain their shapes on a substrate; thus, they must be mixed with other binder materials, such as polymers or a TiO2 slurry containing organic surfactants and binders. We extended the approaches introduced in these works by examining three-dimensional network polymers formed by polymerized monomers that had been cross-linked in-situ with carbon black to robustly fix the carbon black powders onto a substrate. The 3D network polymers were composed of an epoxy monomer and a polyfunctional amine hardener. The chemically XL epoxy polymer provided strong mechanical properties, chemical resistance, thermal resistance, and adhesive properties. Here, we describe the development of novel stainless steel (SS) counter electrodes (CEs) coated with a composite of carbon black and 3D networked polymers to replace conventional CE, Pt-coated fluorine-doped tin oxide (FTO). We coated a conductive corrosion protective layer (CCPL) and a catalytic layer (CL) with a composite of CBs and 3D network polymers onto an SS substrate using spray pyrolysis. The weights of the CB material incorporated into the polymer matrices of the CCPL and CL were 6 and 86%, respectively. The CCPL formed a compact dense structure that prevented corrosion due to electrolyte penetration, whereas the CL formed a nanoporous structure that provided a large surface area for increased catalytic activity.

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Photovoltaic Properties of a New Quinoxaline-based Copolymer with thieno[3,2-b]thiophene as Side Chains for Organic Photovoltaic Cells

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For organic photovoltaic application, we designed and synthesized a new quinoxaline based conjugated polymer poly[(4,8-bis[(2-butyloctyl)oxy]-benzo[1,2-b:4,5-b’]dithiophene)- alt-(2,3-bis(5-octylthieno[3,2-b]thiophene-2-yl)-5,8-di(thiophen-2-yl)quinoxaline)] (PBDT- TTDTQx) by palladium-catalyzed Stille cross coupling reaction. To compare the effect of thieno[3,2-b]thiophene used as side chains with thienyl group on quinoxaline unit, poly[(4,8-bis[(2-butyloctyl)oxy]-benzo[1,2-b:4,5-b’]dithiophene)-alt-(2,3-bis(5-octylthiophene-2-yl)-5,8-di(thiophen-2-yl)quinoxaline)] (PBDT-TDTQx) was also synthesized to compare the optical, electrochemical, morphological, and photovoltaic properties of the polymers. Bulk heterojunction photovoltaic devices are fabricated using the polymers as p-type donors and [6,6]-phenyl C71-butyric acid methyl ester (PC71BM) as the n-type acceptor. The power conversion efficiencies of the devices fabricated using PBDT-TTDTQx and PBDT-TDTQx are 3.42 and 2.26%, respectively. The difference in efficiency is attributed to the broad UV?visible absorption and high crystallinity of PBDT-TTDTQx. The replacement of the alkylthienyl moiety with thieno[3,2-b]thiophene on quinoxaline can yield broad UV-visible absorption due to extended π-conjugation, and enhanced molecular ordering and orientation for organic photovoltaic cells.

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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

New Green Phosphorescent Iridium(III) Complex for Solution-Processed Organic Light-Emitting Diodes

장재호 황도훈* 김희운 이재민[1]

부산대학교 화학과 [1]한국화학연구원 소자재료연구센터

We designed and synthesized a green phosphorescent iridium(III) complex, bis(1,2-dimethyl-4,5-diphenyl-1H-imidazole)iridium(III)(2-(3-(trifluoromethyl)-1H-1,2,4-triazol-5-yl)pyridine) [$(DMDPI)_2$ Ir(tftap)], for solution-processed organic light-emitting diodes (OLEDs). Photoluminescence (PL) spectra of $(DMDPI)_2$ Ir(tftap) showed maximum emission peak (λmax) of 532 nm in dichloromethane solution. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels of $(DMDPI)_2$ Ir(tftap) were measured to be -5.36 and -2.76 eV, respectively. The solution-processed green OLEDs based on $(DMDPI)_2$ Ir(tftap) with the structure of ITO/PEDOT:PSS (30 nm)/26DCzPPy:$(DMDPI)_2$ Ir(tftap) (11%) (40 nm)/TPBi (60 nm)/CsF (1 nm)/Al structure was fabricated. Electroluminescent (EL) spectra of $(DMDPI)_2$ Ir(tftap) exhibited maximum emission peak at 522 nm with a broad full width at half maximum (FWHM) of 115 nm and CIE coordinates of (0.33, 0.54) at 1,000 cd/m^2. The device with 11% doping concentration of $(DMDPI)_2$ Ir(tftap) exhibited maximum luminance of 6,304 cd/m^2, maximum luminous efficiency of 7.14 cd/A, power efficiency of 3.63 lm/W, and external quantum efficiency of 2.59%, respectively. Moreover, white light-emitting devices containing double emissive layer consisting of [$(DMDPI)_2$ Ir(tftap)] as a green dopant and [$(PIQ)_2$ Ir(acac)] as a red dopant were fabricated. The white devices exhibited Commission Internationale de L'Eclairage (CIE) coordinates of (0.42, 0.48) at 1,000 cd/m^2; these values are close to the standard white warm light CIE coordinates of (0.44, 0.40).

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Self-polishing properties of two type of zinc-based copolymers for anti-biofouling applications

김선미 박 현[1] 황도훈*

부산대학교 화학과 [1]부산대학교 첨단조선공학연구센터

Self-polishing copolymers (SPC) containing two different Zn acrylate monomers were synthesized for marine anti-biofouling applications. Zinc methacrylate (ZnMA) is a well-known component of anti-biofouling coatings. In this study, we synthesized zinc 3-(allyloxy)propanoate (ZnAA) as a new SPC to be incorporated with other monomer units like a methyl methacrylate, 2-hydroxyethyl methacrylate, and ethyl acrylate in the desired copolymers. The properties of the new SPC were compared with those of the corresponding polymers containing ZnMA. The SPC containing the new zinc monomers were characterized by proton nuclear magnetic spectroscopy (^{1}H-NMR), gel permeation chromatography (GPC), energy dispersive spectroscopy (EDS), and scanning electron microscopy (SEM). The polishing rate was determined by measuring the film thickness after dynamic immersion tests. The experimental results suggest that new ZnAA-SPCs have the potential to be good candidates for anti-biofouling coatings that can replace ZnMA-SPCs.

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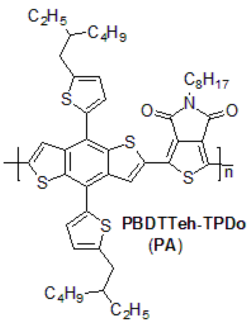
발표종류: 포스터, 발표일시: 금 13:00~14:30

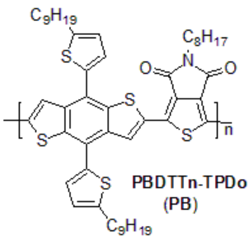
Synthesis and correlation between structure and photovoltaic performance of BDT-TPD conjugated copolymers

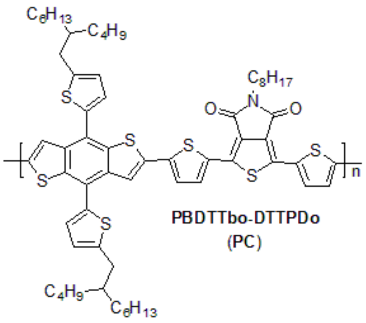
정규관

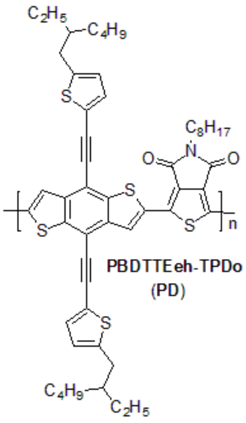
전북대학교 과학교육학부

Four BDT-TPD polymers (PA~PD) were synthesized by modifying alkylthienyl chains on BDT, placing space group between BDT and TPD, and installing extended conjugated side chains on BDT of the polymer in order to investigate the correlation of structure and photovoltaic performance for these polymers. The HOMO levels of the polymers were -5.72, -5.63, -5.48, and -5.61 eV for PA, PB, PC, and PD respectively, indicating very low-lying HOMO energy levels. Bandgaps of these polymers were calculated as in the range of 1.85?1.88 eV. Theoretical calculations clearly show that torsional angles between alkylthienyl group and BDT unit of the simplified dimer correlate with π-orbital delocalization, suggesting that the HOMO π-electrons of vertically aligned conjugated side chains do not well delocalized in the polymers bearing high torsional angles such as PA, PB, and PC. The optimized weight ratios of the polymer to PC61BM were determine to be 1:1 for PA, 1:1.5 for PC, and 1:1 for PD and the average PCEs of the devices were 5.36% for PA, 4.62% for PC, and 2.74% for PD respectively after optimization with DIO.


PBDTTeh-TPDo
(PA)


PBDTTn-TPDo
(PB)


PBDTTbo-DTTPDo
(PC)


PBDTTEeh-TPDo
(PD)

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Conversion from Low-Quality Graphite to High-Quality Graphene Nanoplatelets through Ball-Milling

<u>신선희</u> 전인엽[1] 백종범[*]

울산과학기술대학교(UNIST) 에너지공학부 [1]울산과학기술대학교(UNIST) 에너지 및 화학공학부

Low-quality graphite (L-Graphite) is converted directly and efficiently into high-quality iodinated graphene nanoplatelets (HIGnP) through simple ball-milling method. The resultant HIGnP shows distinguished characteristic such as large specific surface area (969 m2/g), low metal impurity (3.2 wt.%), high iodine content (3.28 at.%), high crystallinity and remarkable electrocatalytic activity with higher selectivity, longer-term stability and better tolerance to methanol crossover/CO poisoning effects.

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UV Curable Materials and Application for 3D Printer

전윤태

애경화학 연구4팀

UV 광경화 메커니즘을 이용한 DLP 3D Printer 에 적용가능한 고기능성 Acryl monomer 를 합성하고, 이를 이용한 UV Curable Solution 을 제작하여 그 성능을 확인하였다.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Photo-responsive helical nanostructure with conductive triphenylamine core

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Evolution of supramolecular chirality from self-assembly of achiral compounds and control over its handedness is closely related to the evolution of life and development of supramolecular materials with desired handedness. Here we report a system where the entire process of induction, control, and locking of supramolecular chirality can be manipulated by light. Combination of triphenylamine and diacetylene moieties in the molecular structure allowed photo-induced self-assembly of the molecule into helical aggregates in a chlorinated solvent by visible light, and covalent fixation of the aggregate via photopolymerization by UV. By utilizing circularly polarized light (CPL), we observed that supramolecular chirality of the resulting helical aggregates was selectively and reversibly controlled by the rotational direction of visible CPL, and the desired supramolecular chirality could be arrested by irradiation of circular polarized ultraviolet light. This methodology opens a route to formation of supramolecular chiral conducting nanostructures from self-assembly of achiral molecules.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Property of Temperature-Responsive Diblock Copolymers having P3HT

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한국과학기술원(KAIST) 화학과 [1]국방과학연구소 제5기술연구본부

Poly(3-hexylthiophene) (P3HT) is one of the conducting polymers having good electrical properties. Self-assembly of P3HT has been studied intensively because electrical properties of the P3HT were sensitive to their nanostructure. 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. Hydrophilic polymers containing oligo(ethylene glycol) methyl ether methacrylate (OEGMA) and 2-(2-methoxyethoxy)ethyl methacrylate (MEO2MA) are well known temperature responsive polymer showing good solubility, and lower critical solution temperature (LCST) in water. In this study, amphiphilic diblock copolymers having P3HT were synthesized. Details on synthetic method and temperature-responsive properties of the amphiphilic diblock copolymers in solution will be presented.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Removal of rare metal element from sulfuric acid solution using a natural based adsorbents

윤해성 이정윤 김연우 이기훈*

서울대학교 바이오시스템소재학부

Rare metals (RMs) are included in the waste of various industries such as mining, refining and semiconductor etc. Because of economical attractions, many researchers focused on the recovery of these RMs from the wastewater. Adsorption using natural based adsorbents is suitable method for the recovery of RMs due to low cost, high efficiency and eco-friendly. Especially in the mining and refining industries, a plenty of sulfuric acid are used and RMs are included in the waste solution. Thus we prepared natural based biosorbents having acidic hydrolysis resistance for applying to the mining and refining waste solution. This study focused on the separations RMs from sulfuric acid solutions and optimization of adsorption experimental conditions.

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Preparation of Polyethylenimine(PEI) modified silk sericin beads as effective hexavalent chromium removal biosorbent

곽효원 주지은 신문주 이기훈*

서울대학교 바이오시스템소재학부

Silk sericin can be used as a low cost adsorbent for organic pollutants and heavy metal removal from water. However, the adsorption capacities of the raw sericin for heavy metals are not very high since the contents of the surface functional groups are insufficient for heavy metal removal. Polyethylenimine (PEI) exhibits strong adsorption ability for heavy metals because of its large number of primary and secondary amine groups. In the present study, A chemically modified silk sericin beads was prepared using polyethylenimine (PEI) as a modification reagent for heavy metal removal. The sericin beads before and after modification were characterized by Fourier transformed infrared spectroscopy, X-ray photoelectron spectroscopy etc. The adsorption capacity of Cr(VI) by the modified sericin beads was investigated with various solution pH and temperature condition. From the results, the Cr (VI) removal capacity of PEI modified sericin beads was 365.38 (mg/g) which was much higher than that of pristine sericin beads (34.56 mg/g). The results herein revealed that the PEI modified sericin beads has high potential as a material for sorption and detoxification of Cr(VI) from aqueous solution.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Inelastic and Quasi Elastic Neutron Scattering Study of Pluronic P85 in aqueous solution

소지용* **Kenji Nakajima**[1]

한국원자력연구원 중성자과학부 [1]*Material Life Science Facility, J-PARC*

Quasi-elastic and inelastic neutron scattering is a unique experimental tool for investigating the dynamics of materials. Especially, the cold neutron time of flight spectrometer can measure wide dynamic range from 100 meV to some tens ueV. This dynamic range is suitable for the research about the dynamics of molecules and polymer. We have measured the aqueous triblock copolymer, Pluronic P85 with additive 5mS in some temperatures using AMATERAS spectrometer in J-PARC (Japan Proton Accelerator Research Complex). Pluronic P85 is a self-assembled unilamella polymeric vesicles and forms a spherical single bilayer structure with a hydrophobic interlayer and a hydrophilic surface. We can expect the dynamics of it can be changed with temperature especially elevation and it will be important for the understanding of its physical and mechanical properties. In this presentation, We compare the dynamics of Pluronic P85 in various temperature. Also, we discuss the physical properties of them comparing with another experimental results, especially SANS.

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발표분야: 공업화학

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발포제 잔사물질의 성분분석을 통한 정밀화학 중간체의 분리 정제 및 물성평가

박수열* 김헌수 이규진[1] 이병민[2]

한국화학연구원 계면재료공정연구그룹 [1]과학기술연합대학원대학교(UST) 한국화학연구원 [2]한국화학연구원 계면화학공정연구센터

본 연구의 목적은 발포제인 ADC(Azodicarbonamide)의 사용 후 대규모로 발생되는 발포 잔사물질을 재활용하여 시아누익 산 또는 시아누익 클로라이드 등의 정밀화학 원료를 수율 개선, 정제법 최적화 및 규모성장을 통하여 상용화하는데 있다. 또한 이들 부산물에서 얻은 화합물의 물성평가를 통하여 다양한 정밀화학 제품(반응성 염료 및 도료, 형광증백제 중간체, 산화방지제, 고분자 첨가제 등)의 중간체로서 활용하는 응용기술을 개발하고자 한다.

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발표코드: **IND.P-81**
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발표종류: 포스터, 발표일시: 금 13:00~14:30

DPP 안료의 표면 개질화 및 시간에 따른 색상 변색에 관한 연구

김헌수 김승회[1] 박수열*

한국화학연구원 계면재료공정연구그룹 [1]단국대학교 화학과

지시 (Indicator) 색소로 사용되는 DPP(Diketo-Pyrrolo-Pyrrol)안료는 다른 색소와 비교하여 내구성, 내열성 등이 우수하여 주로 LCD 칼라필터, 자동차 착색제등의 고급 안료로 사용되고 있다. 그러나 DPP 안료는 염료와 달리 물이나 유기용매에 대한 낮은 용해도를 가지는 단점이 있다. 이들 안료의 근본적 단점을 개선하여 높은 내구성 (열안정성 및 내광성)과 더불어 용해성이 우수한 DPP 안료를 개발 하는 것이 요구 된다. 본 연구에서는 안료의 근본적 단점인 용해성을 개선하여, 기존의 높은 내구성 (열안정성 및 내광성)을 가진 DPP 계 안료를 표면 개질을 통하여 안료형 염료를 개발하고, 이들을 시간에 따른 변색 지시 (Indicator) 색소용 적색 색소로 사용하고자 한다.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

The synthesis of the MHB which is precursor of the AMCA by using industrial waste

정헌주 김종천 김석찬* 유연규[1]

국민대학교 화학과 [1]국민대학교 생명나노화학과

Methyl-4-formylbenzoate(MFB) is a by-product of Dimethyl terephthalate(DMT) produced from oxidation process of P-xylene.. Currently, MFB is no place to apply so that MFB is treated like a industrial waste. Many companies produce DMT are dealing with MFB and MFB is collected and incinerated by the service companies. This kind of incineration has some problems partly it generates severe nasty smell and lots of CO2, and partly it costs a lot. Eventually it leads to environmental pollution. However, when we can get high-purity MFB, we can use it as a precursor of pharmaceuticals, cosmetics, and polymer additives. If we can use MFB, we will use as a high-value green resource from yearly increased industrial waste of the PET usage

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Synthesis and Purification of Aliphatic Isocyanate Applicable to Polyurethane

김종천 정헌주 최근우 박규순 김석찬*

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Xylene diisocyanate(XDI), aliphatic diisocyanate with an aromatic nucleus, give some unique properties. The polyurethanes are widely used for high performance adhesives for flexible packaging, plastic lenses with high refractive indes, outdoor sealant, artificial leathers, coatings, paints, and polyurethane elastromer. XDI synthesized by organic amine with carbonyl dichloride

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Characteristic evaluation of metallocene catalyst for polymerization of polyethylene wax

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In this study, we studied characterization of catalyst that is used for polymerization of polyethylene wax. We compared this catalyst to Ziegler-Natta which is widely used for polymerization of polyethylene. We evaluate hydrogen reactivity and study on charactistics of effected metallocene catalyst in polymerization. We also check hydrogen used for chain transfer agent, molecular weight change and distribution by different ratios of ethylene gas. Finally we suggest proper structure of metallocene catalyst for polymerization of polyethylene wax.

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Silicon-based ETMs(electron-transport materials) with high thermal stability and triplet energy for efficient phosphorescent OLEDs

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A series of electron transporting materials was designed and used in organic light-emitting diodes (OLEDs), exhibiting green phosphorescence. We used the tetrahedral structural motif of silicon atom, which annulated with the 1,2-diphenyl-benzoimidazole (DBI) units in its periphery (1-4) and their thermal, photophysical, and electrochemical properties were investigated. Photophysical and electrochemical properties showed that their LUMO levels can be slightly tuned with an increasing number of DBI units. Furthermore, thermal stability correlated well with an increase in the number of DBI units, showing a gradual increase in Tg values in the range of 100-141°C. The electron-only devices (EOD) based on compounds 2 and 3 were fabricated; EOD device with compound 3 showed higher current densities at the same voltages, indicating higher electron transport (ET) capability compared to compound 2. The electron mobilities of compounds 2 and 3 were estimated as 1.93×10^{-5} cm^2/Vs and 3.67×10^{-5} cm^2/Vs at 1 MV/cm, respectively. We further investigated the excellent ET property of compound 3 via the phosphorescent OLEDs in which the electron-transporting material was coupled with the green emitter, Ir(ppy)3 (Device I). Finally, we compared it with the device based on compound 2 (Device II). The OLED device with compound 3 exhibited maximum current and external quantum efficiencies of 62.8 cd/A and 18.0 %, respectively, with a small efficiency roll-off at high current densities. The devices I and II were fabricated with a structure of ITO (150 nm)/HATCN (10 nm)/TAPC (90 nm)/CBP:Ir(ppy)3 8% (20 nm)/2 or 3 (60 nm)/Liq (1 nm)/Al (150 nm)

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A Combined Computational and Experimental Study of Blue Emitting square-planar Platinum Complexes to develop an efficient, long-lasting blue PHOLED emitter

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Cyclometalated platinum complexes have been the focus of considerable research, driven in large part by their potential use as sensitizers, photocatalysts, and chemosensors. Platinum complexes have also attracted strong interest as luminescent materials for use in organic light emitting diode (OLED) based display and lighting applications due to their ability to harvest both electro-generated singlet and triplet excitons, resulting in a theoretical 100% electron-to-photon conversion efficiency. Despite the dominance of iridium at present, platinum remains an exciting field of study. If the intrinsic electroluminescent properties of phosphorescent platinum complexes can be unmasked and optimized, these complexes can provide a viable alternative to existing iridium emitters and spur further growth in this emerging field. Planar platinum complexes possess excellent structural flexibility, with the ability to employ various cyclometalating ligands. New platinum complexes were synthesized and characterized. These Platinum complexes are highly luminescent, emitting blue to green light in solution. Finally, developed Pt-complexes were tested as dopants in prototype phosphorescent organic light-emitting diode devices and found to show deep blue electroluminescence with high emission efficiency and color purity.

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Study of Ion-Paired Iridium Complexes (Soft Salts) and Hydrogen Evolution via Visible Light-Driven Photoelectrolysis from Neutral Water

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Iridium 을 기반으로 한 cation 과 anion 을 접합시킨 상태의 Ion-paired Ir complexes(soft salts)를 이용하여 새로운 형태의 광촉매 시스템을 구현하는 것에 초점을 맞추었다. 이에 본 연구에서는 cation 은 광촉매로, anion 은 light harvesting 물질로 사용하였다. 세부적으로 동일한 cationic 광촉매에 흡수 영역대가 서로 다른 anionic light harvester 들이 치환 됨에 따라 광물리적 그리고 전기화학적 특성이 크게 변화되는 것이 관측되었으며 cation 의 방출 영역대와 anion 의 흡수 영역대의 겹침정도에 따라 다른 분자 내 에너지 전달 효율이 관찰되었다.

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Intriguing emission properties of *para*- and *meta*-diphenylamine-π-carborane systems

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This investigation has uncovered the origins of different types of emissions in D-π-A systems with a diphenylamino moiety as the donor and *ortho*-carborane as the acceptor. The *para*- and *meta*-substituted D-π-A systems showed three kinds of emission originated from the local excited (LE) state, a twisted intramolecular charge transfer (TICT) state and an aggregation induced emission (AIE). The TICT emission showed strong solvent-polarity dependency, which is attributed to the dipole moment changes in excited TICT state. The strong AIE emission is observed in extremely nonpolar solvent such as *n*-hexane, because the association between solutes caused by low-solubility. Contrast to these, the steric hindrance between donors in *para*-substituted of D-π-A-π-D system prohibited the formation of TICT state, hence the LE and AIE emissions were observed dominantly.

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Designing Bimetallic Complexes for Efficient Light-Driven Redox Catalysis: How to Assign Specific Functions to Each Metal in a Bimetallic Ir(III)-Pt(II) Complex

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The electronic communication between two metal-centers in a bimetallic complex is studied using experimental and computational techniques. Using 2,3-bis(2-pyridyl)pyrazine as a linker, the light-absorbing Ir-chromophore fragment [(2-(4’,6’-difluorophenyl)pyridinato-N,C2)2Ir]+ is coupled to a PtCl2 unit that serves as a model for a redox-active catalyst not absorbing light. The modular design of bimetallic catalysts, in which a chromophore complex and a redox-active metal center can be combined to engineer a photocatalytic system is an attractive general strategy: The chromophore is envisioned to harvest light energy utilizing a metal to ligand charge transfer (MLCT) absorptions, placing activated electrons onto the bridging linker moiety. These electrons must be transferred to the other metal center to be used as reducing equivalents during redox catalysis. Our studies suggest that the bimetallic system does not perform properly as envisioned ? instead of remaining spectroscopically silent, the Pt(II)-center develops enhanced absorption features and the envisioned flow of electrons from the photosensitizer to the redox-center does not take place. Our computational analysis of the electronic structures of each modular fragments and the fully assembled bimetallic complex revealed some simple principles of control: For the Ir-chromophore to remain the main photoactive component in the bimetallic assembly, the Pt-based frontier orbitals must not become one of the highest lying occupied orbitals, as the small energy difference to the ligand-based unoccupied orbitals will give rise to new enhanced absorptions, as was the case in the [Ir]-PtCl2 system. To test this new insight, a new bimetallic complex, [Ir]-Pt(CN)2, was prepared. The much stronger ligand field of the cyanide ligand lowered the Pt-based orbitals, effectively switching off any Pt-based photoactivity and restoring the intended electron flow within the bimetallic assembly. TDDFT calculations are used to quantify the absorptions, but the main qualitative insight is derived from standard MO-diagrams that are intuitively understandable. The workflow showcased here, which integrates computational and experimental techniques, is a general procedural template for rationally designing modular multicomponent catalysts.

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Photocatalytic system (Dye/TiO_2/ReC) using Ni-Cyclam derivatives as a reduction catalyst (ReC) for CO_2 reduction

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화석연료의 사용량 증가로 인한 CO_2 발생량의 폭발적인 증가로 인하여 지구온난화와 기후변화로 기인된 자연폐해가 가속화 됨에 따라 전세계적으로 CO_2 저감 및 활용을 위한 연구개발에 많은 투자가 이루어지고 있는 상황이다. 많은 관련 기술 중 가시광을 이용 CO_2 환원반응의 유도를 위한 방법으로 태양 빛을 이용한 청정공정연구가 각광받고 있는 상황이며 이에 본 연구에서는 TiO_2 에 유기염료인 MOD 와 Ni-Cyclam 유도체를 접합시킨 새로운 Triad-hybrid 구조(Dye/TiO_2/ReC)를 통하여 효율적인 공정시스템을 구현하고자 하였다. 우선적으로 물 속에서 환원촉매로써 효과적인 Ni-Cyclam 을 TiO_2 에 anchoring 하기 위한 방법으로서 ?PO_3H_2 그룹이 치환된 화합물이 고안되었으며 합성 간 NMR, ESI Mass 분석과 X-ray 를 통해 Ni-cyclam 유도체의 합성여부가 확인되었고, 또한 Cyclic voltammetry 측정을 통하여 CO_2 환원에 대한 전기화학적 거동이 확인되었으며 광화학반응을 통한 CO_2 에서 CO 로의 전환효율이 측정 비교되었다.

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High performance of Hydrophilic Organic dyes in photocatalytic CO_2 reduction catalytic system based on Dye/TiO_2/Re(I) Organic-Inorganic Ternary Systems

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이전 연구에서 가시광을 이용하여 CO_2 환원을 시키기 위해 TiO_2 반도체에 흡광체로 유기염료(DMOM)와 CO_2 환원촉매로 Re(I) complex 를 접합시킨 triad 구조가 제시되었다. 가시광 영역인 ≥420 nm 빛을 조사하였을 때, 유기염료가 광자를 흡수하여 들뜬 전자들은 TiO_2 의 conduction band 로 이동되고 그 전자들은 최종적으로 Re(I) complex 위치로 이동하여 CO_2 가 CO 로 환원되는 촉매 메커니즘을 가진다. 또한 전자를 건네 준 염료는 SDN 에 의해 전자를 제공받아 재생되는 catalytic cycle 을 가진다. 본 연구에서는 이전에 보고된 유기염료(DMOM)를 기반으로 Hydrophilic 한 그룹을 치환시키는 것을 통하여 앞서 제시한 triad 시스템을 최적화하는 것에 초점을 맞추었다. Hydrophilic group 이 치환된 OD-NO (R_1 = morpholine-CH_2)와 OD-NN (R_1 = 4-methylpiperazine-CH_2) 염료들이 성공적으로 준비되었으며 좀더 넓은 가시광선영역의 빛을 흡수하기 위한 방법으로 ethylene 그룹이 첨가하여 확장된 conjugation 을 가지는 염료들이 또한 준비되었다. 광반응장치를 통하여 신규 염료들이 흡착된 광촉매시스템의 전환효율이 평가 및 비교되었으며 정확한 메커니즘 분석을 위한 광물리적 그리고 전기화학적 특성이 분석되었다.

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Design of new carborane having thiophene moieties for highly efficient dye-sensitized solar cells

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Oligothiophene functionalities show good electron-donor (ED) character, and they have been utilized as p-type materials for organic electronic materials. Soon, they became essential ingredients in hetero-junction organic solar cells matching properly with C60 based n-type materials such as phenyl-C61-butyric acid methyl ester (PCBM). Since then, electronic alteration in oligothiophenes thus allowing optimum energy levels as EDs for maximum efficiency has become a major hurdle. One approach to the alteration of oligothiophene energy levels involves the incorporation of electron-withdrawing (EW) units such as dicyano-vinyl group at either one or both ends of the oligothiophene to achieve the desired charge separation. Electronic perturbation can therefore facilitate the resulting electronic property adjustment in oligothiophenes.

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Electrocatalytic CO_2 Reduction by Using Cationic Pentamethylcyclopentadienyl-Group 9 Metal Complexes with Symmetrically Substituted Bipyridine Ligands

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Pentamethylcyclopentadienyl-Group 9 Metal Complexes 는 Favourable thermal stability and water solubility, excellent catalytic activity 등의 장점으로 인하여 다양한 화학변환촉매분야에서 활용되었다. 또한 최근에는 Homogeneous Electrocatalytic CO_2 reduction 분야에서도 촉매로 쓰여 우수한 특성을 나타내었다. 하지만 과거 연구사례들의 경우, Photo-induced hydride transfer 능력이 큰 Catalytic intermediate 효과에 대한 고려 없이 진행되었기 때문에 정확한 메커니즘 분석이 확인되지 못하였고, Ligand 의 치환기효과에 대한 연구가 제대로 진행되지 않았다. 이에 본 연구에서는 빛이 없는 조건 하에서 Homogeneous Electrochemical CO_2 reduction 실험을 진행하여 Pentamethylcyclopentadienyl-Group 9 Metal Complexes 촉매의 메커니즘을 연구하였으며 세부적으로 Ligand 의 electronic density 및 3 종의 Group 9 Metal(Ir, Rh, Co) 조절을 통하여 변화효율과 생성물인 H_2와 Formic acid 의 상대적인 비율을 분석하여 비교하였다.

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Studies on the Photochemical Properties of the Iridium Compound Is Replaced with Various *o*-carborane Ligand

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In the last decade, phosphorescent iridium(III) complexes have been widely used in organic light-emitting diodes (OLED) owing to their stable chemical structure, high luminescent efficiency, and tunable excitation and emission wavelength over the whole visible range. However, few carborane-based phosphorescent iridium(III) complexes have been reported. It is anticipated that introduction of carborane cages into phosphorescent iridium(III) complexes may further improve the photophysical properties of these complexes and allow better understanding the roles of carborane groups. In this communication, we synthesized iridium(III) complexes containing *o*-carborane in the various cyclometalated C^N ligand . The tuning of phosphorescence color has usually been achieved by the variation of the substituent on the C^N ligand. The variation in the excited state energy has usually been made by changing the electronic structure of the C^N ligand, which affects the energy levels of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). In this regard, we have recently reported that the introduction of *o*-carborane (1,2-closo-$C_2B_{10}H_{12}$) to the 4- or 5- position of the phenyl ring of a ppy ligand in $(C^\wedge N)_2Ir(acac)$, $(C^\wedge N)_2Ir(pic)$ and $(C^\wedge N)_3Ir$ complexes gives rise to red and blue shifts of the phosphorescence band, respectively, when compared to the emission wavelength of $(tphpy)_2Ir(acac)$, $(tphpy)_2Ir(pic)$ and $Ir(tphpy)_3$.

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Highly Robust Hybrid Photocatalyst for Carbon Dioxide Reduction: Tuning and Optimization of Catalytic Activities of Dye/TiO_2/Re(I) Organic-Inorganic Ternary Systems

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Herein we report a detailed investigation of a highly robust hybrid system (sensitizer/TiO_2/catalyst) for the visible-light reduction of CO_2 to CO; the system comprises 5’-(4-[bis(4-methoxymethylphenyl)amino]phenyl-2,2’-dithiophen-5-yl)cyanoacrylic acid as the sensitizer and (4,4’-bis(methylphosphonic acid)-2,2’-bipyridine)ReI$(CO)_3$Cl as the catalyst, both of which have been anchored on three different types of TiO_2 particles, [001]-facet exposed nanosheets (S-TiO_2) and two commercially available particulate materials (Hombikat and Degussa). The selective reduction of CO_2 to CO was persistently catalyzed by visible-light irradiation of dispersions of the hybrid particles in N,N-dimethylformamide (DMF) at > 420 nm. The reduction efficiencies depended on the TiO_2 sources, indicating that the catalytic activity of the hybrid system is significantly affected by the morphology, size, and agglomeration degree of the TiO_2 particles. It was found that remarkable enhancements in the CO_2 conversion activity of the hybrid photocatalytic system can be achieved by addition of water or such other additives as Li^+, Na^+, and TEOA. For a specific example studied, the photocatalytic CO_2 reduction efficiency was enhanced by approximately 300% upon addition of 3% (v/v) H_2O. To the best of our knowledge, the observed turnover number of CO formation (≥ 360), which was obtained from a single-run photoreaction, is the highest reported for heterogeneous catalytic systems. A series of Mott-Schottky (MS) analyses on nanoparticle TiO_2 films demonstrated that the flat-band potential (V_{fb}) of TiO_2 in dry DMF is substantially negative but positively shifts to considerable degrees in the presence of water or Li^+, indicating that the enhancement effects of the additives on the catalytic activity should mainly arise from optimal alignment of the TiO_2 V_{fb} with respect to the excited-state oxidation potential of the sensitizer and the reduction potential of the catalyst in our ternary system. The present results confirm that the TiO_2

semiconductor in our heterogeneous hybrid system is an essential component that can effectively work as an electron reservoir and as an electron transporting mediator to play essential roles in the persistent photocatalysis activity of the hybrid system in the selective reduction of CO_2 to CO.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Temperature factor : Indication of a disordered structure. An example in alum $KAl(SO_4)_2 \cdot 12H_2O$

오인환[*] 박가람[1]

한국원자력연구소 중성자과학연구부 [1]고려대학교 화학과

Disorder in the crystal structure could be classified into two groups, i) positional disorder and ii) orientational disorder. This disorder may be divided further in i) static and ii) dynamic. Because generally it is difficult to distinguish between dynamic and static disorder using a diffraction method, these two disorders will be ruled out in this study. No atoms in the crystal structure sit in fixed positions and as a result, their motions are described with atomic displacement factor or temperature factor U in the crystal structure analysis. This thermal factor strongly depends on the measured temperature. Heavy atoms in the inorganic condensed matter show the atomic displacement factor between 0.005 and 0.02. The typical values of organic molecular solid lie between 0.02 and 0.06. Loosely bounded terminal atoms may have 0.1 ~ 0.2. If the one of the principal axes of the displacement ellipsoid exceeds 0.2 or 0.3, then this is indicative of the disordered character in the crystal structure. In this presentation, we will present a single-crystal X-ray structure investigation on the well-known α-alum ($KAl(SO_4)_2 \cdot 12H_2O$, Space group : Pa-3, cubic, a=12.172(4)) and how we should treat the data and refine the crystal structure.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

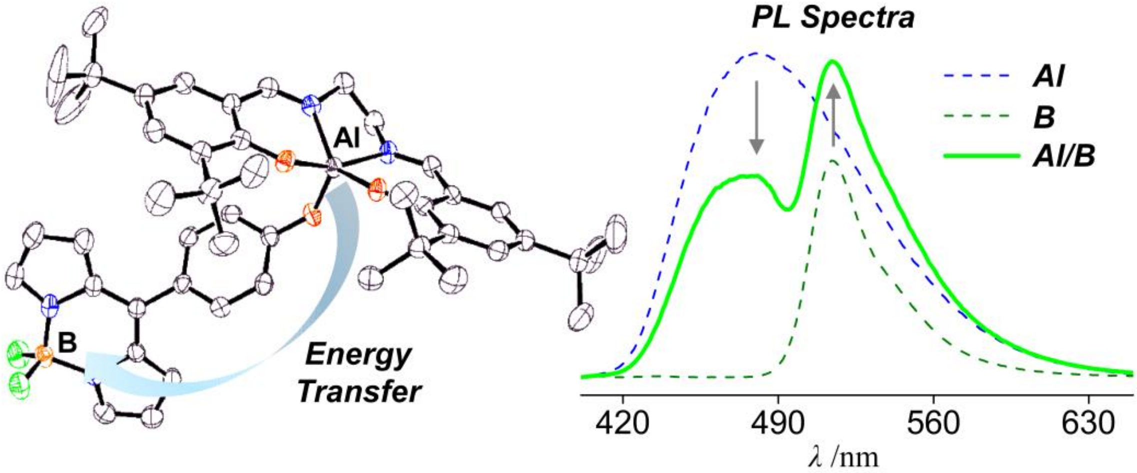
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-2**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoinduced Energy Transfer in BODIPY-containing Aluminum Complexes

손창호 최병훈 이지혜[1] 황현석 박명환[2,*] 이강문[*]

강원대학교 화학과 [1]서울대학교 자연과학대학 화학부 [2]충북대학교 화학교육과

Three aluminum- and borane-centered heterodinuclear complexes, [{salen(3,5-tert-butyl)$_2$}Al-(OC$_6$H$_4$-bodipy)] (10), [{salen(3,5-tert-butyl)$_2$}Al-(OC$_6$F$_2$H$_2$-bodipy)] (11), and [(mq)$_2$Al-(OC$_6$H$_4$-bodipy)] (12) (salen = N,N′-bis(salicylidene)ethylenediamine, BODIPY = 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene, and mq = methyl-8-quinolinolato) were prepared and characterized; furthermore, their optical properties were compared with those of respective aluminum or BODIPY mononuclear compounds. According to the X-ray diffraction results, the crystal structures of 10-12 revealed distorted square-pyramidal geometries around aluminum and evident planarity around borane. Moreover, all heterodinuclear complexes were found to be air stable in the solid and solution states. In particular, the salen-ligand-based heterodinuclear complexes 10 and 11 exhibited thermal stability (T_{d5} = 309 and 306 ^{o}C, respectively) higher than that of their aluminum or BODIPY mononuclear compounds. The UV-vis absorption of the heterodinuclear and partial mononuclear compounds in a chloroform solution (5.0×10^{-5} M) showed that the absorption spectrum of the heterodinuclear complexes is similar to the arithmetic sum of the spectra of both aluminum and BODIPY mononuclear compounds. Density functional calculations revealed independent transition states on only the aluminum moiety or the BODIPY partial moiety in the heterodinuclear complexes, further supporting the experimental features. Notably, the comparison of the emission spectrum of 10 or 11 with that of its BODIPY mononuclear compound suggested that the photoinduced energy transfer from the aluminum moiety to the BODIPY moiety occurs in an intramolecular manner.


Al
B
Energy Transfer
PL Spectra
Al
B
Al/B
420
490
560
630
λ /nm

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **INOR.P-3**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Ruthenocycles involving *s*-tetrazine : binding constants study for polyaromatic guests

전용군 최문근[1,*] 강필재[1] 강혜지[1]

연세대학교 이과대학 화학과 [1]연세대학교 화학과

Metallasupramolecules are synthesized through coordination driven self-assembly process of multidentate ligands and transition metal fragments. Especially, properties of metallamacrocycle which have nano cavity were determined by geometry of chelate ligands and coordination environment of metal centers. These of macrocycles have been attracted with their diverse applications for electrochemical sensor, molecular recognition, size selective catalyst, antitumor agent. Tetraruthenocycle introducing s-tetrazine, six-membered hetero aromatic molecule which possesses extremely poor π-electron density, which induces efficient binding of the ruthenocycle with aromatic guest molecules through donor acceptor interactions has been synthesized and characterized by ^{1}H NMR and elemental analysis. The Molecular structure of ruthenocycle is determined by single crystal X-ray diffraction study. The structure exhibit rectangular shaped macrocycles with nano pores of 13 X 8 Å. These cavity is large enough to encapsulate polyaromatic molecules.The binding constants between ruthenocycle and diverse polyaromatic guests were measured by ^{1}H NMR in acetone-d_6.Conversion from s-tetrazine to pyridazine by inverse Diels-Alder reaction decreased the binding constants between ruthenocycle and aromatic guests with higher π-electron density.

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장소: 대구 EXCO
발표코드: **INOR.P-4**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation of Selenium based Nanoparticles by using Reactivity between Selenium and Ag, Au, and Pt

최지용 송현준[1,*]

KAIST 화학과 [1]한국과학기술원(KAIST) 화학과

Small Se nanoparticles with a diameter of ~20 nm were generated by the reduction of selenium chloride with $NaBH_4$ at -10 ℃. The reaction with Ag at 60 ℃ yielded stable Ag_2Se nanoparticles, which subsequently transformed into MSe nanoparticles (M = Cd, Zn, Pb) via cation exchange reactions with corresponding ions. The reaction with Pt formed Pt layers that were evenly coated on the surface of the Se nanoparticles, and the dissolution of the Se cores with hydrazine yielded uniform Pt hollow nanoparticles. The reaction with Au generated tiny Au clusters on the Se surface, and eventually formed acorn-shaped Au-Se nanoparticles through heat treatment. These results indicate that small Se nanoparticles with diameters of ~20 nm can be used as a versatile platform for the synthesis of metal selenide and metal-selenium hybrid nanoparticles with complex structures.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

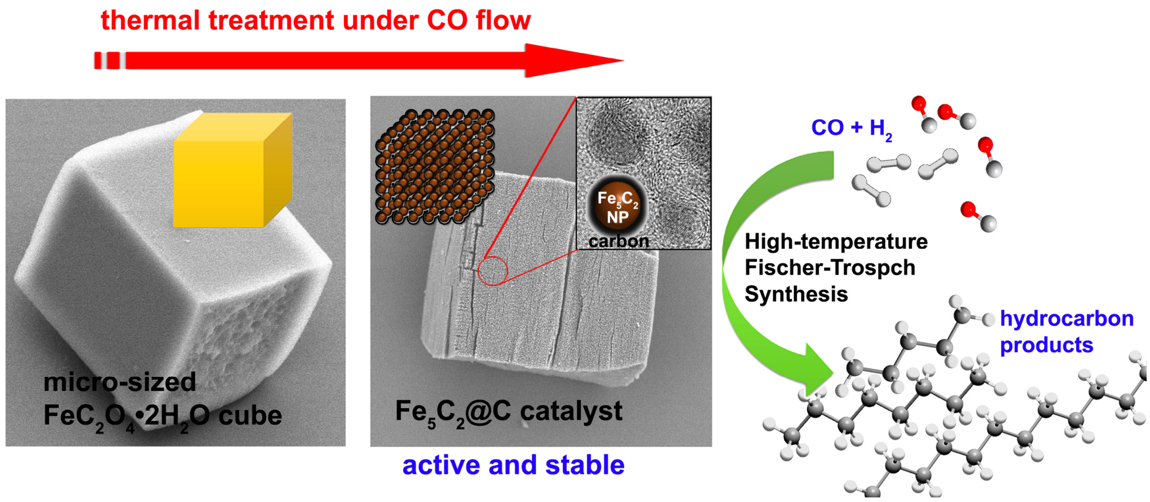
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-5**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A new synthesis of carbon encapsulated Fe5C2 nanoparticles for high-temperature Fischer-Tropsch synthesis

박지찬

한국에너지기술연구원 청정연료연구실

Using the simple thermal treatment under CO flow, uniform micrometer-sized iron oxalate dihydrate cubes prepared by hydrothermal reaction were transformed into Fe5C2@C core-shell nanoparticles to form a mesoporous microreactor framework; the final structure was successfully applied to the high-temperature Fischer-Tropsch reaction and showed high activity (CO conversion=96%, FTY=1.5×10-4 molCO?gFe-1?s-1) and stability.



일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-6**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Temperature dependent investigation on $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) by X-ray powder diffraction

박가람 오인환[1] 박승일[2,*]

고려대학교 화학과 [1]한국원자력연구소 중성자과학연구부 [2]한국원자력연구원 중성자과학연구부

Inorganic-organic perovskite type materials are regarded as a possible new pathway to the multiferroic system. The title compound $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) belongs to the layered inorganic-organic perovskite system. According to the previous report (Polyakov et al., 2012), this material should be multiferroic (ferromagnetic and ferroelectric), although there is an inversion center in the crystal structure. To clarify the inconsistency between the point symmetry and the physical properties, we carried out temperature dependent X-ray powder diffraction measurements. Two structural phase transitions are observed (T_{c1} = 417K and T_{c2} = 367K). Based on our current X-ray diffraction results and the previous optical investigations, Cu-PEA should be ferroelastic. Contrary to the previous investigation, the phase transition at 367K is not the polar phase transition. The color change is caused by an alteration of the optical birefringence associated with an enlargement of the unit-cell. In this work, we will discuss the phase transitions using group-max. subgroup relations.

Reference[1] Polyakov et al., Chem. Mater. Vol. 24, 133 (2012)

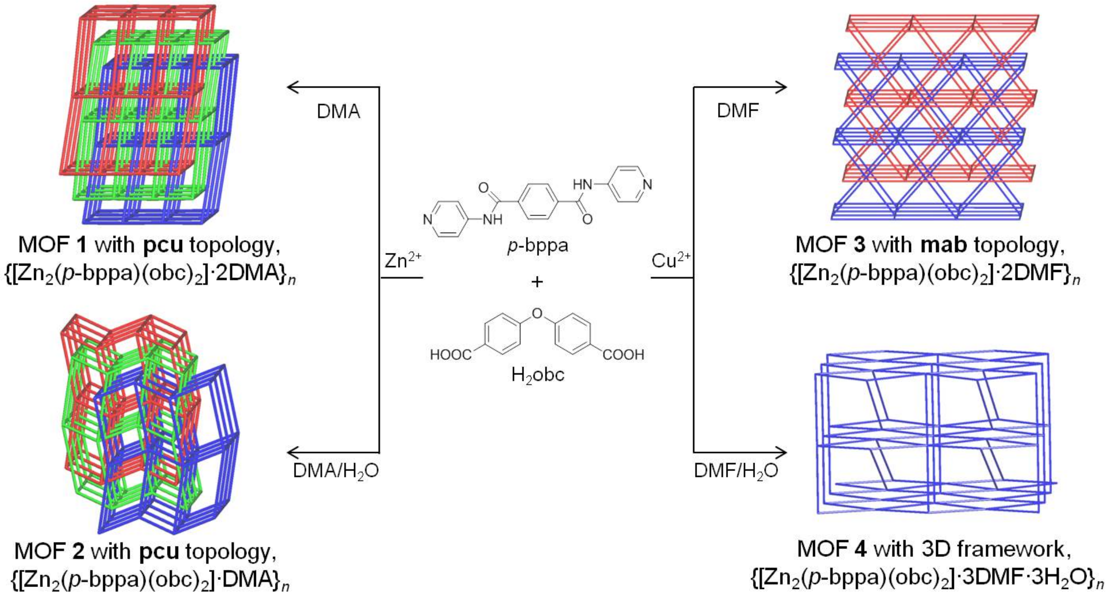
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-7**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solvent-Dependent 3D Zn(II) and Cu(II) MOFs Derived from Binary Ligands Involving Bis(amidopyridine) and Angular Carboxylic Acid

이은지 박기민[1,*] 이심성[*]

경상대학교 화학과 [1]경상대학교 기초과학연구소

Structural characterization and physical properties of Zn(II) and Cu(II) MOFs with 3D frameworks showing different topologies depending on the solvents are reported. MOFs 1-4 were prepared in the solvothermal reactions of Zn(II) and Cu(II) ions with binary ligand system: bis(amidopyridine) ligand (*p*-bppa) and angular carboxylic acid (H_2obc= 4,4′-oxybisbenzoic acid). Reaction of *p*-bppa with $Zn(NO_3)_2\cdot 4H_2O$ in the presence of H_2obc in DMA:0.1M HCl (2:1) afforded a 3-fold interpenetrated 3D MOF, $\{[Zn_2(p\text{-bppa})(obc)_2]\cdot 2DMA\}_n$ (1) with pcu topology. In addition, when H_2O was used instead of 0.1M HCl, $\{[Zn_2(p\text{-bppa})(obc)_2]\cdot DMA\}_n$ (2) adopting a 3-fold interpenetrated 3D MOF was isolated as a supramolecular isomer of 1. Meanwhile, treatment of *p*-bppa with $Cu(NO_3)_2\cdot 3H_2O$ in the presence of H_2obc in DMF:0.1M HCl (2:1) gave a 2-fold interpenetrated 3D MOF, $\{[Cu_2(p\text{-bppa})(obc)_2]\cdot 2DMF\}_n$ (3) with mab topology. Interestingly, when H_2O was used instead of 0.1M HCl, $\{[Cu_2(p\text{-bppa})_2(obc)_2]\cdot 3DMF\cdot 3H_2O\}_n$ (4) adopting a noninterpenetrated 3D MOF was obtained. Among the MOFs prepared, two Zn(II) MOFs (1 and 2) exhibit bright-blue emission (λ_{em} = 439 and 472 nm, respectively) originated from metal-ligand charge transfer (MLCT).


DMA
DMA/H_2O
Zn^{2+}
Cu^{2+}
DMF
DMF/H_2O
O
NH
N
HN
N
O
p-bppa
+
O
HOOC
COOH
H_2obc
MOF **1** with **pcu** topology,
$\{[Zn_2(p\text{-bppa})(obc)_2]\cdot 2DMA\}_n$
MOF **2** with **pcu** topology,
$\{[Zn_2(p\text{-bppa})(obc)_2]\cdot DMA\}_n$
MOF **3** with **mab** topology,
$\{[Zn_2(p\text{-bppa})(obc)_2]\cdot 2DMF\}_n$
MOF **4** with 3D framework,
$\{[Zn_2(p\text{-bppa})(obc)_2]\cdot 3DMF\cdot 3H_2O\}_n$

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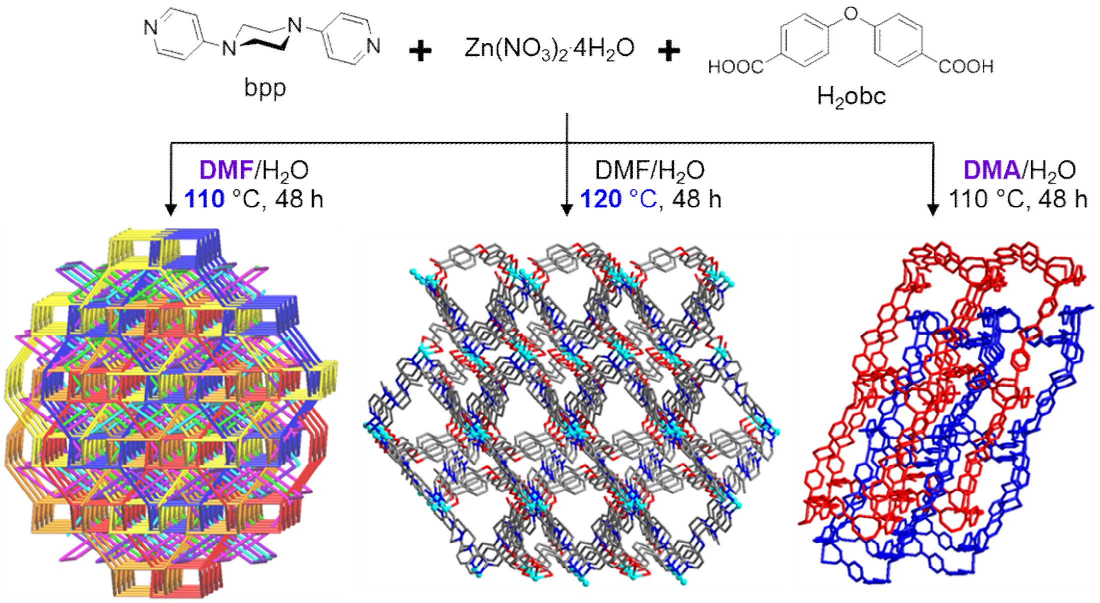
발표코드: **INOR.P-8**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solvent- or Temperature-Dependent Formations of Zn(II) Coordination Polymers Exhibiting Single-Crystal-to-Single-Crystal Transformation

주희영 이심성*

경상대학교 화학과

The intrinsic semi-flexibility of 1,4-bis(4-pyridiyl)piperazine (bpp), 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, bpp was chosen as organic building blocks. Under the different solvothermal condition, the reactions of bpp with zinc(II) in the presence of H_2obc afforded three coordination polymers (1-3). In DMF at 110 °C, for example, a 8-fold interpenetrated 3D framework $[Zn(bpp)(obc)]\cdot 3H_2O\}_n$ (1) showing a sra topology was isolated. In the identical condition but at 120 °C, however, a self-penetrated 3D structure $\{[Zn_3(bpp)_3(obc)_3]\cdot x\mathrm{Solvent}\}_n$ (2) was obtained. The first reaction was repeated employing DMA as a solvent, a 2-fold interpenetrated 3D framework $\{[Zn_2(bpp)_2(obc)]\cdot 2DMA\cdot H_2O\}_n$ (3) with pcu topology was prepared. The solvent-exchange-mediated SCSC transformation induced by acetone converts 3 into another 3D frameworks $\{[Zn_2(bpp)_2(obc)]\cdot 3\mathrm{acetone}\}_n$ (3a) via the conformational changes of the bpp molecule as pillar from *chair* to *twist-boat* form.



8-Fold interpenetrated 3D MOF (**1**) with **sra** topology

Self-penetrated 3D MOF (**2**)

2-Fold interpenetrated 3D MOF (**3**) with **pcu** topology

일시: 2015년 10월 14~16일(수~금) 3일간
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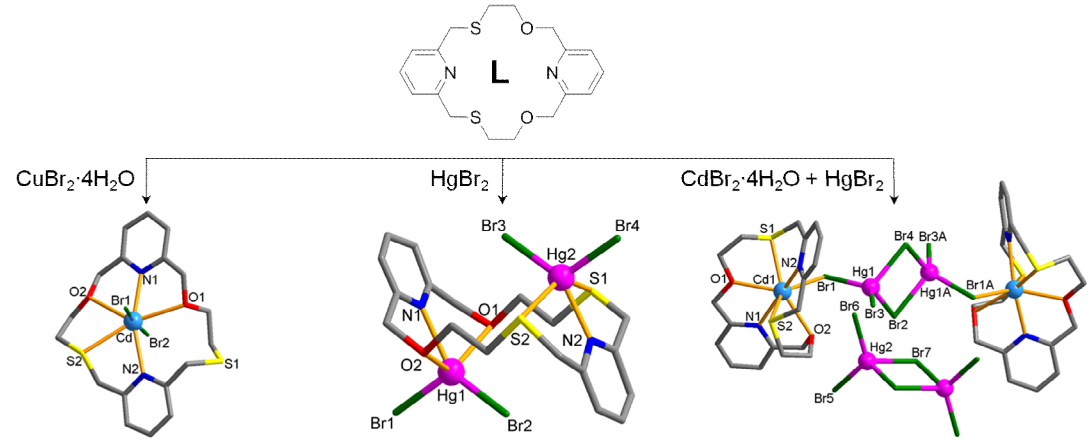
발표코드: **INOR.P-9**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Homo- and Heteronuclear Heavy Metal Complexation of an $N_2O_2S_2$-Donor Macrocycle Possessing Hard and Soft Base Natures

서수진 이은지 이심성*

경상대학교 화학과

We propose a ditopic macrocycle, L, which employs NO_2 and NS_2 donor sets in each side to accommodate one hard and/or one soft metal ion(s). First, Ag(I) salts react with L to give exocyclic 1D coordination polymers of type $\{[Ag(L)]X\}_n$ (1: X = ClO_4^- and 2: X = BF_4^-) with different coordination modes. Also, mercury(II) nitrate gave a 1D coordination polymer of type $\{[Hg_2(L)]NO_3\}_n$ (3) in which macrocyclic dimercury(II) complex units are linked by Hg-Hg contact. A mixture of HgI_2 and CuI afforded an endocyclic monocopper(II) complex $[Cu(L)][Hg_2I_6]$ (4). When $Ni(NO_3)_2{\cdot}6H_2O$ was used, a typical endocyclic mononuclear complex $[Ni(L)](NO_3)_2{\cdot}2H_2O$ (5) was isolated. Similarly, $CdBr_2{\cdot}4H_2O$ afforded an endocyclic mononuclear complex $[Cd(L)Br_2]$ (6). Mercury(II) bromide yielded endocyclic dinuclear complexes $[Hg_2(L)Br_4]$ (7). In addition, one-pot reaction of L with a mixture of $HgBr_2$ and $CdBr_2{\cdot}4H_2O$ afforded a heterotetranuclear dumbbell-liked complex $[Cd_2L_2(\mu_2\text{-}Hg_2Br_6)][Hg_2I_6]$ (8), in which two endocyclic Cd(II) complex units are linked by a square-type Hg_2I_6 cluster as a cationic part. The competitive binding abilities of mercury(II) and cadmium(II) to L in solution were also investigated by the comparative NMR experiments and the results were compared with those in the solid state.



6, [Cd**L**Br$_2$]
Endocyclic 1:1 [Cd(II)/**L**] Complex

7, [Hg$_2$**L**Br$_4$]
Exocyclic 2:1 [Hg(II)/**L**] Complex

8, [Cd$_2$**L**$_2$(μ_2-Hg$_2$Br$_6$)][Hg$_2$Br$_6$]
Endo/Exocyclic Heteronuclear complex

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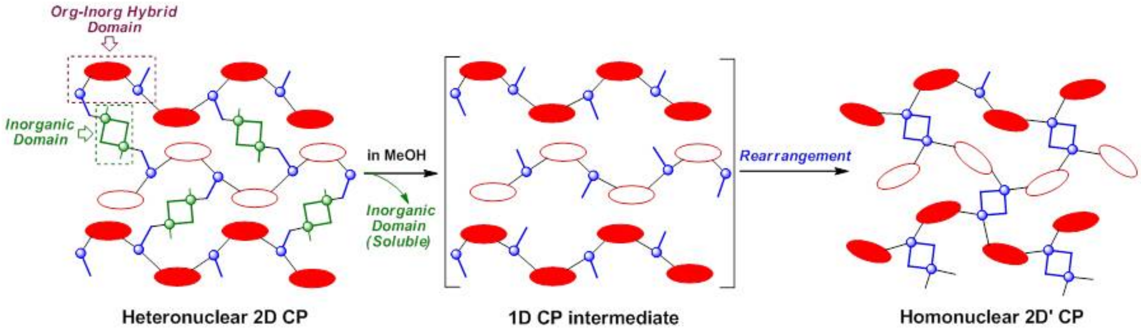
발표코드: **INOR.P-10**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of a Heteronuclear 2D Network and Its Post-Synthetic Modification to a Unique Homonuclear 2D Network via Single-Crystal-to-Single-Crystal Transformation

김슬기 박인혁 이심성*

경상대학교 화학과

The post-synthetic modification of the self-assembled coordination networks via a single-crystal-to-single-crystal transformation (SCSC) transformation is one of the fascinating approaches for the creation of novel materials. We report a significant SCSC transformation of a heteronuclear 2D coordination polymer (CP) to a homonuclear 2D CP by removal of a partial inorganic unit followed by rearrangement. An O_2S_2-macrocycle, L, reacts with a mixture of CuI and HgI_2 to afford the heterometallic 2D CP, $\{[Cu_2(\mu\text{-}Hg_2I_4)(L)_2(CH_3CN)_2I_2]\cdot toluene\}_n$, in which L-Cu-L-Cu 1D wavy chains are cross-linked by μ-Hg_2I_4 bridging clusters, giving rise to the infinite sheet structure. Notably, immersing of the yellow single crystals of the above material in methanol induces the SCSC transformation resulting in the formation of the colorless homonuclear 2D CP, $[(\mu\text{-}Cu_2I_2)(L)]_n$ through the removal of μ-Hg_2I_4 bridging part couple with the rearrangement of the copper(I) coordination sphere as a first case. The mechanism of the conversion was proposed from the AFM data. Additional evidence for the dissolved Hg(II) was obtained by energy dispersive X-ray (EDX) spectrum profile scanning and elemental mapping data.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
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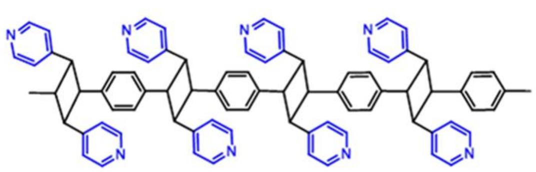
발표코드: **INOR.P-11**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photochemical Formation and Thermal Cleavage of a Syndiotactic Organic Polymer inside a MOF via Single-Crystal-to-Single-Crystal Transformation

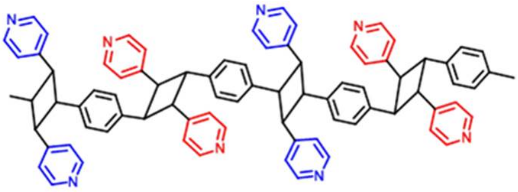
박인혁 Raghavender Medishetty[1] 이형환 Caroline Evania Mulijanto[1] Hong Sheng Quah[1]
이심성[*] Jagadese J. Vittal[1,*]

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

The tacticity control of the organic polymers (isotactic or syndiotactic) is one of the important issues both in academic and industrial areas. We have reported the preparation of the isotactic organic polymer from the metal-organic frameworks (MOFs) with 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb) through the photo-induced [2+2] cycloaddition reaction as a first case in this kind. In the extension of our on-going works on the photochemical approach for the synthesis of organic polymers, we here introduce the formation of the syndiotactic organic polymer ligand inside a MOF. We have synthesized the 3-fold interpenetrated pillared-layer MOF 1 with pcu topology comprising an unusual isomer of the paddle-wheel building block and the trans,cis,trans isomer of bpeb pillar ligand. In MeOH, the single-crystals of 1 were transformed via solvent exchange in a single-crystal to single-crystal (SCSC) manner to yield MOF 2. The guest solvents could be removed without destroying its single crystallinity by heating 2, but on standing in air, it takes water from air to form MOF 3. The spacer ligand bpeb with trans,trans,trans-conformation in 3 undergoes pedal motion to trans,cis,trans-conformation prior to [2+2] photo-cycloaddition reaction and yield single crystals of MOF 4 containing 2D network fused with the syndiotactic organic polymer. We also found that the prepared syndiotactic organic polymer in the single crystal form is depolymerized reversibly by cleaving the cyclobutane rings upon heating. These MOFs also show interesting photoluminescent properties and sensing of small organic molecules.



isotactic polymer



syndiotactic polymer

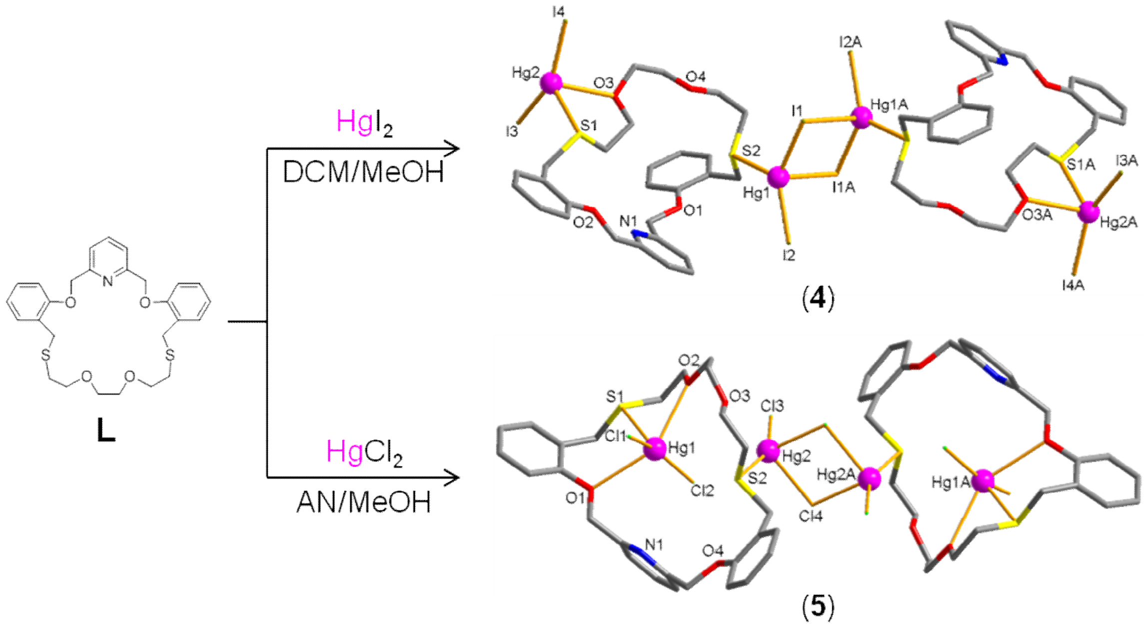
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-12**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Soft Metal Complexes of a 23-Membered NO_4S_2-Macrocycle: Anion-Controlled Endo/Exo-Coordination and NMR Titration

신민경 주희영 이심성*

경상대학교 화학과

A 23-membered NO_4S_2-macrocycle (L) has been synthesized and its complexation behaviors in solid and solution states have been investigated by X-ray crystallography and NMR titration experiment, respectively. Reactions of L with $AgClO_4$ and $Cu(ClO_4)_2 \cdot 3H_2O$ afforded typical endocyclic 1:1 complexes $[Ag(L)]ClO_4$ (1) and $[Cu^{I}(L)]ClO_4$ (2), respectively. In contrast, the reaction of L with copper(I) chloride yielded an endocyclic complex $[Cu^{II}(L)Cl_2] \cdot CH_3CN$ (3) exhibiting the oxidation of copper(I) to copper(II). The reaction of mercury(II) iodide with L afforded a discrete 4:2 (metal-to-ligand) complex of a formula $[Hg_4(L)_2I_8]$ (4) in which two exocyclic HgI_2 macrocyclic complex units are linked by $[Hg_2I_4]$ cluster. The $HgCl_2$ gave a same stoichiometric species $[Hg_4(L)_2Cl_8]$ (5) but the $HgCl_2$ exists in the cavity. When a mixture of CdI_2 and HgI_2 was used in the reaction with L, a discrete complex with two separated parts of a formula $[Cd(L)I]_2[Hg_2I_6]$ (6) was isolated. An NMR titration of the formation of 1 confirmed that the Ag^+/L stoichiometry of 1:1 found in the solid state is also maintained in solution.


L
HgI2
DCM/MeOH
HgCl2
AN/MeOH
I4
Hg2
O3
O4
I3
S1
S2
I2A
I1
Hg1A
Hg1
I1A
O2
N1
O1
I2
S1A
I3A
O3A
Hg2A
I4A
(4)
O2
O3
S1
Cl3
Cl1
Hg1
Hg2
Cl2
S2
Hg2A
Hg1A
O1
Cl4
N1
O4
(5)

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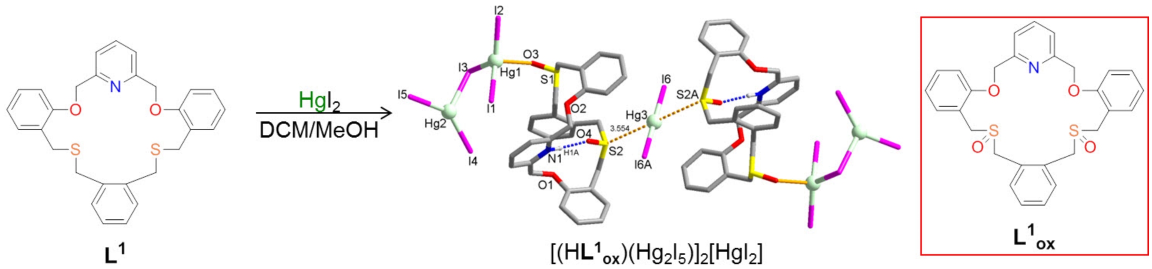
19- and 38-Membered Thiaoxaaza-Macrocycles via 1:1 and 2:2 Cyclizations and Their Supramolecular Complexes

강윤지 박인혁 이심성*

경상대학교 화학과

There is a growing interest in a large macrocyclic ligand system that can form binuclear complexes exhibiting electron transport, charge transfer, and allosteric behavior. In this presentation, supramolecular complexation behaviors of a 19-membered NO_2S_2-macrocycle L^1 and a 38-membered $N_2O_4S_4$-macrocycle L^2 (a 2:2 cyclization byproduct) are reported. Four metal complexes (1-4) of L^1 with silver(I), cadmium(II), copper(I), or mercury(II) were prepared and structurally characterized. When $AgNO_3$ was employed in the reaction with L^1, a typical endocyclic mononuclear complex, $[Ag(L^1)]NO_3$ (1), was obtained. In the cadmium(II) iodide complex of L^1, two mononuclear macrocyclic complex units are doubly linked by two bridging iodide atoms, adopting a double-decker type dimeric complex featuring two separated units of formula $[Cd_2I_2)_2(L^1)_2][Cd_2I_6]$ (2). When CuI was reacted with L^1 in the presence of CdI_2, we obtained a mixed metallic complex featuring two separated units of formula $[Cu(L^1)][Cd_2I_6]$ (3). The most fascinating product with L^1 is a pseudo-dimeric mercury(II) iodide complex, $[(HL^1_{ox})(Hg_2I_5)]_2[HgI_2]$ (4) in which the macrocycle was oxidized to the disulfoxide form (L^1_{ox}) under present complexation condition. In 4, one sulfoxide of HL^1_{ox} coordinates to one Hg atom in the Hg_2I_5 cluster, while another sulfoxide interacts with protonated pyridine unit via intramolecular H-bond. The two exocyclic complex units are linked by HgI_2 via long range interactions between Hg and S atoms. More metal complexes of L^1 and L^2 will be presented and discussed.


L^1
HgI_2
DCM/MeOH
I2
I3
O3
Hg1
I5
S1
I1
O2
Hg2
O4
I4
N1
H1A
S2
O1
3.554
Hg3
I6
S2A
I6A
$[(HL^1_{ox})(Hg_2I_5)]_2[HgI_2]$
L^1_{ox}

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Crystal Structures of Macrocyclic Nickel(II) Complexes Bearing 1,4-chdc (chdc = Cyclohexanedicarboxylate) Ligands

김태영 서초현 서성용 김주창*

부경대학교 화학과

Two macrocyclic nickel(II) complexes, {[Ni(cyclam)(*a*,*e*-*cis*-1,4-chdc)]·4H_2O}n (1) and [{(H_2O)Ni(cyclam)}$_2$(*e*,*e*-*trans*-1,4-chdc)] (2), have been obtained and characterized by X-ray diffraction methods, elemental analyses, IR spectra, and thermal analyses. The complex 1 bearing an *a*,*e*-*cis*-1,4-chdc conformation is separated from the starting *a*,*e*-*cis*-/*e*,*e*-*trans*-1,4-chdcH_2 mixture in basic DMF/H_2O. In 1, the *a*,*e*-*cis*-1,4-chdc ligand bridges nickel(II) macrocycles to form an undulated 1D coordination polymer. Each 1D chain in 1 is further connected by hydrogen bonds, resulting in the formation of a 2D supramolecule. The dimeric complex 2 in which the *e*,*e*-*trans*-1,4-chdc ligand bridges two nickel(II) cyclams has been obtained from the same reactants in basic H_2O. The dimer 2 extends its structure by hydrogen bonds to form a 2D supramolecule containing cavities. The crystallization of 1 and 2 from the reaction of nickel(II) cyclam and *a*,*e*-*cis*-/*e*,*e*-*trans*-1,4-chdcH_2 mixture depends on the solvents employed. The *a*,*e*-*cis*-1,4-chdc ligand in 1 which is more polar "L shape" prefers to crystallize the 1D coordination polymer in basic DMF/H_2O, whereas the linear *e*,*e*-*trans*-1,4-chdc ligand leads to the formation of the dimer 2 in basic H_2O.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Intercalation Route to Complex Perovskites $AM_{0.2}Nb_{0.8}O_{3-x}N_x$(A= Sr, Ba; M=Li, Na, Mg)

문건호 김영일[1,*]

영남대학교 에너지융합공학과 [1]영남대학교 화학과

Oxynitride-type complex perovskites, $AM_{0.2}Nb_{0.8}O_{3-x}N_x$ (A=Sr, Ba; M=Li, Na, Mg) were synthesized by the ammonolytic heating of a layered perovskite, $A_5Nb_4O_{15}$, with $0.5M_2CO_3$ or $MgCl_2$. A Rietveld refinement of the X-ray powder patterns confirmed the complete structural transformation from a hexagonal layered-perovskite to a three-dimensional perovskite type, as well as the stablilization of alkali cations on the octahedral sites rather than on the dodecahedral sites in the latter. In all six compounds, M^+ and Nb^{5+} were disordered completely despite a charge difference as much as 4. The crystal summetry of the average structure depended on the size of the dodecahedral cation: simple cubic for $BaM_{0.2}Nb_{0.8}O_{3-x}N_x$ and body-centered tetragonal for $SrM_{0.2}Nb_{0.8}O_{3-x}N_x$. This trend coincides with the symmetry transition from $BaNbO_2N$(Pm-3m) to $SrNbO_2N$(I4/mcm). In both $SrM_{0.2}Nb_{0.8}O_{3-x}N_x$, nitrogen atoms preferentially occupied the c-axial 4a site of the tetragonal cell. The optical band gaps are estimated from diffuse reflectance spectra as follows : $BaLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$, 1.4eV; $BaNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$, 1.6eV; $SrLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$, 1.8eV; $SrNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$, 1.6eV; $SrMg_{0.2}Nb_{0.8}O_{2.6}N_{0.4}$, 1.3eV; Solid state magic angel spinning resonance spectroscopy showed that $SrNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$ and $BaNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$ exhibited marked downfield shifts of 23Na, manifesting an octaheral coordination. On the other hand, the 7Li NMR of $SrLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$ and $BaLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$ indicated a highly symmetrical coordination environment of Li.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

New macrocyclic complexes of a five-membered ring consisting of an organic isocyanate dimer and group 10 metals

김용주* 최준환 김건우 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

New macrocylic complexes, tetramers of a five-membered ring consisting of an organic isocyanate dimer and Pd or Pt atom were obtained from five-menbered metallacyclic complexes with elemental sulfur. Isocyanate cyclotrimerization with tetrameric or single palladacycles was carried out. Experimental detail will be discussed.

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Synthesis and properties of Pd(II) and Pt(II) complexes having pyrrole or indole ligand

김용주* 김남수 김건우 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

New Pd-N or Pt-N bonded bis(phosphine) Pd(II) or Pt(II) complexes were prepared by the metathesis of MCl2L2 (M = Pd, Pt; L = PR3) with n-lithiated pyrrole or indole reagents. Isolated complexes were characterized for IR, NMR and elemental analysis. Some compounds were determined from X-ray diffraction method. In addition, Suzuki-miyaura C-C coupling reactions were carried out.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: 무기화학
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Highly enhanced gas-sorption capacities of N-doped porous carbon spheres by hot NH3 and CO2 treatments

김희수 강민석 유원철*

한양대학교 응용화학과

Highly enhanced CO2 and H2 adsorption properties were achieved from a series of different phenolic resin-based carbon spheres (resorcinol-formaldehyde carbon (RFC) and phenol-formaldehyde carbon (PFC)) by carbonization of RF and PF polymer (RFP and PFP) spheres synthesized sol-gel reaction method and subsequent activations with hot CO2 and NH3 gas treatments A series of CO2-activated and N-doped RFC and PFC spheres show almost perfect correlation (R2 = 0.99) between CO2 adsorption capacities and accumulated volumes of fine micropores (ultra micropore < 1 nm). When NH3 activation employed, surprisingly, hot NH3 treatment serves as not only an effective way for nitrogen doping into the carbon framework but also an excellent activation process that can fine-tune surface area and pore size distribution (PSD). Moreover, prolonged activation processes for RFC and PFC spheres showing ultra high surface area with the highly H2 uptake capacity which is one of the best H2 storage media among carbonaceous materials and metal-organic frameworks (MOFs).

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

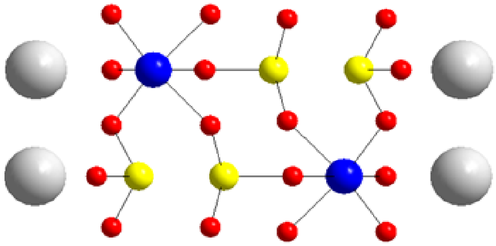
Syntheses, Structure and Characterizations of new Quaternary Alkali Metal NiobiumSelenites

김봉수 옥강민*

중앙대학교 화학과

Pure polycrystalline phases and single crystals of four new quaternary alkali metal niobiumselenites, $ANbO(SeO_3)_2$ (A = Na, K, Rb, and Cs)have been synthesized by solid-state and hydrothermal reactions. The stoichiometrically similar materials reveal uni-dimensional chains and two-dimensional framework structures consisting of SeO_3 polyhedra and NbO_6octahedra. The local unsymmetrical coordination environment of the constituent polyhedra is attributed to the second-order Jahn-Teller (SOJT) distortions arising from the NbO_6 octahedra and the stereoactive lone pairs on Se^{4+} cations.

Full characterizations including X-ray diffraction, Scanning Electron Microscopy (SEM), infrared and UV-Vis diffuse reflectance spectroscopies, thermal analyses, and dipolemoment calculations for the new alkali metal niobium selenites will be presented.



일시: 2015년 10월 14~16일(수~금) 3일간

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발표코드: **INOR.P-20**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Nonlinear Optical (NLO) and Photoluminescence (PL) Properties ofNoncentrosymmetric (NCS) Polar Perovskite Solid Solutions

김형구 옥강민*

중앙대학교 화학과

Hyung Gu Kim and Kang Min Ok*Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, 156-756, Republic of Korea.Several new noncentrosymmetric (NCS) layered perovskite solid solutions containing both families of second-order Jahn-Teller distortive cations have been prepared through standard solid state reactions. X-ray diffraction has been utilized to determine the polar structures of the reported mixed metal oxide materials. The structures of the solid solutions consist of statically disordered A-cations, Bi^{3+} and Eu^{3+}, and corner-shared NbO_6 octahedra. Detailed structural analysis suggests that the nonlinear optical (NLO) properties of the solid solutions are strongly influenced by the alignment of the polarizable lone pair cation, Bi^{3+}. Photoluminescence (PL) excitation and emission spectra of the reported materials exhibit the charge transfer transition bands and f-f electric dipole transition bands, respectively. The PL emission spectra strongly suggest the asymmetric coordination environment of the A-cations site in the reported solid solutions.

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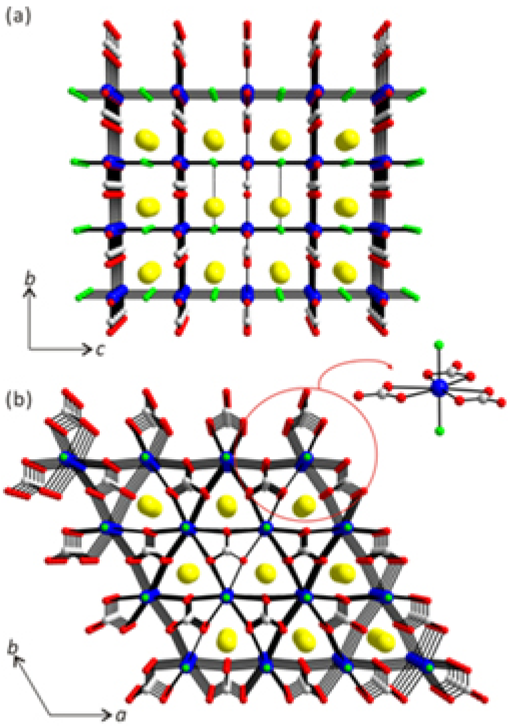
$ACdCO_3F$ (A = K and Rb): Nonlinear optical materials with strong second-harmonic generation

Zouguohong 옥강민*

중앙대학교 화학과

Nonlinear optical (NLO) materials have become increasingly important and are attracting more and more attention owing to their promising applications in laser science and technology. However it presents a particularly difficult challenge in searching for suitable materials with high NLO coefficients and wide transparency. A general strategy to synthesize new NLO materials is suggested to employ noncentrosymmetric (NCS) chromophores as building units which consist of borate π-orbital systems or distorted polyhedra with a d^0 cation center resulting from a second-order Jahn-Teller (SOJT) effect, polar displacement of a d^{10} cation center, or distortion from stereochemically active lone pair (SCALP) effect of cation.

In this research, we introduced d^{10} cation Cd^{2+} into carbonates and successfully synthesized two new noncentrosymmetric (NCS) materials, namely, $ACdCO_3F$ (A = K and Rb). $ACdCO_3F$ exhibits a 3-dimensional structure that is composed of the stacked layers of $[Cd(CO_3)]\infty$. Each $[Cd(CO_3)]\infty$ layer is connected by infinite Cd?F?Cd chains and the $[CO_3]$ triangles are oriented in the same direction with a coplanar alignment. $KCdCO_3F$ and $RbCdCO_3F$ reveal remarkably strong second-harmonic generation (SHG) responses of approximately 9.0 and 7.2 times that of potassium dihydrogen phosphate (KDP), respectively, and both materials are phase-matchable. $ACdCO_3F$ exhibit wide transparent regions ranging from far UV to mid IR suggesting that they are very promising NLO materials.


(a)
b
c
(b)
b
a

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, Structure, and Optical Properties of Ln (III) - doped Bismuth Tellurium Oxide (Ln = Ce, Eu)

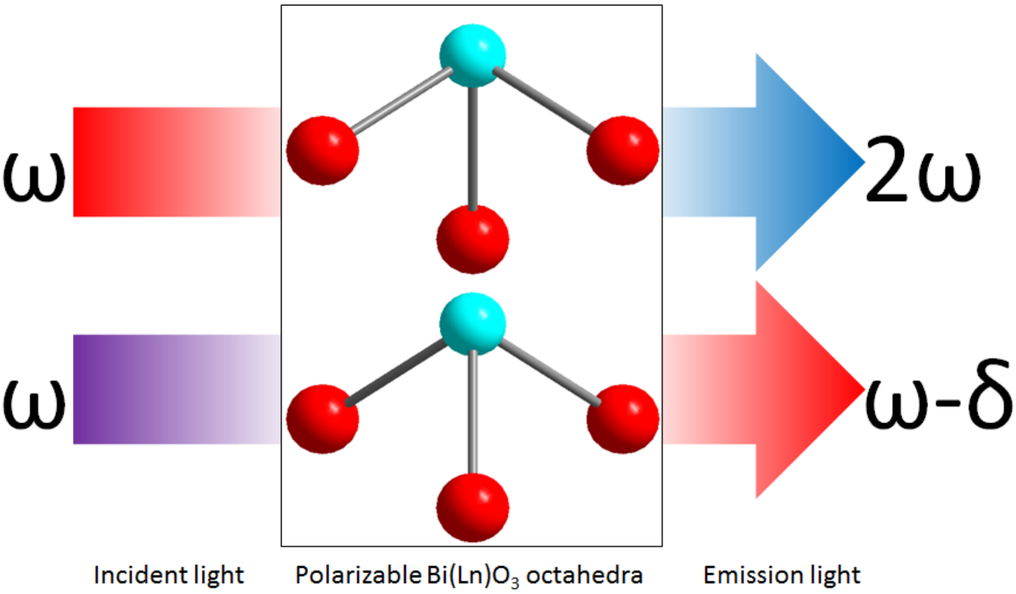
조홍일 옥강민*

중앙대학교 화학과

Bi_2TeO_5 is a bismuth tellurium oxide material consisting of only lone pair cations, Bi^{3+} and Te^{4+}. Bi_2TeO_5 has large second-harmonic generation (SHG) efficiency attributable to the polarization arising from the alignment of lone pairs.

In this study, we have tried to introduce luminescent cations into the asymmetric coordination sites in Bi_2TeO_5. Ce^{3+}- and Eu^{3+}-doped noncentrosymmetric (NCS) bistmuth tellurite solid solutions have been successfully synthesized by standard solid state reactions. We found that the NCS materials reveal both of the nonlinear optical (NLO) and photoluminescence properties. Detailed photoluminescence properties at variable temperatures will be presented.

Powder X-ray diffraction, energy dispersive analysis by X-ray, UV-vis diffuse-reflectance spectroscopy, infrared spectroscopy, nonlinear optical property, and structural analysis will be also introduced.


ω
ω
2ω
ω-δ
Incident light
Polarizable Bi(Ln)O_3 octahedra
Emission light

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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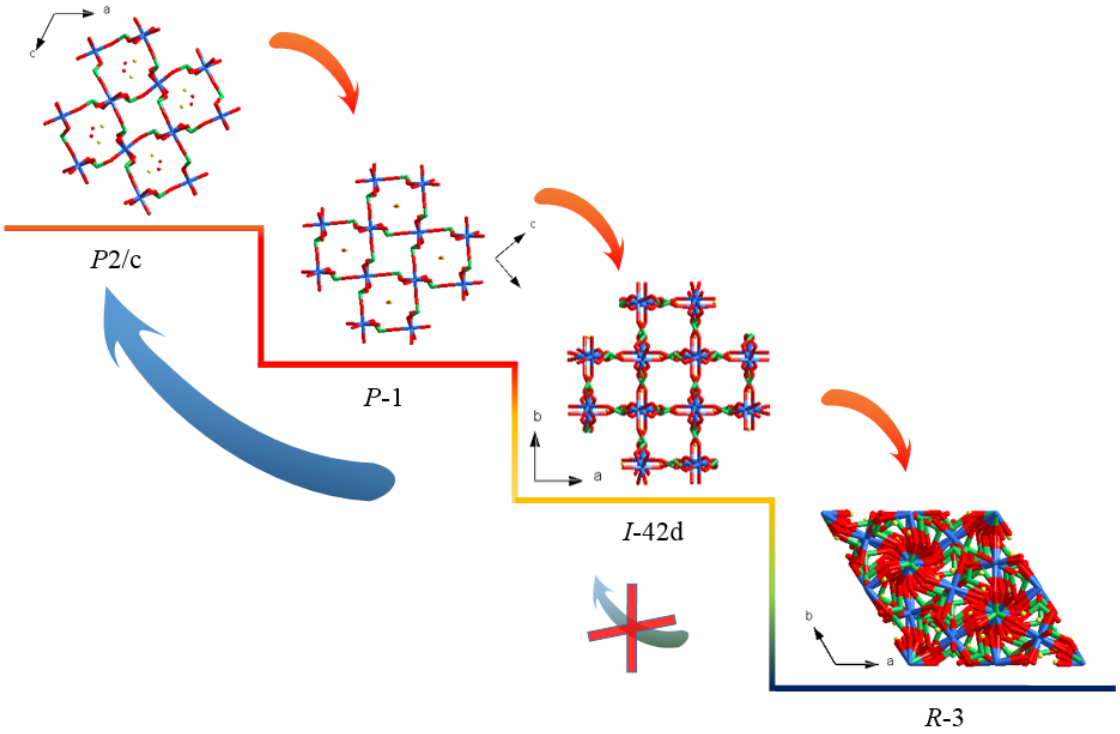
Reversible Single-Crystal-to-Single-Crystal Transformations in a Series of Lithium Scandium Selenites

송승윤 옥강민*

중앙대학교 화학과

Four new stoichiometrically equivalent quaternary lithium scandium selenites, α-$LiSc(SeO_3)_2$, $LiSc(SeO_3)_2 \cdot H_2O$, $LiSc(SeO_3)_2 \cdot nH_2O$ ($0.26 \le n \le 0.54$), β-$LiSc(SeO_3)_2$, have been synthesized by hydrothermal reactions using Li_2CO_3, Sc_2O_3, and SeO_2 as starting materials. All four materials share similar bond networks that are composed of corner-shared distorted ScO_6 octahedra and SeO_3 trigonal pyramids. However, each material reveals different frameworks and centricities. Detailed structural analysis suggests that the structural variation is attributed to the hydrogen bonding and coordination environments of Li^+ cations. Interesting reversible single-crystal-to-single-crystal transformations are observed in water at different temperatures. Powder second-harmonic generation (SHG) measurements on noncentrosymmetric (NCS) β-$LiSc(SeO_3)_2$ show that the compound has an SHG efficiency of 3 times that of α-SiO_2. Thorough characterizations such as spectroscopic, thermal, and elemental analyses for the new materials are presented as are dipole moment and out-of-center distortion calculations.


a
c
P2/c
P-1
c
b
a
I-42d
b
a
R-3

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Calix[4]arene-based Metal Organic Frameworks (CalixMOFs)

박기민* 이은지[1] 김영훈[2] 주희영[1] 허정석[2]

경상대학교 기초과학연구소 [1]경상대학교 화학과 [2]충남대학교 화학과

The metallation of 1,3-Alternate calix[4]arene derivative (H_4CTA) with four acetic acid arms at the low rim has allowed the creation of 1-D and higher-order metal organic frameworks (calixMOFs) including metallopolycapsular networks. Assembly of calix[4]arene tetraacetate (CTA) with $AgClO_4$ afford a two-metal-mediated tube-type calixMOF of the formula $\{[Ag_2(Ag_2@CTA)]\cdot 4H_2O\}_n$.[1] The use of H_4CTA with $Pb(NO_3)_2$ give a three-dimensional calixMOF of the formula $\{[Pb_2@CTA]\cdot 2DMF\}_n$, which undergoes single-crystal to single-crystal transformation induced by the desolvation process.[2] Additionally, the use of H_4CTA with $Zn(NO_3)_2$ in the presence of α,ω-diaminoalkanes result in the formation of two-dimensional metallopolycapsular networks.[3] These metallopolycapsular networks are built up of metallocapsules that consist of two CTA and two Zn(II) ions. Short alkanediyldiammonium ($^+NH_3\text{-}(CH_2)_n\text{-}NH_3^+$, $n = 2, 3, 4$) guest ions are accommodated in each capsule of the metallopolycapsular network through a variety of supramolecular interactions.

[1] Park, K.-M.; Lee, E.; Park, C. S.; Lee, S. S. *Inorg. Chem.* 2011, *50*, 12085.

[2] Lee, E.; Kim, Y.; Heo, J.; Park, K.-M. *Cryst. Growth Des.* 2015, *15*, 3556.

[3] Lee, J.; Ju, H.; Kang, Y.; Lee, S. S.; Park, K.-M. *Chem. Eur. J.* 2015, *21*, 6052.

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발표코드: **INOR.P-25**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Unusual Enhancement of Hydrogen Photoproduction by a Pyrene-pendant Rh Catalyst Immobilized to Reduced Graphene Oxide

김진홍* 김수진 박솔지[1] 이성은[1] 박유미[2]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학나노과학

The assembly of nanomaterials has been extensively studied for their promising optoelectric applications. Reduced graphene oxide (rGO), which is highly dispersed in water due to its hydrophilic oxygen functional groups and has electric properties superior to those of graphene oxide (GO), is intensively utilized to prepare efficient systems for optical sensors, catalysts, light antennas, and other applications. The photoexcited electrons of most chromophores are rapidly transferred to rGO when they are in close contact. rGO attached with organic chromophores was recently used to collect wide-range visible light energy for a photoregeneration system of 1,4-dihydronicotinamide adenine dinucleotide (NADH) with a molecular Rh catalyst, but direct interaction between rGO and Rh catalyst was not investigated. A cyclopentadienyl rhodium catalyst derivatized with pyrene was used to study the effects of a reduced graphene oxide (rGO) on visible light driven photocatalytic hydrogen production using formate and Pt nanoparticles. The pyrene-derivatized rhodium catalyst was immobilized on rGO by pi-pi stacking interactions. A tight formation of the Rh catalyst on rGO surprisingly enhanced the hydrogen production upon visible light irradiation, in contrast with the results using a thin formation of the catalyst or the unfunctionalized Rh catalyst. Our results also demonstrated that the catalytic stability of the pyrene-functionalized Rh complex dramatically increased when it was immobilized to rGO during the photocatalytic reaction cycle. RGO played a crucial role in efficiently transferring electrons from the Rh(III)-hydrides to the platinum nanoparticles

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Selective Assay of Anions Using a Thioamide-based Probe Containing Phenol and Pyridyl Groups

김진홍* 김 철[1] 김수진 박유미[2]

이화여자대학교 화학·나노과학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터 [2]이화여자대학교 화학나노과학

The selective assay of cyanide ions with a thioamide compound (HNPTU) containing phenol and pyridine as a chemosensor is reported using absorbance changes in a buffered aqueous solution (50 mM HEPES, pH 7.4) containing ethanol. Upon treatment with cyanide ions, the colorless solution of HNPTU turned to yellow. No significant changes were observed with other comparable anions, such as F-, Cl-, Br-, I-, and CH3COO-. The color change of HNPTU upon treatment with CN- was maintained even in the presence of the comparable monovalent anions. The complex stability constant (Ka = 2.6 x 103) for the stoichiometric 1:1 complexation of HNPTU with cyanide ions was obtained based on absorbance titrations. The interaction of HNPTU with cyanide ions was proposed to be deprotonation, as shown by NMR and Cu(II) treatment experiments..

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Methyl methacrylate polymerization study of copper(II) complexes having *N*-(2-pyridinylmethyl)aniline derivatives and *N*-(2-pyridinylmethyl)cycloalkylamines

안승현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New series of Cu(II) complexes, namely polynuclear $[L_aCuCl_2]_n$, dinuclear $[L_nCu(\mu\text{-}Cl)Cl]_2$ ($L_n = L_b$, L_d, L_e, L_f) and mononuclear $[L_cCuCl_2]$ were prepared by the reaction between $[CuCl_2.2H_2O]$ and *N,N'*-bidentate ligands, L_n [L_n = *N*-(2-pyridinylmethyl)aniline (L_a), 2,4,6-trimethyl-*N*-(2-pyridinylmethyl)aniline (L_b), 2,6-dimethyl-*N*-(2-pyridinylmethyl)aniline (L_c), *N*-(2-pyridinylmethyl)cyclopentanamine (L_d), *N*-(2-pyridinylmethyl)cyclohexanamine (L_e) and *N*-(2-furanylmethyl)-2-pyridinylmethylamine (L_f)], respectively. Monomeric $[L_cCuCl_2]$ showed a distorted square planar geometry around copper metal based on x-ray crystallography. The polymeric $[L_aCuCl_2]_n$ and representative dimeric $[L_bCu(\mu\text{-}Cl)Cl]_2$ had a chloro-bridged 5-coordinated and a distorted square pyramidal geometry around the Cu(II) center. $[L_cCuCl_2]$ showed the highest catalytic activity for the polymerisation of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 2.1×10^4 g PMMA/molCat?h at 60 °C and resulted in syndiotactic poly(methylmethacrylate) (PMMA).

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and catalytic properties of Zinc(II) and Cd(II) complexes containing bispyrazolyl ligand

안승현 신수진 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The bis(pyrazolyl) based ligands L^1 and L^2, where L^1 is *N*,*N*-bis((1H-pyrazol-1-yl)methyl)cyclohexanamine and L^2 is *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)cyclohexanamine, reacted with $ZnCl_2$ and $CdBr_2{\cdot}4H_2O$, respectively and resulted in mononuclear $[L_nMX_2]$ ($L_n = L^1, L^2$, M = Zn, Cd, X = Cl, Br) complexes in facile yield and high purity. The synthesized complexes have been characterized spectroscopically and crystallographically. The molecular structure of 4-coordinate $[L^1ZnCl_2]$ was best described as a distorted tetrahedral whereas 5-coordinate $[L^1CdBr_2]$ and $[L^2CdBr_2]$ exhibited distorted trigonal bipyramidal geometry involving the metal centres. $[L^1ZnCl_2]$ showed the highest catalytic activity for the polymerisation of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 4.40×10^4 g PMMA/molCat?h at 60 °C and resulted in syndiotactic poly(methylmethacrylate) (PMMA).

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MMA polymerization study of complexes [(nmpc)MCl_2] (M = Co, Cu, Zn) containing ligand *N*-methyl-*N*-((pyridin-2-yl)methyl)cyclohexanamine (nmpc)

안승현 **ruqia bibi**[1] 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [(nmpc)MCl_2] (M = Co, Cu, Zn) were synthesized by the reaction of the corresponding metal starting materials, [$ZnCl_2$], [$CoCl_2 \cdot 6H_2O$] and [$CuCl_2 \cdot 2H_2O$] with *N*,*N'*-bidentate *N*-methyl-*N*-((pyridin-2-yl)methyl)cyclohexanamine (nmpc), respectively. Molecular structure of [(nmpc)$ZnCl_2$] and [(nmpc)$CoCl_2$] were best described as a distorted tetrahedral geometry around metal centers. However,[(nmpc)Cu(μ-Cl)Cl]$_2$ was dimeric species which has a distorted trigonalbipyramidal geometry around metal center. [(nmpc)$CoCl_2$] showed the highest catalytic activity for the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 7.45×10^4 g PMMA/molCo·h at 60°C among the others compared to the reference complex [$CoCl_2$] (4.03×10^4 g PMMA/molCo·h) or [$CoCl_2 \cdot 6H_2O$] (4.73×10^4 g PMMA/molCo·h) or [$CoCl_2 \cdot 6H_2O$] (4.73×10^4 g PMMA/molCo·h).

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Solution-based Synthetic Protocol for Group IV Single-layer 2D (Transition Metal Chalcogenides (TMCs) Nanosheets

한정희 천진우*

연세대학교 화학과

Single-layer 2D TMCs nanosheets have huge potential for application in photocatalysis, optoelectronics, and solar energy harvesting due to their remarkable electronic and optical properties. Although single-layer 2D TMCs nanosheets are advantageous for their various application, obtaining them is still challenging, since the multilayer structures are readily formed as stable products. Here, we present a solution-based synthetic protocol, which takes advantage of controlling chalcogen source (e.g., H_2S) influx, for the formation of group IV single-layer 2D TMCs (ZrS_2, TaS_2, HfS_2).While the burst influx of H_2S at the beginning forms group IV multilayer TMCs nanodiscs, the single-layer nanosheets could be obtained through the continuous and diluted H_2S influx in the entire reaction.Therefore, this study serves a new approach for altering the growth mode of 2D TMCs nanosheets in solution system, which can be achieved by controlling influx rate of precursor, providing the possibilities to be utilized for synthesizing various kinds of single-layer 2D TMCs nanosheets.

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Reduction of *N*-Cyanomethyl Groups on a Macrocyclic Nickel(Ⅱ) Complexes Using Sodium Borohydride

김현자 강신걸*

대구대학교 화학과

The nickel(Ⅱ) complexes $[Ni(L^3)]^{2+}$(L^3=2-(2-aminoethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0.$^{7.12}$]docosane) bearing one *N*-$CH_2CH_2NH_2$ pendant arms and $[Ni(L^4)]^{2+}$(L^4=2-(2-hydroxyethyl)-13-(2-aminoethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0.$^{7.12}$]docosane) bearing one *N*-$CH_2CH_2NH_2$ and one *N*-CH_2CH_2OH pendant arms have been prepared by the metal-assisted reaction of $[Ni(L^1)]^{2+}$(L^1=2-(*N*-cyanomethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0.$^{7.12}$]docosane) or $[Ni(L^2)]^{2+}$(L^2=2-(2-hydroxyethyl)-13-(cyanomethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.0.$^{7.12}$]docosane) with sodium borohydride under relatively mild conditions. In acid aqueous solutions, the *N*-$CH_2CH_2NH_2$ group of $[Ni(L^3)]^{2+}$ or $[Ni(L^4)]^{2+}$ is protonated to produce $[Ni(HL^3)]^{3+}$ or $[Ni(HL^4)]^{3+}$. Synthesis and characterization of the complexes bearing one *N*-$CH_2CH_2NH_2$ pendant arm are presented.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Pyrimidyl functionalizaion of schiff base type of bimetallic metal complex

김부현 허정석*

충남대학교 화학과

Many reports on, bimetallic complex revealed outstanding catalytic activities compared to monometallic metal complexes. To exploit its superiority, we've been researched bimetallic metal complex to find potent catalyst candidates enough to be applied for surface attached catalyst. We have developed synthetic route which allows one step synthesis of bimetallic complex. Our group developed new bimetallic complex with aldehyde group for further functionalization that has both sides consisted of pyrimidine type. Its aldehyde groups were converted to pyrimidyl group upon reaction with diamine compound. This result demonstrates our bimetallic complex is useful for the application of surface anchored type of catalyst. In the poster session, detailed synthesis, X-ray structure and characterization results of the bimetallic metal complex will be presented.

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Synthesis of Palladium(II) complexes containing phosphine and NHC ligands with bulky aryl group and their catalytic activity towards norbornene polymerization

이동진 이익모*

인하대학교 화학과

Pd(II) complexes containing various NHC(N-heterocyclic carbene) ligands have been successfully synthesized by the reaction with phosphines.Treatments of dinuclear Pd-Phosphine complexes $[(PPh_3)_2Pd_2(Ph)_2(\mu\text{-}OH)_2]$, with NHC salt such as IPr·HCl, IMes·HCl resulted in new $[(PPh_3)Pd(Ph)(NHC)Cl]$ complexes and these complexes are characterized by NMR and elemental anaylsis.Moreover, these new palladium complexes showed moderate to good catalytic activities towards norbornene polymerization.

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Reactivity Comparison of Cobalt(III)-Peroxo and Cobalt(III)-Hydroperoxo Complexes

신봉기 조재홍*

대구경북과학기술원(DGIST) 신물질과학

Metal-dioxygen adducts, such as metal-peroxo and -hydroperoxo species, are key intermediates that observed in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. Previously, manganese(III)-hydroperoxo complex, $[Mn(III)(TMC)(OOH)]^{2+}$ (TMC=1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane) was characterized and reactivity of this intermediate has been shown electrophilic character. In this work, using Me_3-TPADP (Me_3-TPADP=3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane) ligand, $[Co(Me_3\text{-TPADP})(CH_3CN)_2]^{2+}$ was synthesized and characterized by various physicochemical methods. Cobalt-peroxo complex, $[Co(Me_3\text{-TPADP})(O_2)]$+, was synthesized with H_2O_2 in the presence of triethylamine. Upon protonation, Co(III)-peroxo complex was converted into a Co(III)-hydroperoxo complex, $[Co(Me_3\text{-TPADP})(OOH)(CH_3CN)]^{2+}$. Interestingly, the Co(III)-hydroperoxo complex shows both nucleophilic and electrophilic reactivity. Nucleophilic reactivity of Co(III)-hydroperoxo complex is higher than that of Co(III)-peroxo complex.

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Porous 3-Dimensional Networks Consist of Cu(II) complexes: Catechol Oxidation Catalysis and Solvent Adsorption

김도언 정옥상*

부산대학교 화학과

The reaction of CuX_2 (X^- = ClO_4^- and BF_4^-) with a new 1,3,5-tris(isonicotinoyloxymethyl)benzene (L) ligand gives rise to 3D coordination networks, $[Cu_3L_4(CH_3CN)_6](X)_6$, with new topology of a Schl?fli point symbol, $\{4\cdot8^2\}_4\{4^2\cdot8^2\cdot10^2\}_2\{8^4\cdot12^2\}$. The 3D networks basically have oval-shaped pores with the dimensions of 11.2 × 11.2 × 24.8 Å^3 and 11.1 × 11.1 × 24.4 Å^3 for $[Cu_3L_4(CH_3CN)_6](ClO_4)_6$ and $[Cu_3L_4(CH_3CN)_6](BF_4)_6$, respectively.The 3D porous coordination networks act as good heterogeneous catalysts, which oxidize the catachols in the order of 3,5-DBuCat > 4-BuCat > 4-ClCat. The catalytic effect of $[Cu_3L_4(CH_3CN)_6](BF_4)_6$ is slightly higher than that of $[Cu_3L_4(CH_3CN)_6](ClO_4)_6$. The pores of the 3D networks reversibly adsorb the solvents in the order of $CHCl_3$ > THF > Me_2CO.

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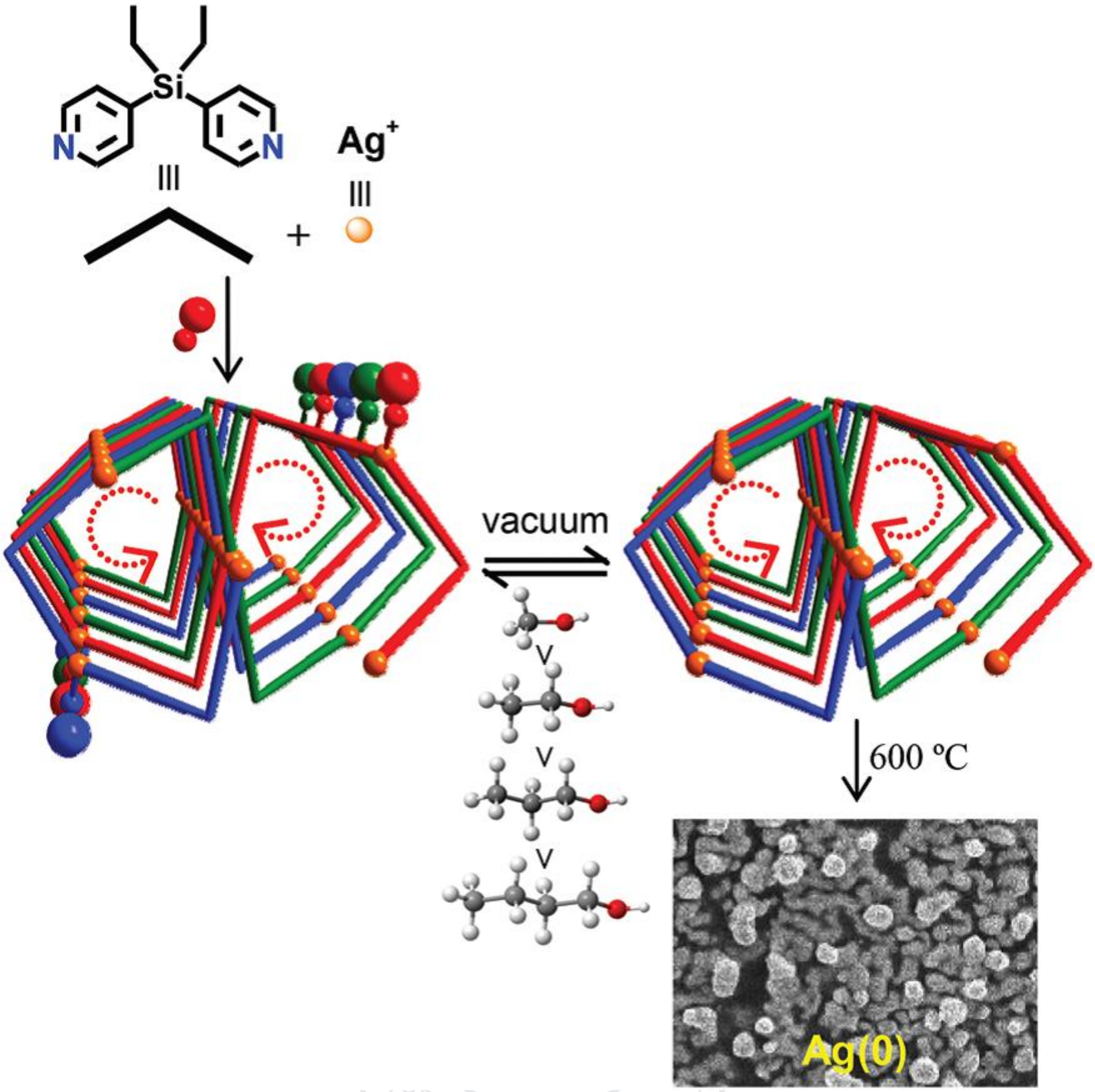
Synthesis and Characterization of Ag complexes of a diethylbis(4-pyridyl)silane

최은경 정옥상*

부산대학교 화학과

Designed helical coordination polymers' construction and functionalization have become hot issues in the field of multi-disciplinary supramolecular science over the past two decades, owing to their practical applications in asymmetric catalysis, chiral separation, non-linear optics, template precursors, memory devices, and molecular-level reaction vessels. The recent construction of a new type of helical motif, then, has been met with great interest.Self-assembly of silver triflate with L in alcohol solvent produces characteristic triple-meso helices $[Ag_3(L)_3(ROH)](CF_3SO_3)_3$ (L = diethylbis(4-pyridyl)silane; R = Me, Et, *n*-Pr, and *n*-Bu) with six units in each turn. Their unit cell volumes are sensitive to the size of the coordinated alcohol molecules. An unusual "alcohol molecules at triple-*meso* helices" system is a characteristic reversible alcohol container and discriminator via appropriate association/dissociation. The helical crystalline solids are favored in the order MeOH > EtOH > *n*-PrOH > *n*-BuOH via an interaction between the silver(I) ion and the alcohol molecule. The crystals evaporate the coordinated alcohol molecules at low temperatures, and finally calcination at 600 °C produces micro-sized chaotic surface materials consisting of silver(0) without silicon(IV) oxide.


Si
N
N
Ag+
vacuum
V
V
V
600 ºC
Ag(0)

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Cyclodimeric Copper(II) Complexes of 1,4-Bis(dimethyl(quinolin-3-yl)silyl)benzene: Steric Effects and Substrates on Catechol Oxidation Catalysis

김혜은 정옥상*

부산대학교 화학과

Reaction of CuX_2 with new ligand, 1,4-bis(dimethyl(quinolin-3yl)silyl)benzene (L), in alcohol affords C_2-symmetric double-alkoxy-supported cyclodimeric copper(II) complexes, $[Cu(\mu\text{-}OR)(L)]_2(X)_2$ (R = Me, Et, ^{i}Pr; X^- = ClO_4^-, BF_4^-) in high yields. These cyclodimeric species with intracyclic Cu…Cu distances of 2.92-2.98 Å show the significant catalytic effects on the catechol oxidation catalysis in chloroform in the order $[Cu(\mu\text{-}OMe)(L)]_2(X)_2$ > $[Cu(\mu\text{-}OEt)(L)]_2(X)_2$ > $[Cu(\mu\text{-}O^iPr)(L)]_2(X)_2$. Furthermore, the catalytic efficiency is strongly substrate-dependent in the order 4-BuCat > 4-ClCat > 3,5-DBuCat > Cat. Such notable catalytic effects potentially can be explained by the steric hindrance of both catalysts and substrates.

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Crystallization and Photoluminescence Properties of Silver(I) Complexes According to the Anion Effects

김정균 정옥상*

부산대학교 화학과

The anion effects on the formation and photoluminescence (PL) of a series of AgX (X^- = NO_2^-, NO_3^-, ClO_4^-, and PF_6^-) compounds with naphthalene-2,3-diyl-diisonicotinate (L) were investigated. According to the single-crystal X-ray structures, the NO_2^-, NO_3^-, and ClO_4^- anions act as anionic ligands rather than as simple counteranions whereas the PF_6^- anion acts as a simple counteranion. Correspondingly, the dinitroargentate anionic species, $Ag(NO_2)_2^-$, was observed in the solid state. The PL intensity of the present compounds, moreover, was proportional to the Ag…X distance, namely the metallophilicity of the anions. The weak- or non-coordinating anions, ClO_4^- and PF_6^-, could be smoothly exchanged with the NO_2^- or NO_3^- anion, whereas the reverse exchanges did not occur. The compounds' physicochemical properties were characterized by means of infrared (IR) spectroscopy, thermogravimetric analysis (TGA)/differential scanning calorimetry (DSC), and photoluminescence (PL).

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-39**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ensembles of Metallacyclodimeric Zinc(II) Complexes for Recognition of Dihalomethane Molecules

조윤정 정옥상*

부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with 2,7-bis(nicotinoyloxy)naphthalene (L) as a hemi-circular bidentate ligand containing chromophore moiety yields a systematic metallacyclodimeric unit, $[ZnX_2(L)]_2$. These basic skeletons constitute, via interdigitated π…π interactions, a unique columnar ensemble forming a suprachannel. This can then be employed as an unusual "diiodomethane within the suprachannel" host-guest system, $CH_2I_2@[ZnX_2(L)]_2$. Specifically, the suprachannel significantly stabilizes the CH_2I_2 molecules in the order $[ZnI_2(L)]_2 > [ZnBr2(L)]_2 > [ZnCl_2(L)]_2$. This suprachannel has significant halogen effects on the photoluminescence (PL), thermal properties, and host-guest inclusion.

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장소: 대구 EXCO
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Organization and Properties of Cyclodimeric Cu(II) Complexes Containing Free Nitrogen-Donors via Crystal-Facial Effects

이해리 김병주 정옥상*

부산대학교 화학과

Reaction of MX_2 (M = Cu(II), Hg(II); X^- = Cl^-, Br^-) with C_3-symmetric tris(6-quinolyl)trimesic ester (L) produces crystals consisting of C_2-symmetric metallacyclodimeric species with two free quinolinyl *N*-donors, $[CuX_2L]_2$. The crystals self-aggregate each other in aqueous media. Furthermore, the reaction with cotton threads and glass-fibers form unique crystal organization on/with cotton threads and glass fibers, respectively. Such crystal aggregation/organization may be ascribed to the hydrogen bonding interactions between the free quinolinyl *N*-donors and the hydroxyl (-OH) groups of water, cotton-threads, or glass-fibers. The composite organization of crystals on/with glass-fiber, $[CuX_2L]_2$@glass, is an effective recyclable heterogeneous catalytic system on catechol oxidation, indicating that the free quinolinyl N-donors on the crystal surface play a significant role in the catalysis. The treatment of $[CuX_2L]_2$ crystals with K_2PdCl_4 produces a conceptually advanced composite materials $PdCl_2$@$[CuX_2L]_2$ via Pd(II)-N interaction, which are useful to Suzuki-Miyaura C-C coupling reaction.Reference[1] Kim, B. J.; Lee, H.; Noh, T. H.; Jung, O.-S. CrystEngComm 2015, 17, 4241-4410.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-41**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Modulation of Amyloid-β Aggregation Pathways by Iridium(III) Complexes

강주혜 이신정[1] 권태혁[2,*] 임미희[*]

울산과학기술대학교(UNIST) 자연과학부/화학과 [1]포항공과대학교(POSTECH) 화학과 [2]울산과학기술대학교(UNIST) 친환경에너지 공학부

Iridium(III) complexes are known to have properties to convert triplet dioxygen into singlet dioxygen or superoxide anion upon the treatment with light. These produced reactive oxygen species are shown to oxidize peptides and proteins and further induce their crosslinking. Utilizing such properties, we have applied Ir(III) complexes to modulate the aggregation pathways of amyloidogenic peptides. The aggregated amyloidogenic peptides are found in brains of neurodegenerative disease [*e.g.*, amyloid-β (Aβ) aggregates in the brain of Alzheimer's disease] and are suggested to be linked to neuropathogenesis. Thus, significant efforts on developing chemical reagents capable of controlling the aggregation of amyloidogenic peptides have been recently made. Herein, we will present the synthesis, characterization, and reactivity of Ir(III) complexes, newly designed for regulating Aβ aggregation based on their photophysical properties. Some mechanistic studies for the anti-amyloidogenic activity of our Ir(III) complexes will also be discussed.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간

장소: 대구 EXCO

발표코드: **INOR.P-42**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Porphyrin Nanoparticles of Heterometallic Porphyrins Assembled by Cooperative Coordination of Tin(IV) and Zinc(II) Porphyrins

조민경 김희준*

금오공과대학교 응용화학과

Multiporphyrin architectures have been much used as photosynthtic system mimics, and for the creation of artificial enzymes and functional molecular devices. Porphyrin nanoparticles are promising components of advanced materials because of the rich photochemistry, stability, and proven catalytic activity. It is expected that nanoparticles of porphyrins will have unique photonic properties not obtainable by larger-scaled materials containing the macrocycle, or by the molecules themselves. Here we present heterometallic porphyrin nanoparticles assembled by the cooperative coordination of tin- and zinc-porphyrins with complementary building blocks.

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장소: 대구 EXCO
발표코드: **INOR.P-43**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Oxygen Vacancy Mediated Pt Deposition Process on In_2O_3 Nanocrystal Investigated at the Interior Cavity Protected by a Hollow Silica Nanoshell

조영신 이인수[1,*]

포항공대 화학과 [1]포항공과대학교(POSTECH) 화학과

The inorganic surface of nanomaterial is regarded as an active element that takes part in a diverse range of interfacial reactions with ions and molecules dissolved in a solution. Over the past decade, the chemical and morphological changes during surface-involving reactions has been exploited to devise post-synthetic transformation strategies for complex hybrid nanoparticles, which render pre-synthesized nanoparticles of more complicated structure or of heterojuction interface between dissimilar materials. In particular, redox reactions between metal oxide and dissolved metal ions, which involves the growth of in-situ reduced metallic species on the surface of non-colloidal semiconductor material, were very recently adopted by pioneering researchers for producing semiconductor/noble-metal hybrid nanocomposites with intimately contacting heterojuction interfaces, such as TiO_2/M (M = Au, Pt, Ag) and WO_3/M (M = Rh, Au, Pt, Ag), which exhibited the improved activity and stability in the photocatalytic performance. Notwithstanding this extendible applicability, the innate surface-reactivity of the inorganic nanoparticles has not been investigated thoroughly due to the impediment of surface-capping organic surfactants which is required for their colloidal dispersion. In other hand, the alternative attempt with surfactant-free nanoparticles, which are subject to the sintering or aggregation in suspension, mostly has led to the inhomogeneity in reactivity among nanoparticles or regions of their surfaces. In this paper, we presents our efforts to explore the newly discovered Pt deposition phenomenon on the In_2O_3 semiconductor nanoparticle, by employing the hollow silica nanosphere as a nanosized incubation-box which allows for the in-depth examination of the reaction of the intact In_2O_3 surface under the systematic variation of surface parameters such as curvature, crystallinity, exposed facets, and density of the defect. The hollow silica nanosphere can be considered to best suits the purpose of this study on account of the ability to isolate a single nanoparticle inside the cavity and maintain all its surface area accessible to the reaction, without using any interfering organic surfactants or even after the high-temperature treatment for alternating its surface parameters. The confined reaction within the protected interior space was envisioned to provide the reacting inorganic surface for undisturbed and consistent environment, thus allowing for the homogeneous reactivity for all the nanoparticles and over a broad range of reaction conditions. In addition, the porous silica nanoshell, which is selectively permeable for dissolved solution species, also can help to identify the surface-involving reaction from those occurring in the outer solution. Accordingly, the hollow nanoreactor-based investigation identified that the Pt deposition is templated by the defective In_2O_3 surface via the spontaneous redox process including the reduction of Pt^{2+} species by the oxygen vacancy of the In_2O_3 lattice whose density could be manipulated by changing the annealing temperature. The acquired insight into the controllable reactivity of the In_2O_3 surface led to the surfactant-free and electroless strategy of uniformly decorating In_2O_3 nanoparticle with directly grown Pt nanocrystals, which can help to modulate band gaps and charge-transfer properties of semiconductors and also endows supported metal catalysts with increased activity and durability. In this context, this study also attempted to develop a novel protocol for the modification of indium tin oxide (ITO) electrode with Pt-catalyst-decorated In_2O_3 nanoparticles (In_2O_3@Pts), which may enable more sensitive and stable performance in electrogenerated chemiluminescence (ECL)-based analyses, thus proving the extensibility and usefulness of the newly explored Pt deposition strategy. This paper reports the highly enhanced electrochemical activity of transparent In_2O_3@Pts?modified ITO electrode in oxidizing $Ru(bpy)_3^{2+}$/tripropylamine (TPrA) system, resulting in much increased ECL emission.

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발표코드: **INOR.P-44**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of nickel(II) complexes of hexadentate Schiff base ligands derived from bis(ethylamine)

임종완

심인고등학교 화학

The nickel (II) complex with Schiff base ligand derived from the condensation of bis(ethylamine) and salicylaldehyde have been prepared and investigated using different chemical techniques such as elemental analysis, infra-red, electronic spectra, NMR and magnetic moment. The crystallographic analysis of the complex revealed that the two Nickel compex is dinuclear structure.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-45**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Water as an agent for the morphology modification of mixed metal oxalate materials on the nanoscale: from sheets to rods

김민옥 박규순[1] 윤성호[2,*]

국민대학교 화학과/생명나노화학 [1]국민대학교 화학과 [2]국민대학교 생명나노화학과

Mixed metal oxide has been of interest to improve the performance of metal oxides, which have pros (e.g. high chemical stability, conductivity, mechanical flexibility, harmlessness and economic nature) and cons (e.g. low sensitivity, high working temperature, long response and recovery time), as pigments, gas sensor, catalyst, supercapacitors, and Li-ion batteries. Moreover, facile synthesis methods that control crystal architecture are of great interest because the nanoscale morphology of metal oxides alters the physical and chemical properties of bulk materials. Precursors for metal oxide have been continuously studied because they can often be tailored structurally; Metal oxalates, where oxalate (C2O4) is the simplest dicarboxylate, are known to transform into the corresponding metal oxides with high degrees of shape retention or similarity as well as the advantages of low cost, various preparation methods, and easy transformation at relatively low temperatures.A number of approaches have been used to control the shape of metal oxalates, which often used as precursors for metal oxide nanomaterials. However, attempts to use water as a regulator have not been reported. Here in we report systematic studies on related topics: nanosheets, composed of 1-dimensional [Zn3/4M1/4(C2O4)(EG)] (M=Co or Ni) polymeric structure, could be transformed into nanorods by using water as an shape-shifting agent. In addition, heat-treatment of these nanomaterials with diverse morphologies resulted in porous metal oxides with high degrees of shape retention.We acknowledged the financial support by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean government.

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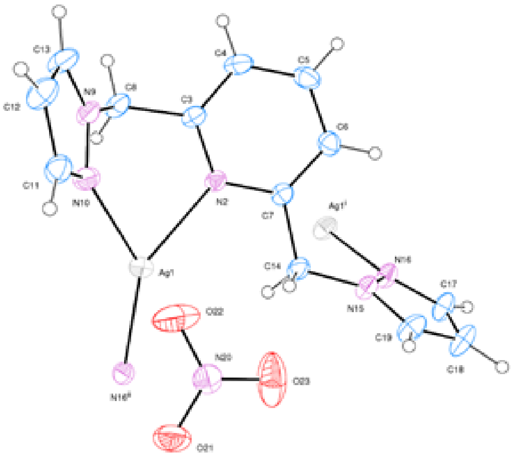
장소: 대구 EXCO
발표코드: **INOR.P-46**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

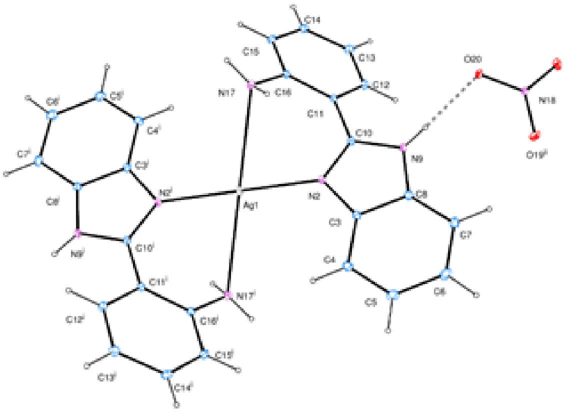
Synthesis and Structures of Ag(I) Complexes with Heterocyclic N-donor Ligands

김용태 김대영 강성권*

충남대학교 화학과

[Ag(PMP)]·(NO_3) and [Ag(APBI)$_2$]·(NO_3) complexes are synthesized and characterized by UV, IR and single crystal X-ray diffractometer. In the crystal structure of [Ag(PMP)]·(NO_3) complex, the coordination geometry around the Ag(I) metal center is a distorted trigonal planar, with three N atoms of two bidentate/monodentate pyrazoylpyridyl (PMP) ligands. The complex cations are arranged in polymeric chains along the *c*-axis direction, with the nitrate counter anions situated in the lattice.The [Ag(APBI)$_2$]·(NO_3) complex adopts a distorted square planar geometry with four coordinated N atoms of two bidentate 2-(1*H*-benzimidazol-2-yl)aniline (APBI) ligands. This Ag(I) cations are linked by intermolecular hydrogen bonds in zig-zag chains along the *c*-axis direction.





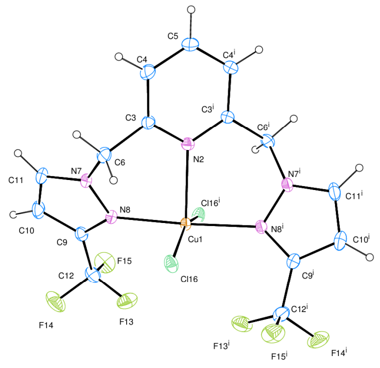
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-47**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

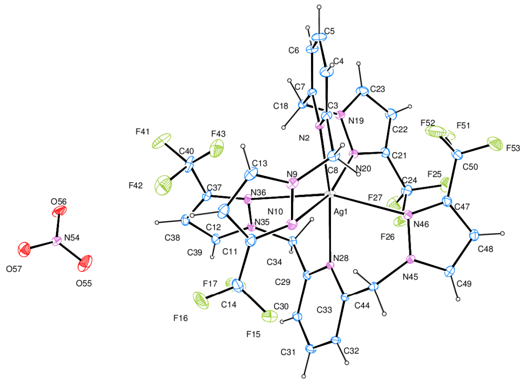
Synthesis and Structures of Cu(II) and Ag(I) Complexes with 2,6-bis((3-(trifluoromethyl)-1*H*-pyrazol-1-yl)methyl)pyridine Ligand

김용태 강성권*

충남대학교 화학과

Tridentate NNN ligand, 2,6-bis((3-(trifluoromethyl)-1*H*-pyrazol-1-yl)methyl)pyridine (TPMP), is designed and synthesized to investigate the related metal complexes. [Cu(TPMP)·Cl_2] and $[Ag(TPMP)_2]\cdot(NO_3)$ complexes are characterized by UV, IR and single crystal X-ray diffractometer. The coordination geometry around the metal Cu(II) center is square pyramidal with three N atoms of TPMP ligand and two Cl atoms. Ag(I) complex adopts a distorted trigonal antiprism geometry with six N atoms of two TPMP ligands.





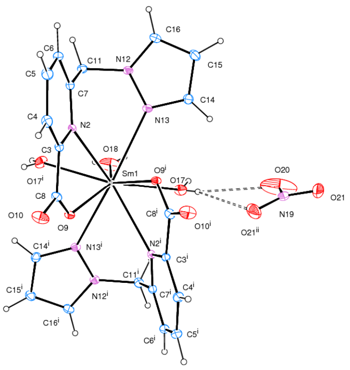
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-48**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

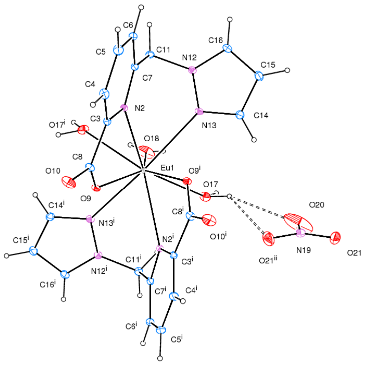
Photoluminescence and Crystal Structures of Lanthanide Metal Complexes with 6-((1*H*-pyrazol-1-yl)methyl)picolinate(PMPN) Ligand

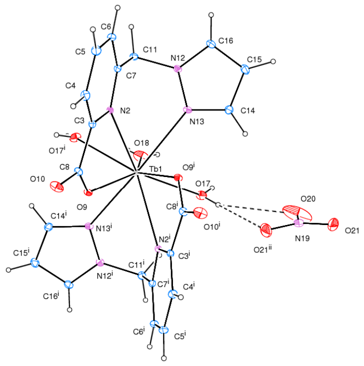
김대영 강성권*

충남대학교 화학과

Tridentate NNN ligand, 2,6-bis((1*H*-pyrazol-1-yl)methyl)pyridine(PMP), is designed and synthesized to investigate the related metal complexes. PMP ligand is oxidized to 6-((1*H*-pyrazol-1-yl)methyl)picolinate(PMPN) by nitrate anion of metal salts. $[Ln(PMPN)_2(H_2O)_3]\cdot(NO_3)$ (Ln = Sm, Eu, and Tb) complexes are synthesized and characterized by UV, PL spectra and single crystal X-ray crystallography. The coordination geometry around the metal center is a distorted tricapped trigonal prism, with the metal nine-coordinated by O atoms and N atoms from PMPN and aqua ligand. The unit cells and volumes of theses complexes show the lanthanide contraction.







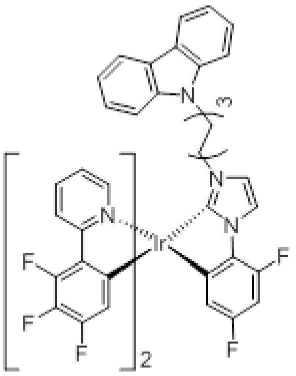
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-49**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

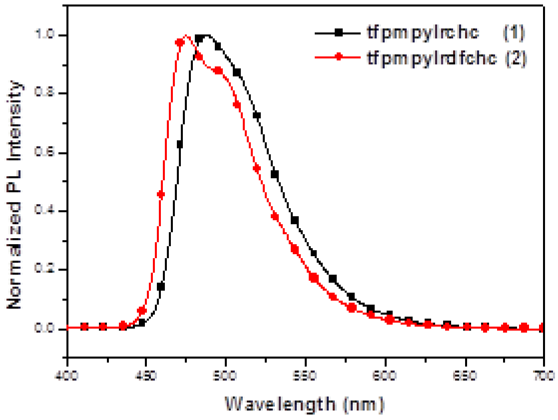
Sky-blue Phosporescent Iridium(III) Complexes with Carbene as Ancillary Ligands for Organic Light-Emitting Diodes (OLEDs)

최지혜 김영인* 송영광[1] 전진실

부산대학교 화학교육과 [1]부산대학교 화학소재과

Organic lignt-emiting diodes (OLEDs) with high performances phosphorescent materials have attracted broad attentions. In addition, cyclometalated iridium(III) complexes have property to achieve the theoretical upper limit of external quantum efficiency for red, green and blue phosphorescent organic light-emitting devices. We synthesized and characterized the carbene based ancillary ligands for efficient iridium(III) complexes ; tfpmpyIrchc (1), tfpmpyIrdfchc (2) (tfpmpy = 4-methyl-2-(2,3,4-trifluoromethyl)pyridine ; chc = 1-phenyl-3-hexylcarbazolylimidazolin-2-ylidene ; dfchc = 1-(2,4-difluorophenyl)-3-hexylcarbazolylimidazolin-2-ylidene). In addition, the photophysical and electrophysical properties of this complexes were investigated.The phosphorescence properties of complexes (1) and (2) showed sky-blue emission at 487, 474 nm in PL spectra and exhibited quantum yield at 42, 47% in dichloromethane solution, respectively. The complexes (1) and (2) showed band gap of sky-blue region as 2.76, 2.81 eV, respectively.


N
3
N
N
N
Ir
F
F
F
F
F
2


tfpmpyIrchc (1)
tfpmpyIrdfchc (2)
Normalized PL Intensity
0.0
0.2
0.4
0.6
0.8
1.0
400
450
500
550
600
650
700
Wavelength (nm)

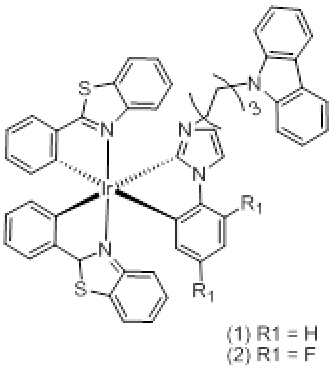
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-50**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

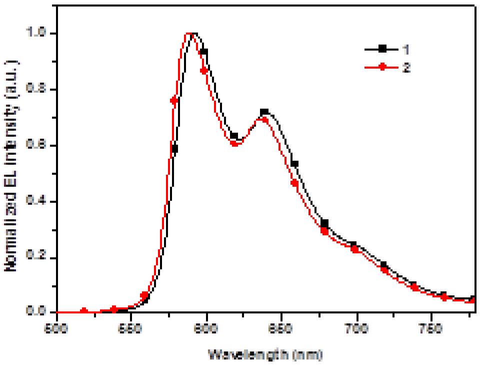
Orange-red Phosporescent Iridium(III) Complexes Showing Wide Region Emission for Organic Light?Emitting Diodes (OLEDs)

송영광 김영인[1,*] 최지혜[1] 전진실[1]

부산대학교 화학소재과 [1]부산대학교 화학교육과

we have reported phosphorescent heteroleptic cyclometallated iridium(III) complexes for their application for organic light-emitting diode(OLEDs) due to their high performance in the devices and easy control of color tuning. In this research, we designed and synthesized two cyclometalated Ir(III) complexes containing two 2-phenylbenzothiazole and one carbene derivative as C^C ancillary ligand ; pbtIrchc (1), pbtIrdfchc (2), (pbt = 2-phenylbenzothiazole ; chc = 1-phenyl-3-hexylcarbazolylimidazolin-2-ylidene and dfchc = 1-(2,4-difluorophenyl)-3-hexylcarbazolylimidazolin-2-ylidene). In addition, the photophysical, electrophysical properties and devices performance of complex (1) and (2) were investigated.Two complexes showed similar band gap of orange-red region as 2.47 eV for (1) and (2), respectively. The complex (1), (2) showed wide region phosphorescent emissions with shoulder. The complex (1) showed maximum PL spectra at 586.4, 689.8 nm, the complex (2) showed 583.6, 625.8 nm in solution and exhibited good quantum yields of 1.94, 1.71 % in dichloromethane solution, respectively.


S
N
Ir
N
S
N
N
3
N
R1
R1
(1) R1 = H
(2) R1 = F


Normalized EL intensity (a.u.)
Wavelength (nm)
1.0
0.8
0.6
0.4
0.2
0.0
500
550
600
650
700
750
1
2

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-51**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Zn(II) and Cu(II) Complexes Containing (1R)-(+)-Camphor imino-based with N^2-alkyl Derivatives for Ring Opening Polymerization from *rac*-Lactide

권경섭 정종화*

경북대학교 화학과

New zinc complexes based on bidentate ligands, (E)-N^1,N^1-dimethyl-N^2-(1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene)ethane-1,2-diamine and (E)-N^1,N^1-diethyl-N^2-(1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene)ethane-1,2-diamine have been synthesized in high yield and purity. The crystal structures of the complexes were determined by X-ray crystallography. The well characterized complexes were employed as an initiator for ring opening polymerization of *rac*-Lactide. The active catalyst species was generated by treating air and moisture stable $ZnCl_2$ complex and $CuCl_2$ complex with $LiOCH(CH_3)_2$, *in situ*. The complexes were found to be highly efficient initiator yielding the PLA with well molecular control and narrow molecular weight distribution. Furthermore, the heterotactic PLA with P_r up to 0.90 can be obtained by initiating ROP of *rac*-lactide in CH_2Cl_2. The molecular weight of the polymer was determined by ^{1}H-NMR spectra and GPC.

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Synthesis and Molecular Structure of Copper(II) Complexes Bearing *N*,*N*-Pyrazolylpyridinyl Group Substituted (*S*)-1-Phenylethylamine

함지혜 정종화*

경북대학교 화학과

Novel three dichloro copper(II) complexes ligated by the tridentate ligands, L^1 ? L^3, where L^1 is *N*-((1*H*-pyrazol-1-yl)methyl)-1-phenyl-*N*-((pyridin-2-yl)methyl)ethanamine, L^2 is *N*-((3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)-1-phenyl-*N*-((pyridine-2-yl)methyl)ethanamine, and L^3 is *N*-((3,5-diisopropyl-1*H*-pyrazol-1-yl)methyl)-1-phenyl-*N*-((pyridine-2-yl)methyl)ethanamine, have been synthesized in high yield and purity. The molecular structures of the Cu(II) complexes were determined by X-ray crystallography. Interestingly, two diastereomer of (C_S N_R) and (C_S N_S) are co-crystallized therefore the asymmetric unit contains the diastereomer pair. All Cu(II) complexes were five-coordinate and mildly distorted trigonal bipyramidal depending on the ligand employed as centers linked with three nitrogen atoms of the ligand in tridentate coordination mode along with two chlorido ligands.

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Metal-Organic Frameworks로부터 유래된 계층적 다공성 탄소 나노 소재의 방사성 요오드 및 이산화탄소 흡착 성능 평가

김혜련 이창연[1,*]

인천대학교 에너지화학공학과 [1]인천대학교 에너지 화학공학과

다공성 탄소 소재는 높은 표면적 및 공극률과 함께 열적/화학적 안정성을 지닌 물질로 기체의 저장과 분리, 촉매 작용, 에너지 저장과 전환 등의 다양한 분야에 걸쳐 응용되고 있다. 이 소재는 제올라이트나 실리카 메조포러스를 고체 주형으로 사용하여 정렬된 나노 혹은 메조 탄소 세공체를 합성하는 이른바 nanocasting 방법을 사용하여 합성되고 있다. 최근 금속-유기 골격체(Metal-Organic Framework, MOF)를 템플릿 또는 전구체로 이용하여 다공성 탄소 소재를 합성하는 연구가 시도되어 왔다. MOF 는 금속 이온 또는 금속 클러스터가 유기 리간드에 의해 연결되어 3 차원 골격 구조를 형성한 다공성 물질로 표면적과 기공 부피가 크고 화학적 특성을 조절할 수 있다는 장점을 지닌다. 특히 MOF 의 특성 중 하나인 규칙적으로 정렬된 내부 구조와 풍부한 유기 리간드는 정렬된 구조를 가지는 다공성 탄소 소재를 형성시키기에 적합하다. 이러한 특성으로 인해 템플릿 또는 전구체로써 MOF 를 열분해시켜 다공성 탄소 소재를 형성시키는 방법이 연구되어 왔다. 다공성 탄소 소재는 용도에 따라 요구되는 특성이 다르기 때문에 적절한 합성 조건에 대한 연구가 필요하다. 본 연구에서는 방사성 요오드와 주요 온실 기체인 이산화탄소 포획을 위한 흡착제 개발을 목표로 다공성 탄소 소재를 합성하였다. 합성 과정에서 전구체인 MOF 의 종류와 열분해 조건을 조절하여 다공성 탄소 소재의 기공 구조와 heteroatom 의 도핑 등 물질의 특성이 흡착 성능에 미치는 영향을 연구하였다. Acknowledgments This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis and Characterization of Copper(I) Iodide Coordination Polymers Based on Hexagonal Ring Shaped Thioether Ligands

장호재 강기행 권은진 김태호* 김재상*

경상대학교 화학과

The cuprous ion as one of soft acids favors to coordinate soft base ligands containing S donor atoms. The reactions of CuI and hexagonal ring shaped ligands which are pentamethylene sulfide (L^1) and 1,4-thioxane (L^2) yield two coordination polymers (CPs), $[Cu_8I_8L^1_4(MeCN)_2]_n$ (1) and $[Cu_6I_6L^2_4(MeCN)_2]_n$ (2), respectively. CP 1 shows a 1D chain structure based on S shaped ladder Cu_8I_8 cluster units. CP 2 shows a 1D chain structure based on the combination of Cu_2I_2 rhombiod dimers and Cu_4I_4 stair step tetramers. CP 1 has bright orange color luminescence under ultraviolet irradiation whereas CP 2 has no luminescence. Syntheses, structural characterizations, thermal and photoluminescence properties of two new Cu(I) CPs 1 and 2 are presented.

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Photophysical and Structural Properties of Cu(I) Coordination Polymers Based on N/S Mixed Donor Ligands

임한수 강기행 권은진 장호재 김태호* 김진은*

경상대학교 화학과

The pyridyl ligands (L^1 and L^2) with thioether substituents were synthesized by the reaction of 2-chloroethyl cyclohexyl sulphide or 2-chloroethyl benzyl sulphide and 3-hydroxypyridine. Two Cu(I) coordination polymers (CPs), $[CuIL^1]_n$ (1) and$[CuIL^2]_n$ (2) were prepared by the reaction of CuI and ligands, L^1 and L^2. CPs 1 show a 2D network structure and CPs 2 show a 1D loop chain structure, based on a rhomboid Cu_2I_2 cluster node. We report crystal structures, thermal behaviors and photophysical properties of the CPs based on N/S mixed donor ligands.

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Reversible Solvent Exchange, Crystal Transformation and Photophysical Properties of Cu(I) Coordination Polymers Based on 4-(2-(Cyclohexylthio)ethoxy)pyridine

박현진 권은진 강기행 김태호* 김진은*

경상대학교 화학과

Solvent-responsive four Cu(I) coordination polymers (CPs) $[Cu_4I_4\mathbf{L}_2]n$ (**1**), $\{[Cu_4I_4\mathbf{L}_2]\cdot CHCl_3\}n$ (**2**), $\{[Cu_4I_4\mathbf{L}_2]\cdot CHCl_2\}n$ (**3**) and$\{[Cu_4I_4\mathbf{L}_2]\cdot C_6H_6\}n$ (**4**) were prepared by the reaction of CuI and 4-(2-(Cyclohexylthio)ethoxy)pyridine (**L**). CPs **1-4** are pseodupolymorphic supramolecular isomers with a 1D loop chain structure, based on cubane-like Cu_4I_4 cluster nodes. Crystal-to-crystal transformation of CP **2** to **3** were reversible under appropriate solvent coordination (chloroform or dichloromethane). We report crystal structures, thermal behaviors and photophysical properties of the CPs based on **L** with N/S mixed donor atoms.

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Luminescence Solvatochromism and Reversible Crystal Conversion of Cu(I) Supramolecular Isomers

권은진 강기행 장호재 김태호* 김진은*

경상대학교 화학과

Four solvent-responsive copper(I) coordination polymers (CPs), namely $[Cu_2I_2L_2]_n$ (1), $[Cu_4I_4L_2]_n$ (2), $\{[Cu_4I_4L_2]\cdot CH_2Cl_2\}_n$ (3), and $\{[Cu_2I_2L]\cdot 0.5C_7H_8\}_n$ (4) were prepared by the reaction of CuI with 3-(2-(*tert*-butylthio)ethoxy)pyridine (L) via self-assembly under varying solvent conditions. CP 1 is composed of butterfly-like Cu_2I_2 cluster nodes and CPs 2-4 are composed of cubane-like Cu_4I_4 cluster nodes. CP 1 shows blue light emission under UV irradiation and CPs 2-4 emit green, yellow, yellow green light, respectively. Crystal-to-crystal transformations of CP 2 to 3 or 4 occurred reversibly in solvents such as dichloromethane or toluene. The results of our investigation including syntheses, structural characterization, thermal and photoluminescence properties of four new Cu(I) CPs 1-4 are presented.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Reversible Luminescence Vapochromism and Crystal-to-Amorphous-to-Crystal Transformations of Pseudopolymorphic Cu(I) Coordination Polymers

강기행 권은진 장호재 김태호* 김진은*

경상대학교 화학과

Four solvent-responsive one-dimensional copper(I) coordination polymers (CPs), namely $\{[Cu_4I_4L(MeCN)_2]CH_2Cl_2\}_n$ (1), $\{[Cu_4I_4L(MeCN)_2]CHCl_3\}_n$ (2), $\{[Cu_4I_4L(MeCN)_2]0.5p\text{-xylene}\}_n$ (3), and $[Cu_4I_4L(MeCN)_2]_n$ (4), were prepared by reaction of CuI with *N*,*N′*-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide (L) via self-assembly under varying solvent conditions. CPs 1-4, which are pseudopolymorphic supramolecular isomers derived from solvent molecules, are composed of Cu_4I_4 cubane clusters. The ligands in CPs 1-3 adopted a *syn*-conformation, whereas in CP 4 they were observed in the *anti*-conformation. This occurred via *syn* to *anti* transitions of MeCN vapor upon heating. In addition, a reversible anti to *syn* transition was achieved by agitating in mixed organic solvents. It was shown that ligand transition from the *syn*- to the *anti*-conformation occurred through crystal-to-amorphous-to-crystal (CAC) transformations. Furthermore, CPs 1-3 exhibited reversible solvent exchange and crystal transformation of vapors from volatile organic compounds (VOCs).

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Structural Variations and Reactivity of Transition Metal Complexes with N,N'-(ethylene-di-p-phenylene)bis(pyridine-2-carboxamide)

김오연 김유정[1] 정종화 이홍인[*]

경북대학교 화학과 [1]이화여자대학교 과학교육과

Carboxamide group, found in the primary structure of proteins, is an important ligand construction unit for coordination chemistry. Especially, metal complexes containing phenyl-pyridyl-carboxamide groups have been found to be useful in asymmetric catalysis, molecular receptors and dendrimer synthesis. To investigate the diversities of the complex structures and reactivities, we have developed a tetradentate ligand, H_2EBPP (=N,N'-(ethylene-di-p-phenylene)bis(pyridine-2-carboxyamide)), to be utilized for synthesizing vanadium, chromium, manganese, iron, cobalt, nickel, copper, and ruthenium complexes. Crystallographic studies of the complexes revealed the variations of the structures from monomeric to tetrameric metal complexes depending on the metal ions, their oxidation states and the first coordination spheres. Catecholase (catechol oxidase), catalyzing the oxidation of catechols to the corresponding o-quinones accompanying with the four-electron reduction of O_2 to $2H_2O$, is a type-3 copper protein containing dinuclear copper center. Many model copper complexes have been reported to show catecholase activities. Recent development of non-copper metal complexes with catecholase activities have attracted considerable interests in the catalytic mechanism of catecholase reactions. Among the complexes containing the EBPP ligand, copper, manganese and cobalt complexes showed unexpectedly-high catecholase activity when the complexes were treated with 3,5-di-tertbutylcatechol (3,5-DTBC) in the presence of air at basic condition. First part of this poster will present the crystallographic investigations of the vanadium, chromium, manganese, iron, cobalt, nickel, copper and ruthenium complexes containing EBPP ligand. Second part will present the reaction pathway of catecholase activities of the copper, manganese and cobalt complexes, revealed by EPR, ESI-MS and UV-Vis kinetic measurements.

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Fluorescent Chemosensing of Aromatic Compounds by Supramolecular Porphyrin-Viologen-Cucurbit[8]uril System

손정인 김희준*

금오공과대학교 응용화학과

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

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Inter- and Intra-Molecular Interaction in Organic-Inorganic Alucone Polymeric Films using Molecular Layer Deposition

박이슬 김혜인 이진석*

숙명여자대학교 화학과

Molecular layer deposition (MLD) is sequential, self-limiting surface reaction to form conformal and ultrathin polymer film. This technique typically uses bifunctional precursors for stepwise sequential surface reaction and entirely organic polymer films. Also, in comparison with solution-based technique, because MLD is vapor-phase deposition based on ALD, it allows epitaxial growth of molecular layer on substrate and is especially good for surface reaction or coating of nanostructure such as nanopore, nanochannel, nanwire array and so on. 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. But this tendency of linear growth of the films versus number of MLD cycles is confirmed to reduce with increasing of the number of alkyl chains. 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.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Orientation Controlled Growth of Organic Polyurea Films by Molecular Layer Deposition

김혜인 박이슬 이진석*

숙명여자대학교 화학과

Molecular layer deposition (MLD) is sequential, self-limiting surface reaction to form conformal and ultrathin polymer film. This technique typically uses bifunctional precursors for stepwise sequential surface reaction and entirely organic polymer films. Also, in comparison with solution-based technique, because MLD is vapor-phase deposition based on ALD, it allows epitaxial growth of molecular layer on substrate and is especially good for surface reaction or coating of nanostructure such as nanopore, nanochannel, nanwire array and so on. In this study, polyurea film that consisted of phenylenediisocyanate(PDI) and phenylenediamine(PDA) was formed by MLD technique. In situ Fourier Transform Infrared (FTIR) measurement on high surface area SiO2 substrate was used to monitor the growth of polyurea film. Also, to investigate orientation of chemical bonding formed polymer film, plan-polarized grazing angle FTIR spectroscopy and raman spectroscopy were used. It showed epitaxial growth and uniform orientation of polyurea films.

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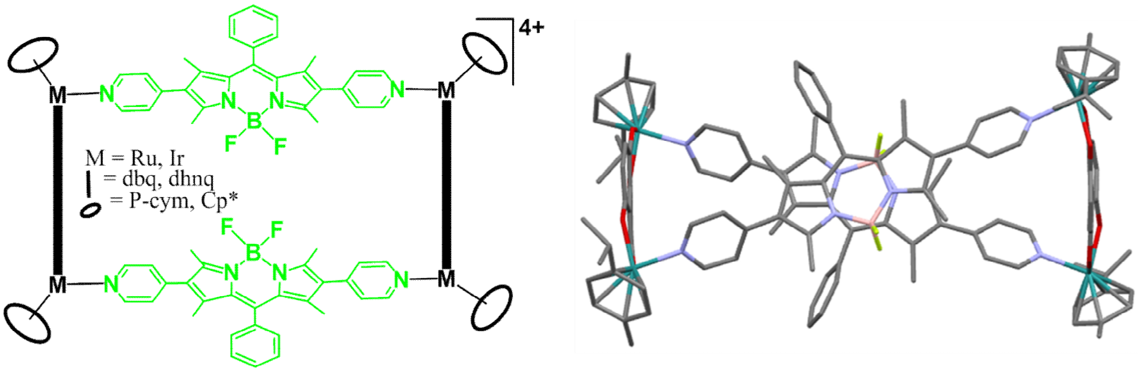
FIRST EXAMPLES OF BODIPY BASED Ru AND Ir RECTANGLES

GUPTA GAJENDRA 김탁현[1] 이창연[*]

인천대학교 에너지 화학공학과 [1]인천대학교 에너지화학공학과

Combining the excellent biological properties of arene based metal complexes[1] with the fluorescent properties of BODIPY[2], we hereby, present the first examples of arene Ru and Ir metalla-rectangles comprising a pyridine-fictionalized BODIPY ligand. The formation of these rectangles (Fig.1) were fully confirmed by different spectroscopic and analytical techniques. The single crystal X-ray structure of one of the Ru rectangle shows unusual interesting twisted molecular structure (Fig.1). The anticancer activities of these complexes were performed on different cancer cell lines. Rectangles Ru-dhnq and Ir-dhnq (dhnq = 5,8-dihydroxy-1,4-naphthoquinone) showed potent inhibitory activities against the proliferation of U87 (glioblatoma), HeLa (cervical), A549 (Lung carcinoma) and MCF-7 (breast carcinoma) cells, as compared to the rest. As expected, the BODIPY ligand as such did not show any pronounced effect on any of the cell lines. Moreover when their respective effects on normal cells (WI 38) were checked, Ru-dbq (dbq = 2,5-dihydroxy-1,4-benzoquinone) showed a substantially higher IC_{50} value as compared to its activity against MCF-7, indicating its selectivity to inhibit the growth of carcinoma against normal cells. The study on photodynamic activities on these complexes are underway.Fig. 1: Molecular structures of the rectangles (left) and X-ray structure of a Ru rectangle (right).1.H. -K. Liu and P. J. Sadler, Acc. Chem. Res., 44, 2011, 349-356.2.T. Kowada, H. Maeda and K. Kikuchi, Chem. Soc. Rev., 44, 2015, 4953-4972.AcknowledgementsThis research is supported by Post-Doctor Research Program (2015) through Incheon National University (INU), Incheon, Republic of Korea


4+
M
N
B
F
M = Ru, Ir
= dbq, dhnq
= P-cym, Cp*

일시: 2015년 10월 14~16일(수~금) 3일간
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Crystal Structures and Magnetic Properties of Azide-bridged Tetranuclear Complex and 1-D Polymer with *N*-(2-Pyridylmethyl)iminodipropanol (H_2pmidp)

신종원 문도현*

포항가속기연구소 빔라인운영부 생명화학소재팀

To investigate the magnetic properties of coordination compounds, the tetradentate ligand, *N*-(2-Pyridylmethyl)iminodipropanol (H_2pmidp) that has pyridine, amine and two propanol groups has been synthesized and acts as a bridging ligand as well as a capping ligand to form the various coordination compounds with transition metal ions, because the hydroxyl groups can be easily deprotonated by the reaction of the various metal ions. The reactions of stoichiometric amount of nickel(II) acetate tetrahydrate, copper(II) acetate monohydrate, sodium azide and H_2pmidp ligand afford the double cubane tetranuclear complex, $Na[Ni_4(Hpmidp)(CH_3CO_2)(N_3)_4]?CH_3OH$ (1), and coordination polymer, $[Cu(H_2pmidp)(N_3)_2]$ (2), in good yield under an air atmosphere, respectively. The asymmetric unit of 1 contains four different nickel(II) ions, two nickel (Ni1, Ni3) ions are coordinated with a monodeprotonated Hpmidp- ligand, two azide ions, and an acetate ion, while the others (Ni2, Ni4) are bonded with two azide ions, two acetate ions, and two bridged oxygen atoms. As contrasted with 1, the copper(II) ion of 2 is coordinated with the H_2pmidp ligand and two azide ions and is linked by bridging azide ions to from an one dimensional coordination polymer.The compound 1 and 2 display interesting ferromagnetic couplings between the metal ion through the bridging azide ions (end-on and end-to-end mode) in the temperature range from 2 to 300 K. In this poster, we will explain the detailed preparation, crystal structure, interesting magnetic properties.

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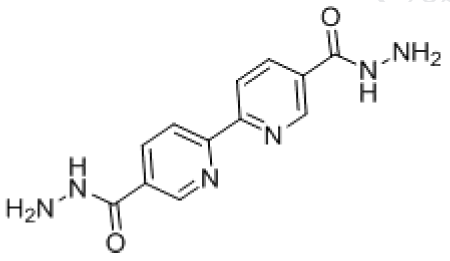
Chirality Control of Triple Helix Gels with Chiral Dopant

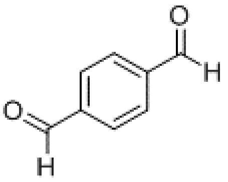
최희경 이지하 정성호 서효원 정종화[*]

경상대학교 화학과

Bipyridine-based compound 1 and 2 were synthesized by hydrazone reaction. Compound 1 and 2 could be gelated in DMSO with and without (1*S*,2*S*)-(+)-1,2-Cyclohexanediamine by hydrazone reaction. The gel 1 was characterized by SEM, CD, Rheometer. SEM images of gel 1 showed the fiber structure. In particular, CD spectrum of gel 1 with Fe^{2+} exhibited higher than that of without Fe^{2+}. The results indicate that gel 1 with Fe^{2+} forms the triple helical structure. We also observed CD spectra of gel 1 with and without Fe^{2+} by changing temperature. The CD intensity changes of gel 1 with Fe^{2+} were smaller than that of without Fe^{2+}. In this conference, we will present on triple helix of bipyridine gel 1 with Fe^{2+}.



Compound **1**



Compound **2**

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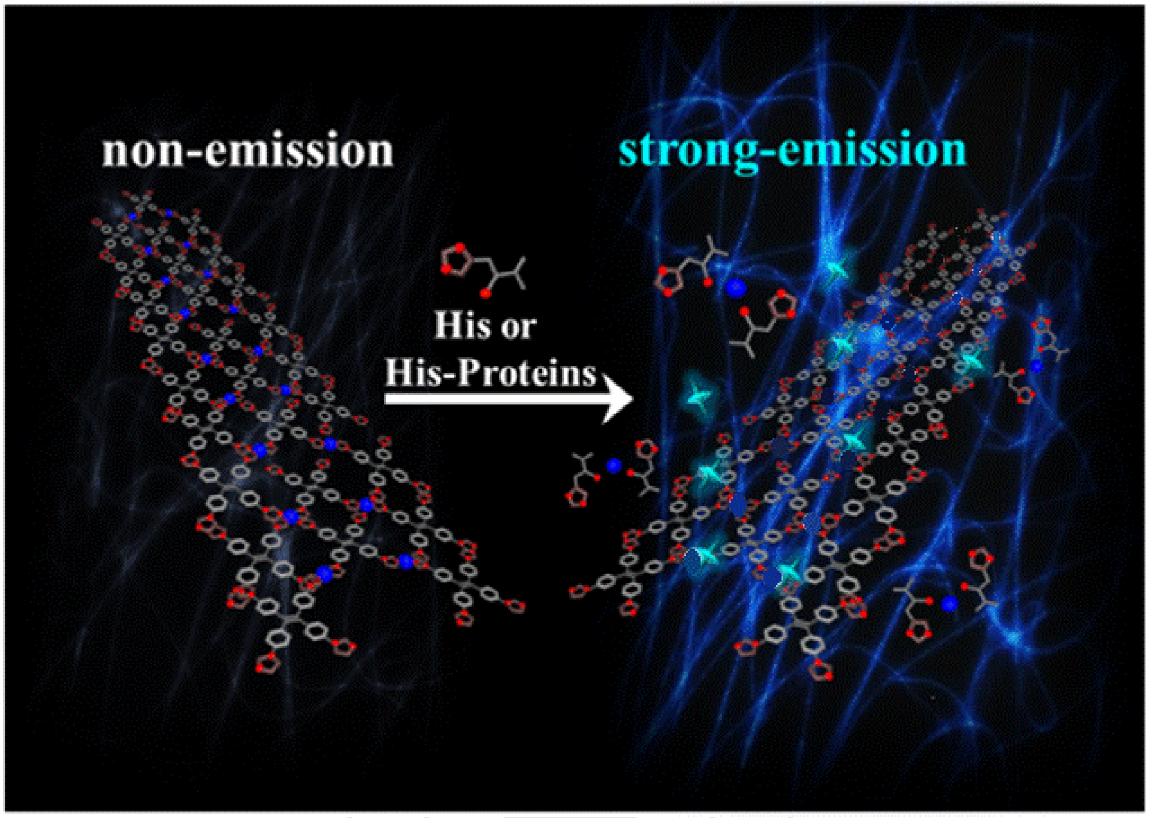
Tetra-imidazole-appended *p*-phenylene-Cu(II) embedded nanofibrous membrane film (IP-Cu-NF) as a portable chemoprobe

김가영 정성호 정종화*

경상대학교 화학과

A tetra-imidazole-appended *p*-phenylene-Cu(II) doped nanofibrous membrane (IP-Cu-NM) as a portable chemoprobe was prepared by the electrospinning method. Fluorescence changes were observed upon dropping amino acids and proteins containing histidine residues onto the surface. IP-Cu-NM prepared with 1.0 equivalent of Cu(II) showed non-emissive properties, indicating that Cu(II) induced the quenching with aggregation-caused quenching (ACQ) effect. The fluorescence intensity of IP-Cu-NM was enhanced approximately 25-fold upon dropping histidine onto the film, which is “turn-on” system. In contrast, no significant fluorescence intensities were observed upon dropping other amino acids, such as valine, serine, phenylalanine, alanine, cysteine, lysine, leucine, asparagine, glutamic acid, glycine, methionine and arginine. IP-Cu-NM achieved a low detection limit of 6.24 ppb observed by the fluorescence change. The results indicate that IP-Cu-NM could be used to selectively detect histidine. More interestingly, the fluorescence of IP-Cu-NM exhibited a strong emission with “turn-on” when proteins containing different numbers of His were dropped onto IP-Cu-NM, and the intensity was dependent on the numbers of His residues in the protein. The enhanced fluorescence of IP-Cu-NM with His could be recovered by treatment with Cu(II) solution, suggesting the fluorescence reversibility of IP-Cu-NM. Furthermore, this advanced convenient method was found to be valid up to 80% with excellent linearity for His detection over the range of 0 ? 10 ppm in urine as a biological sample.


non-emission
His or
His-Proteins
strong-emission

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Duplex DNA-gold nanoparticle probe composed as colorimetric biosensor for sequence-specific DNA-binding protein

안준호 정종화* 이준화

경상대학교 화학과

A colorimetric biosensing strategy for visual detection of specific DNA-binding proteins, SQUAMOSA promoter binding protein-like 12(SPL12), was developed using DNA duplex-formed AuNPs cluster. Interaction between double-stranded DNA, wild type SPL14 sequence and SPL12 lead to form intrinsic aggregation of AuNPs. DNA-modified AuNPs were prepared by a mixed thiol-DNA in the presence of excess of NaCl. In this reaction, two different type DNAs were immobilized onto AuNPs respectively. Single-stranded and double-stranded DNA attached onto AuNPs cluster were characterized by IR spectroscopy, UV-Vis spectroscopy, TEM. Color change of double-stranded DNA prepared by single strand DNA-AuNPs upon addition of SPL12 was observed from purple to blue. Detection ranges of SPL12 were 5 to 15 ?M. In control experiment using BSA, no color changes were observed. The color change from purple to blue was due to intrinsic interaction SPL12 with specific sequences of double-stranded DNA. The result revealed that the method allowed a specific and simple colorimetric assay of the target protein with a response range from 5 to 15 ?M

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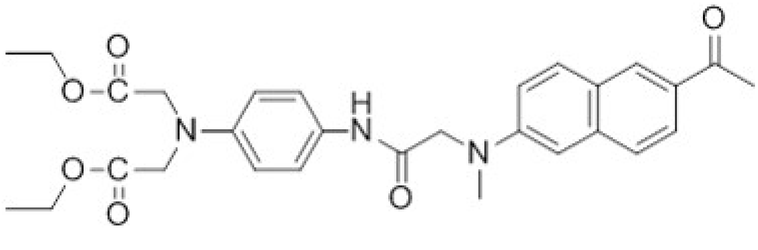
철(Ⅲ) 이온에 대해서만 형광 세기의 감소 현상을 보여주는 화학센서

문규리 정성호 정종화*

경상대학교 화학과

철(Ⅲ) 이온에 선택적인 리간드 1 의 형광단은 나프탈렌기이다. 리간드 1 과 철(Ⅲ) 이온의 착물의 색깔은 노란색을 나타내었다. 또한 그 상호작용은 365 nm UV 램프를 비추었을 때, 육안으로도 형광의 세기가 철(Ⅲ) 이온에 대해서만 감소하는 것을 관찰할 수 있었다. 리간드 1 의 분광학적 특징은 자외선 및 가시광선, 형광 분광기를 통해 측정하였다. 들뜸 파장 360 nm, 방출 파장 480 nm 에서 아세토나이트릴, 메탄올, 다이메틸 설폭사이드와 같이 용매에 따라 리간드 1 은 각각 다른 형광 세기를 나타내었다. 과량의 다른 금속에 대해서, 리간드 1 은 철(Ⅲ) 이온에 선택성을 보여주었다. 경쟁금속실험에서도 마찬가지의 실험 결과를 얻을 수 있었다. 1H NMR 적정실험에서 철(Ⅲ) 이온을 당량별로 첨가했을 때 피크의 이동을 통해, 리간드 1 과 철(Ⅲ) 이온의 결합자리를 확인하였다. 리간드 1 은 용액에서뿐만 아니라 고체화 되었을 때에도 철(Ⅲ) 이온에 선택성을 보여주었다.



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Synthesis of triphenylphosphate derivative as drug delivery system to mitochondria

백영은 정성호 이지하 고미선 정종화*

경상대학교 화학과

A mitochondria-targeting drug delivery system for anticancer activity has been developed in this research. A coumarin-based triphenylphosphate derivative which have fluorescent property was synthesized for mitochondria-targeting, and it was used as precursor of micelle. 50~200 nm of micelle size distribution could be confirmed by DSL analysis and images of the micelle particles were obtained by SEM. Doxorubicin and micelle precursor were dissolved in phosphate buffer solution and the mixture was heated to load the drug into the micelle precursor. Decrease of fluorescent intensity at 408 nm of coumarin was observed by PL. The loaded doxorubicin could be released by modulating condition of pH 3~5. As a result of the modulation, fluorescent intensity of coumarin increased again. Overall, delivery and release system of doxorubicin will be represented in this symposium.

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Conjugated microporous polymer의 합성 및 CO_2, I_2 포집 연구

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인천대학교 에너지화학공학과 [1]인천대학교 에너지 화학공학과

화석 연료의 사용으로 발생되는 이산화탄소는 지구온난화에 있어 가장 큰 주범으로 작용하고 있으며, 핵 폐기물로부터 발생되는 방사성동위원소인 Iodine 은 반감기가 길고, 환경적인 문제가 있어 두 물질 모두 포집과 저장에 대한 관심이 대두되고 있다. Conjugated microporous polymers(CMPs)는 π-conjugation 되어 형성되는 다공성 물질로, 유사 다공성 소재인 Metal-organic frameworks (MOFs) 의 약한 금속-리간드 의 배위결합 대신 강한 공유결합을 사용 하기 때문에 기존 MOFs 가 가지고 있던 화학적 불안정성을 해결한 신소재로 주목 받고 있다. 따라서 본 연구에서는 porphyrin 과 pyrene 을 사용하여 Sonogashira?Hagihara crosscoupling 반응을 통해 CMPs 를 합성하였으며, 합성된 CMPs 는 FT-IR, Solid state ^{13}C NMR, N_2 , CO_2 isotherm 등을 통해 특성을 파악하였다. 또한 광학적 특성을 UV-Vis 을 사용하여 관찰하였으며, 시간에 따른 I_2 포집을 측정하여 흡착제로서의 성능을 확인하였다.Acknowledgement : This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

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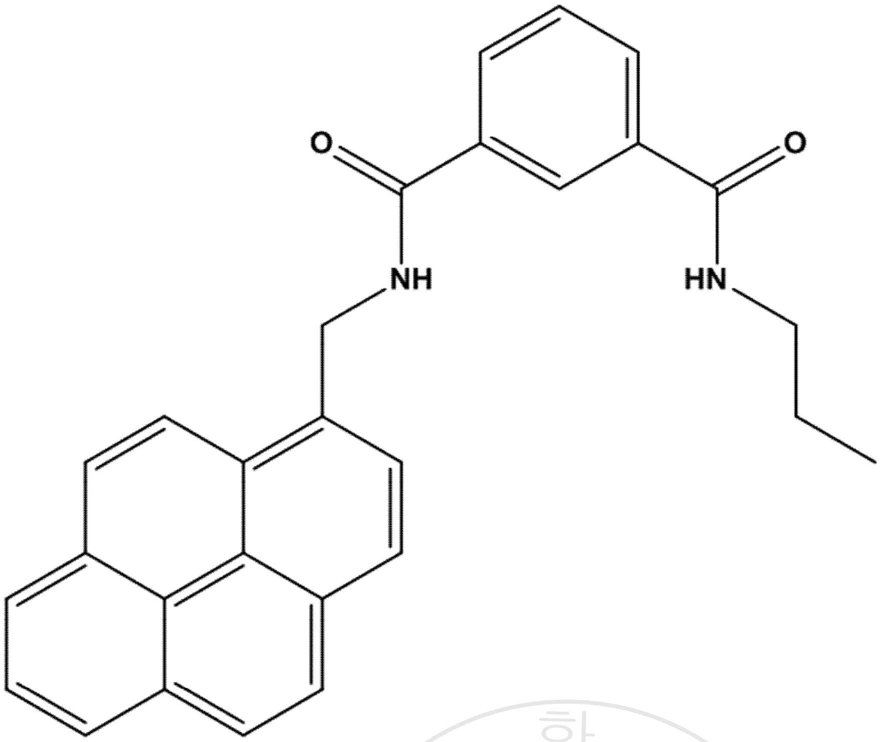
Development of fluorescent probe for nitro compounds by electrospinning of a pyrene-based compound

최연원 김성국* 정종화*

경상대학교 화학과

New fluorescent probe has been prepared by electrospinning process on a pyrene-based compound (1) and tested for its ability to detect nitro compounds. Fibrous morphology of the probe was confirmed by scanning electron microscope (SEM) and confocal microscope. The probe displayed turn-off behavior upon exposure to several nitro compounds, especially, fluorescent intensity was dramatically reduced with trinitrobenzene (TNB), Nitroaniline (NA) and trinitrotoluene (TNT) among others. In the case of the three nitro compounds, they could be detected by the probe even in nanomolar level of concentration. Also, the fluorescent turn-off behavior was apparent to the naked eye by confocal fluorescence microscope.



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pyrene 과 porphyrin을 이용한 MOF 합성 및 에너지 이동에 대한 특성 연구

박경철 조진희 이창연[1,*]

인천대학교 에너지화학공학과 [1]인천대학교 에너지 화학공학과

Metal Organic Frameworks(MOF)는 금속 이온 또는 금속 클러스터가 유기 리간드와 배위결합을 통해 이루어져 연결된 다공성 물질로 표면적과 기공 부피가 크고, 리간드를 변화시킴에 따라 화학적 특성이나 기공 크기를 조절 할 수 있는 특성들로 인해 MOF 는 기체 저장 및 분리, 촉매, 약물 전달, 센서의 분야에서도 많은 연구가 이루어 지고 있다. 또한 MOF 는 규칙적으로 정렬된 내부 구조를 지니고 있는 특성이 있어, 리간드 사이의 에너지 이동이 효과적이다.본 연구에서는 SBU 가 동일한 MOF 인 NU1000 과 PCN-222 의 두가지 리간드를 혼합하여 새로운 형태의 MOF 를 제조하고 에너지 이동을 관측하는 연구를 진행하였다.합성된 MOF 는 NMR, OM 등을 통해 특성을 파악하고 관측하였으며, 에너지 이동에 대한 특성을 파악하기 위해 UV-Vis spectrum 과 Emission and excitation spectrum 을 관측하고 분석하였다.AcknowledgmentsThis research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

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리간드의 구조적 특성을 이용한 배위 고분자형 입자의 형태 연구

차유빈 정성호 정종화*

경상대학교 화학과

본 연구는 MOF(Metal-Organic Frameworks)형 CPPs(Coordination Polymer Patricles)를 제조하여 가스저장, 촉매 등의 분야에 응용 하기 위해 진행하였다. 카이랄 센터를 가지는 기능적 C_3-리간드와 심플한 구조를 가지는 선형 리간드를 이용하여 아연이온의 존재 하에서 다양한 조건변화를 통해 MOF 형 CPPs 를 제조하고 형태 제어를 연구하였다. C_3-리간드인 L-TMTAH_3(L-TrimesoylTriAlanine)가 선형 리간드인 Terephthalic Acid 보다 많을 경우에는 구형의 모폴로지가 형성되었으며, 선형 리간드가 더 많을 경우에는 반대로 큐브형 모폴로지가 형성 되는 것을 SEM(Scanning Electron Microscope)을 이용하여 확인하였다. 그 결과 리간드의 몰비율과 온도, 시간등의 조건변화에 따라 다양한 CPPs 의 형태를 제어 할 수 있었다.

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칼릭스[4]아렌 유도체를 이용한 세슘 이온 형광 센서

박정수 정성호 최연원 임나영 정종화*

경상대학교 화학과

본 연구에서는 Cs^+을 검출 하기 위해 선택성이 기대되는 칼릭스[4]아렌 유도체를 합성하고 이 리간드를 이용한 유기-무기 하이브리드 센서 개발을 목적으로 한다. 형광 센서를 만들기 위해 naphthalene 기를 도입하고 Cs^+을 선택적으로 검출 하기 위해서 1,3-alternate 칼릭스[4]아렌에 crown ether 그룹을 도입하여 리간드 1 을 합성하였다. 리간드 1 은 선택적으로 Cs^+과 착물을 형성 했을 때, PET(photoinduced electron transfer)효과에 의해 형광이 감소 하였다. 따라서 리간드 1 은 Cs^+의 검출을 위한 형광센서로 이용 할 수 있을 것으로 판단된다.

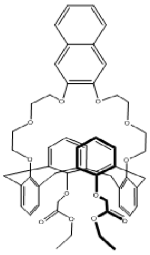
리간드 **1**

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Photo-activated NO-releasing Ru(NO) Complexes

김민영 조장훈[*] 정종화[*] 임만호[1,*] 이태곤[1,*] 이홍인[*]

경북대학교 화학과 [1]부산대학교 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 developed a new Ru-nitrosyl bis-pyridyl/biscarboxamide compound, [Ru(III)(ebpp)(Cl)(NO)], where H2ebpp = N,N'-(ethylene di-p-phenylene)bis(pyridine-2-carboxamide), to be tested as a model NO-releasing agent. Here, we present the strategies to develop visible-light sensitive NO-releasing Ru complexes with higher quantum yield. We introduced new series of ligands, bis-salophen and bis-naphophen, to develop Ru-nitrosyl complexes. In this study, we describe our progress in designing photoactive ruthenium nitrosyls and the properties of the photo-activated NO-releasing of the complexes monitored by UV-VIS, EPR, X-ray crystallography and femtosecond mid-IR spectroscopy.

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Synthesis and Structure of Dinuclear Copper Complex : Catechol Oxidase Mimic Activity, Spectroscopy

조장훈 이홍인*

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Model enzymes are being developed and extensive studies were conducted in order to gain an understanding of the factors underlying the relationship between coordination geometry and the nature of donor ligands. Dinuclear copper proteins like hemocyanin, tyrosinase and catechol oxidase are known as type-3 copper proteins. The active site contains dicopper core in which both copper ions are surrounded by three nitrogen donor atoms of histidine residues. Recently, many dinuclear copper(II) complexes have been reported as model compounds of catechol oxidase. In this study, we have synthesized dinuclear copper(II) complex (Cu_2L_2) derived from a tetradentate dicarboximide ligand(H_2L=N,N'-(ethane-1,2-diyldi-o-phenylene)-bis(3-methylpicolinamide). Single crystal X-ray crystallography of Cu_2L_2 revealed that the copper sites are non-coupled containing copper centers at 6.598 ? apart, 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 catalytic activities were followed in dichloromethane solvent and monitored by the UV-VIS, CV and EPR spectroscopy.

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Syntheses of Porphyrin Dyes with Electronic Push-Pull Groups for Dye-Sensitized Solar Cells

김남길 김호준 김희준*

금오공과대학교 응용화학과

With advantages of low cost, low weight, coloring, and easy processing, dye-sensitized solar cells (DSSCs) are prospective alternatives for future devices for the conversion of solar energy. Inspired by the important role that porphyrins play in natural photosynthesis, researchers have tested numerous derivatives of this substrate class as sensitizers for DSCs, but conversion efficiencies obtained so far have largely remained below 8%. Recently, porphyrin dyes with electron push-porphyrin-electron pull systems have been attracted for dye-sensitized solar cells. We here report syntheses of the porphyrin dyes with a new acceptors of 2,1,3-benzothiadiazole (BTD).

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Fundamental study for improvement of road visibility at night by Al2O3 and phosphorescence powder with rare earth metals

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한국건설기술연구원 화재안전연구소 [1]동덕여자대학교 약학대학

기존의 도로 노면 표시는 TiO_2 안료를 기반으로한 백색 도료를 사용하였다. 백색도료는 태양광이 존재하는 낮시간에는 시인성이 좋지만 태양광이 없는 야간의 경우에는 차량 전조등에 의한 차선반사에 의존하여 시인성을 확보해야하는 문제점이 있다. 특히 무조명구간의 야간 도로에서 차선인식이 어렵고 야간 교통사고의 위험은 주간에 비해 3 배에 이르고 있다. 이러한 문제점을 해결하기 위하여 본 연구에서는 희토류금속의 인광(phosphorescence)을 활용하여 노면표시 도료를 제작하고, 축광 후 일정시간 인광을 유지하여 야간 시인성을 확보하도록 하였다. 그러나 Eu, Sr 원소에 의한 인광은 녹색 또는 주황색으로 기존 노면표시 도료의 백색과 아스팔트의 흑색의 명도대비에 비해 시인성이 작다. 야간 시인성 및 희토류의 인광을 증폭시키키기 위해 Al_2O_3 를 노면표시도료에 혼합하여 반사효율을 개선하였다. Al_2O_3 는 희토류의 인광효과에 추가적인 발광(luminescence)을 높이기 때문에 도로 시인성 개선에 효과적이었으며, 상대적으로 경제성이 있는 Al_2O_3 는 희토류 사용량을 최소화하여, 상용화 및 대중적인 사용 가능성을 제시하였다.

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Morphological and Structural Evolutions of Metal-Organic Framework Particles from Amorphous Spheres to Crystalline Hexagonal Rods

김두영 위정훈 이희정 오문현*

연세대학교 화학과

The compositions of micro- and nanoparticles as well as their morphologies and structures are important factors that define their properties and applications. Thus, understanding the morphology and structure changes of particles in response to their composition change is vital for the controlled formation of particles. Herein, we wish to report the morphological and structural evolutions of metal-organic framework (MOF) particles according to the different contributions of the two organic linkers, isophthalic acid (H_2IPA) and 1,4-benzenedicarboxylic acid (H_2BDC). Porous crystalline MOF particles were generated when the contribution of BDC linkers was dominant; however, non-porous amorphous MOF particles resulted when the contribution of the IPA linkers was dominant.

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Hydrogen-Bonded Networks of Purine Derivatives and Their Guest Inclusion Properties

노경규 오유진 심재웅 임나래 김자헌*

숭실대학교 화학과

Alkylated purine derivatives are synthesized and their crystal structures were determined. In crystals, they are assembled via hydrogen bonds to form 2-dimensional hydrogen-bonded networks. The layers are further stacked with bilayers via π- π interactions. The alkyl chains introduced to the purine derivatives are directed perpendicularly to the layer plane, and fill the space between the bilayers. Various aliphatic and aromatic molecules can be intercalated between the bilayers with maintaining the characteristic hydrogen bond patterns of the host molecules.

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Comparative study of 64Cu-Biconjugates for αvβ3 integrin targeting and in vivo imaging

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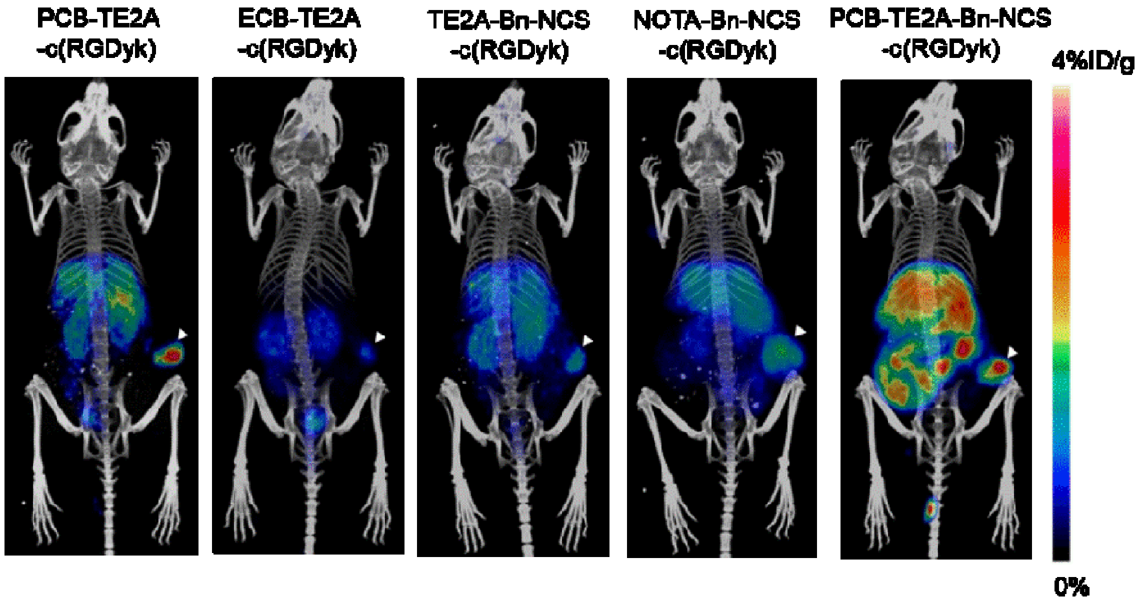
Bifunctional chelator (BFC) is a key component in developing 64Cu-based imaging agents. The accuracy of metal based tumor imaging often relies on the stability of metal-BFC complex as less stable metal-complex leads to unwanted background from non-targeted organs. Various comparative studies were thus executed to uncover superior bio-conjugates, but mainly focused on TETA or DOTA based chelates. In our previous communications, we have introduced TE2A and PCB-TE2A and modified thereafter for in vivo applications. Herein we described a full comparative study of five different BFCs. All BFCs are known to form highly stable copper complex. The chelates were conjugated with c(RGDyK) and were evaluated for tumor targeting efficacy in U87MG tumor model by various studies like bio-distribution, in vivo stability, and PET imaging. Among all chelates, cross-bridged macrocycles gave high tumor uptake in compare to non-cross bridged macrocycles. Although, ECB-TE2A-RGD cleared out fast in compare to other cross-bridged analogues, but, PCB-TE2A-RGD was found to give excellent contrast image at 24 h p.i with high tumor to background ratio as revealed in the adjoining figure. Studies will then be focused in near future with PCB-TE2A to evaluate its therapeutic potential with Cu-67.Figure 1. PET images of 64Cu-BFC-c(RGDyK) at 24 h p.i in U87MG tumor bearing nude mice.


PCB-TE2A -c(RGDyk)
ECB-TE2A -c(RGDyk)
TE2A-Bn-NCS -c(RGDyk)
NOTA-Bn-NCS -c(RGDyk)
PCB-TE2A-Bn-NCS -c(RGDyk)
4%ID/g
0%

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Novel Metal Precursors Prepared by Newly Designed Multidentate Amide-type Ligands

남지현 전동주[1,*] 정택모[2] 김창균[3] 박보근[3]

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For metal and metal oxide thin films which diverse applications to electronic devices novel precursors have been continuously required. Vacuum technology such as metal organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) is used for the thin films, and the development of metal precursors having desirable properties such as high vapor pressure and thermal stability is most important, and for obtaining the desirable precursors, design and preparing suitable organic ligands is indispensable. As a result of extensively focusing on the development of diverse metal precursors using the newly designed organic ligands for many years, we have successfully developed excellent metal precursors and adopted them to deposit metal and metal oxide thin films using CVD and ALD for advanced electronic devices. Here we will discuss our recent results on new metal precursors having multi-dentate amide-type ligands which were synthesized by molecular design

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Guest Selectivity Control in a Metal-Organic Framework via Simple Post-modification

홍지수 최판규 우경택 김자헌*

숭실대학교 화학과

MOF-14 is a pto-type metal-organic framework (MOF) composed of Cu(II) and benzene-1,3,5-tribenzoate (BTB). Due to its framework interpenetration, two pairs of facing Cu(II) ions in the portal of pore window come to have uneven separation with interatomic distances of 7.66 and 14.00 Å, respectively. In our previous work on a Zn(II) version of MOF-14 (Zn-MOF-14), it was possible to link the shorter pair of metal centers with 2-methyl-imidazolate. Similarly to this work but now with simple insertion of an extrinsic neutral bridging ligand, we could connect two facing Cu(II) centers to block the windows in part, leading to selective gas adsorption and guest inclusion properties not shown in MOF-14.

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Novel Metal Precursors Synthesis by Ligands Having Chelate Amino Group for MOCVD and ALD

이가연 전동주[1,*] 정택모[2] 김창균[3] 박보근[3]

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New precursors have been required continuously for metal and metal oxide thin films which diverse applications to electronic devices. For preparing desirable thin films chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) are performed mainly, and there the metal precursors having desirable properties such as high vapor pressure and thermal stability are most important, and so design and preparing suitable organic ligands is indispensable for good precursors. As a result of extensively focusing on the development of diverse metal precursors using the newly designed organic ligands for many years, we have successfully developed excellent metal precursors, especially containing amino alcohol-type ligands and adopted them to deposit metal and metal oxide thin films using CVD and ALD for advanced electronic devices. In this presentation we will discuss our recent results on new metal precursors synthesized from various ligands getting chelate amino moiety such as amino alcohol, amino thiol, amino amine-type ligands by molecular design.

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Real time monitoring of sulfidation with Au@Ag core-shell nanocubes at high temperature

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Sulfidation reactions of silver has been applied widely for synthesizing elaborate nanostructures as frameworks of cation exchange as well as for utilizing themselves as calorimetric sensing techniques. Using reactions, the addition of sulfide ions into the Au@Ag core-shell nanocubes yields stable Au@Ag/Ag_2S nanocubes. Herein, changes of optical properties from Ag to Ag_2S is monitored at the single-particle level by means of in situ characterization tool. This tool enables to examine the kinetics of sulfidation reactions with flow cell setup at two different temperatures. we found that the reaction at 80 ℃ is more abrupt relative to that at 25 ℃. Accordingly, the in situ monitoring at the single-particle level has a great potential for analyzing the rate of reaction. Furthermore, experimental data can be confirmed by performing theoretical simulations such as finite-difference time-domain(FDTD) calculation method. It is helpful to understand the mechanisms of s variety of reactions more in detail and control the reactions more delicately.

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Super-hydrophobic Zeolite Adsorbents with Microporous Organic Network Shells

강성아 김보룡 손성욱*

성균관대학교 화학과

Hydrophilic surface of ZSM-5 nanoparticles were modified by the coating of microporous organic networks (MONs). The MONs were prepared via the Sonogashira coupling reaction of tetrakis(4-ethynylphenyl)methane and 1,4-diiodobenzene. Scanning electron microscopy verified the homogeneous coating of MON on the surface of ZSM-5. By adjusting the amount of building blocks, the thickness of MON coating was controlled. After etching ZSM-5 with hydrofluoric acid, the thickness of MON coating was measured as 10 nm, 20 nm and 42 nm by transmittance electron microscopy. Hydrophobic property of ZSM@MON hybrid material was investigated by observing water contact angle. Contact angle was changed from 118˚ to 152˚ depending on the amount of building blocks. Especially, ZSM@MON-3 which has a thick MON coating showed super-hydrophobic property (contact angle>150˚). Only one third of ammonia adsorption capacity was retained for untreated ZSM-5 at 43% relative humidity. However, almost 90% of ammonia adsorption capacity of was retained for ZSM@MOP at 43% relative humidity. These observations resulted from the efficient blocking of competitive water adsorption to ZSM-5 by the hydrophobic MON coating.

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New Methodology for the Surface Area Enhancement of Microporous Organic Networks

김보룡 강성아 손성욱*

성균관대학교 화학과

Recently, various porous molecular materials have been synthesized by scientists. Microporous organic networks (MONs) prepared by various coupling reaction became an important class of porous materials. Due to the high surface area and porosity, the MON materials have been applied for diverse purposes including catalysis, adsorption, and sensing. Because the functional performance of MON materials is dependent on the porosity, many scientists have tried to find the methodology to improve the surface area. This presentation introduces the new methodology for the enhancement of porosity of MON materials and our suggestion for the underlying structural reasons.

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Diffusion Pathway Effect in the Photocatalytic Performance of Hollow Microporous Organic Networks Bearing Triphenylamines and Anthraquinones

강성아 김보룡 손성욱*

성균관대학교 화학과

In recent years, microporous organic networks (MONs) have attracted great attention as versatile functional materials. Among various functions of MONs, the photocatalytic properties have attracted significant attention. The conjugated extension of building blocks resulted in the gradual red shift of the absorption bands to the visible light region. These photo-active MON materials could promote photochemical reactions under visible light irradiation. In this presentation, we will introduce the diffusion pathway effect of hollow MON materials in the photocatalytic function in visible light-driven oxidative coupling of benzyl amines.The hollow MON materials were prepared by using silica spheres as the template and tris(4-ethynylphenyl)amine and 2,6-diiodo-9,10-anthraquinone as the building blocks for the Sonogashira coupling. The resultant hollow MON materials bearing triphenylamine and anthraquinone moieties showed efficient visible light absorption and catalytic activities in the photochemical oxidative coupling of benzylamines. Via the comparison studies of hollow and nonhollow catalytic materials, the diffusion pathway effect of the substrates was investigated in the photochemical conversion of benzylamines.

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Preparation of Tin(IV) Porphyrin-Silica Hybrid Nanoparticles with Core-Shell Structure

이수지 김희준*

금오공과대학교 응용화학과

Metalloporphyrins are popular molecular components in supramolecular assembled nano-materials because they possess a rigid and well-defined geometry, ease of synthesis, and good spectroscopic characteristics; in addition the coordination chemistry of metalloporphyrins can be tuned by varying the central metal ion. Tin(IV) porphyrins readily form stable six-coordinate complexes with the two trans axial ligands of oxyanions such as carboxylates and alkoxides due to the oxophilic nature of the tin(IV) center. We have been thus interested in the assembly of tin(IV) porphyrins on silica surfaces by layer-by-layer method using metal-ligand coordinative interactions and the preparation of tin(IV) porphyrin-silica hybrid nanoparticles with core-shell structure. Here we present our efforts on the preparation of porphyrin hybrid nano-materials.

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Synthesis and Structure of 1D-chain of Cu Tetrathiafulvalene (TTF) Complex

KhanMohammadSherjeelJaved 조장훈 정종화 이홍인*

경북대학교 화학과

There is a continuing interest in the chemistry of polyazamacrocycles because of their chemical and biochemical application. Structural factors, such as ligand rigidity and the electron-donating properties of the nitrogen atoms create the polyaza network and their disposition play a significant role in determining the binding features towards metal cations. The complexation is governed mainly by the ring size and ionic radii of the metal ions. Interest in the salts and charge-transfer compounds of TTF prompted us to investigate the possibility of preparing substituted derivatives by means of desulfurization of dimethyl 2-thioxo-1,3-dithiole-4,5 dicarboxylate with phosphorus (III) compounds. TTF and its derivatives are renowned organic π donors which have been largely studied for distinct applications,particularly in the area of conducting organic materials including intermolecular charge-transfer interactions with several π -accepting molecules. An array of mono- or polydentate coordinating functional groups has been adhered to the TTF moiety and the interrelated metal complexes have been divulged. The structural and electronic properties of TTF are considered to be important determinants of electrical-transport properties in crystals of conductive materials. Transition metal 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). It has been characterized by various analytical methods

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Coodination Chemistry of Trinuclear Nickel(II) and Cobalt(II/III) Complexes with N_2O_2-type Ligands

정아림 신종원[1] 민길식[2,*]

경북대학교 화학과 [1]포항가속기연구소 빔라인운영부 생명화학소재팀 [2]경북대학교 사범대학 화학교육과

Tetradentate ligands containing hydroxyl groups are useful for the preparation of diverse compounds. These ligands are can be used for constructing various coordination complexes such as dimer, trimer, and tetramer because hydroxyl groups are easy to deprotonation by coordination. Recently, we have synthesized three new trinuclear complexes, $[(Hpmide)_2Ni_3(OAc)_4]$ (1), $[(Hpmide)_2Co_3(OAc)_4]$ (2), and $[(pmidip)_2Co_3(OAc)_4]$ (3), by the N_2O_2-type ligands, *N*-(2-pyridylmethyl)iminodiethanol (H_2pmide) and *N*-(2-pyridylmethyl)iminodiisopropanol (H_2pmidip), with nickel(II) and cobalt(II/III) ions. In 1 and 2, the central nickel(II)/cobalt(II) ion is bonded to four oxygen atoms of acetate anion and to two bridged oxygen atoms of Hpmide ligand, respectively. Two terminal nickel(II)/cobalt(II) units are coordinated Hpmide$^-$ and two acetate anions, respectively. In 3, two terminal cobalt(III) ions are bonded pmidip$^-$ and two acetate anions. The terminal units are each linked to a central cobalt(II) cation through two oxygen atoms of pmidip$^-$ and one oxygen atom of acetate anion, giving rise to a linear trinuclear mixed-valence cobalt complex. Complex 1 and 2 shows a weak ferromagnetic and antiferromagnetic interaction through the bridging oxygen atoms, respectively. Additionally, complex 3 behaves as a paramagnetic cobalt(II) monomer, due to the diamagnetic cobalt(III) ions in the terminal units. In this poster, we will present the detailed preparation of the ligand and cobalt compounds, crystal structures, magnetic properties.

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Synthesis of Carbon-Coated V_2O_5 Nanoparticles Prepared from MIL-47(V) Metal-Organic Framework as a Cathode Material for Lithium-Ion Batteries

김태경 김종식*

동아대학교 화학과

Vanadium pentoxide (V_2O_5) is one of the most promising cathode materials for lithium-ion batteries (LIBs) due to the easy synthesis, abundant sources, and relatively high theoretical capacity (about 294 $mAhg^{-1}$ at 2.1-4.0 V), compared with more commonly used cathode materials such as $LiCoO_2$ (140 mAh g^{-1}) and $LiFePO_4$ (170 mAh g^{-1}). Despite these advantages, the capacity retention of V_2O_5 is relatively worse because of its poor structural stability, low electroconductivity, and sluggish Li ion diffusion. For these reasons, practical application of V_2O_5 is hindered. In this work, the carbon-coated V_2O_5 nanoparticles are simply synthesized through a controlled thermal decomposition of MIL-47(V) metal-organic framework (MOF) used as a vanadium precursor. MIL-47(V) is built up from infinite chains of corner-sharing VO_6 octahedra interconnected by dicarboxylate groups, which act as a carbon source. The highly crystalline V_2O_5 nanoparticles prepared from MIL-47(V) are coated with a carbon layer of thickness approximately 3-7 nm. The carbon-coated V_2O_5 nanoparticles exhibit an enhanced initial discharge capacity of about 286 mAh g^{-1} with the capacity fading of 8.68 % after 50 cycles at 0.1 C in the voltage range of 2.1-4.0 V. Even at an increased current density of 1 C, the excellent cycling stability is still observed with the capacity fading rate of 0.48 % per cycle.

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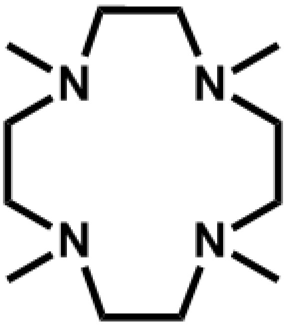
Comparisons of the structure and reactivity for ‘side-on’ nickel(lll)-peroxo complexes

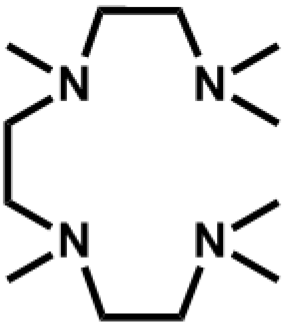
윤성근 조재흥[1,*]

대구경북과학기술원(DGIST) 신물질과학전공 [1]대구경북과학기술원(DGIST) 신물질과학

Transition metal-dioxygen species are of basic importance in industrial chemistry and biology. A wide variety of metalloenzyme active sites form characteristic metal-dioxygen adducts as key intermediates in the catalytic cycle of dioxygen activation. Among the metal-dioxygen species, there are two types of ligands where the one is "macrocycle" such as porphyrin in cytochrome P450 and the other is "open chain" sticking on amino acid residues. The synthesis and spectroscopic characterization of an side-on nickel(lll)-peroxo complex with a 12-membered macrocyclic ligand was reported previously.[1] In this work, mononuclear nickel(lll)-peroxo complex, $[Ni(Me_6\text{-trien})(O_2)]^+$ (Me6-trien = 1,1,4,7,10,10-Hexamethyltriethylenetetramine), was synthesized in the reaction of $[Ni(Me_6\text{-trien})](ClO_4)_2$ in the presence of H_2O_2 and triethylamine. The nickel(lll)-peroxo complex was characterized by ESI-MS, UV-Vis, EPR and XRD. We will compare the reactivity of the nickel(lll)-peroxo complexes which have two different types of ligands. [1] J. Cho, R. Sarangi, J. Annaraj, S. Y. Kim, M. Kubo, T. Ogura, E. I. Solomon, W. Nam, “Geometric and electronic structure and reactivity of a mononuclear ‘side-on’ nickel(III)-peroxo complex” Nature Chem. 1, 568, 2009



12-TMC



Me$_6$trien

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발표코드: **INOR.P-94**
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Zintl Phase with the Mixed Cations for the Thermoelectric Material Application: the $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1.5-3.5) Series

남근우 유태수*

충북대학교 화학과

A series of $Ca_{5-x}Yb_xAl_2Sb_6$ ($x = 1.5$-3.5) compounds has been synthesized using the arc-melting method under an argon atmosphere. The crystal structures have been characterized by both powder and single crystal X-ray diffractions. Two Ca-richer compounds adopted the orthorhombic $Ca_5Ga_2Sb_6$-type structure (space group *Pbam*, Pearson code *oP*26) with lattice parameters of $a = 11.96$, $b = 13.93$ and $c = 4.43$ for $Ca_{3.5}Yb_{1.5}Al_2Sb_6$, and $a = 12.03$, $b = 14.02$ and $c = 4.45$ Å for $Ca_3Yb_2Al_2Sb_6$. On the other hand, the Yb-richer $Ca_{1.5}Yb_{3.5}Al_2Sb_6$ crystallized in the orthorhombic $Ba_5Al_2Bi_6$-type structure (space group *Pbam*, Pearson code *oP*26) with lattice parameters as follows: $a = 7.32$, $b = 22.90$ and $c = 4.41$ Å. Energy dispersive X-ray spectroscopy (EDXS) verified the chemical composition of $Ca_{5-x}Yb_xAl_2Sb_6$ ($x = 1.5, 2$) compound: $Ca_{2.71}Yb_{1.28}Al_{3.48}Sb_{5.52}$ for $Ca_{3.5}Yb_{1.5}Al_2Sb_6$ and $Ca_{2.34}Yb_{1.94}Al_{3.21}Sb_{5.51}$ for $Ca_3Yb_2Al_2Sb_6$. The structural correlation between the Ca-richer $Ca_{5-x}Yb_xAl_2Sb_6$ ($x = 1.5, 2$) compounds ($Ca_5Ga_2sb_6$-type) and the Yb-richer $Ca_{1.5}Yb_{3.5}Al_2Sb_6$ ($Ba_5Al_2Bi_6$-type) has been thoroughly investigated, where two crystal structures share a certain portion of structural similarities including the one-dimensional $[Al_2Sb_6]^{10-}$ double chain composed of the $[AlSb_4]$ tetrahedra and the connecting Sb_2 dimers, and the space filling Yb^{2+} and Ca^{2+} cations. However, a subtle distinction in spatial distributions of the $[AlSb_4]$ tetrahedra and the Yb^{2+}/Ca^{2+} cations differentiates two structure types. Electronic structure calculations using tight-binding linear muffin-tin orbital (TM-LMTO) method were performed for a structural model of $Ca_{2.5}Yb_{2.5}Al_2Sb_6$, and density of states (DOS) and crystal orbital Hamilton population (COHP) curves were thoroughly interrogated. Thermal gravimetric analysis (TGA) and thermoelectric property measurements including electrical resistivity, Seebeck coefficient as well as thermal conductivity were also conducted.

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Synthesis, Spectroscopic Characterization, and Reactivity of Cobalt(III)-Peroxo and Hydroperoxo Complexes

노현주 조재홍*

대구경북과학기술원(DGIST) 신물질과학

Mononuclear metal-dioxygen adducts are key intermediates in catalytic cycles of dioxygen activation by metalloenzymes in our body. In this work, cobalt(III)-peroxo complex bearing a macrocyclic pyridinophane ligand, N,N’-di-tert-butyl-2,11-diaza[3.3](2,6)pyridinophane (TBDAP), $[Co(III)(TBDAP)(O_2)]^+$, was synthesized with H_2O_2 and trimethylamine and characterized by various spectroscopic techniques. Upon protonation with perchloric acid, the cobalt(III)-peroxo complex was converted into an cobalt(III)-hydroperoxo complex, $[Co(III)(TBDAP)(OOH)]^{2+}$. The O-O bond stretching frequency of $[Co(III)(TBDAP)(O_2)]^+$ and $[Co(III)(TBDAP)(OOH)]^{2+}$ were detected to be 839 cm^{-1} and 807 cm^{-1} respectively by the resonance Raman spectroscopy. The reactivity of the cobalt-peroxo complex shows the nucleophilic character in aldehyde deformylation. Electrophilic reactivities were observed in the cobalt(III)-hydroperoxo complex such as sulfur oxidation and phosphine oxidation. In conclusion, we have shown the synthesis, spectroscopic characterization, and reactivities of mononuclear cobalt-peroxo and -hydroperoxo intermediate complexes.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis of Silole and Thienosilole Derivatives and their Copolymerization with Dichlorodisubstitutedsilane

민용기 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1,3,4-tetraphenylsilole as monomer was prepared by the intramolecular reductive cyclizations of diphenylbis(phenylethynyl)silane with treatments of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide in situ. We have synthesized polymeric materials of polycarbosilanes containing 1,1,3,4-tetraphenyl-2,5-silolene and disubstitutedsilylene along the polymer main chain by copolymerization of 2,5-dibromo-1,1,3,4-tetraphenylsilole with several dichlorodisubstitutedsilanes using *n*-butyllithium.4,4-Diphenyl-2,6-bis(trimethylsilyl)dithienosilole was synthesized by the intramolecular cyclization reaction of 3,3'-dibromo-5,5'-bis(trimethylsilyl)-2,2'-bithiophene using 4 mol n-buthyllithium. 2,6-Dibromo-4,4-diphenyldithienosilole was synthesized by the substitution with bromine at -90 ℃ to 4,4-diphenyl-2,6-bis(trimethylsiltl)dithienosilole. We also have synthesized new polymeric materials of polycarbosilanes containing 4,4-diphenyldithienosilolene and disubstitutedsilylene along the polymer main chain by copolymerization of 2,6-Dibromo-4,4-diphenyldithienosilole with several dichlorodisubstituedsilanes using *n*-butyllithium. The obtained polycarbosilanes-silole and thienosilole derivatives are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, ^{1}H, ^{13}C NMR, and FT-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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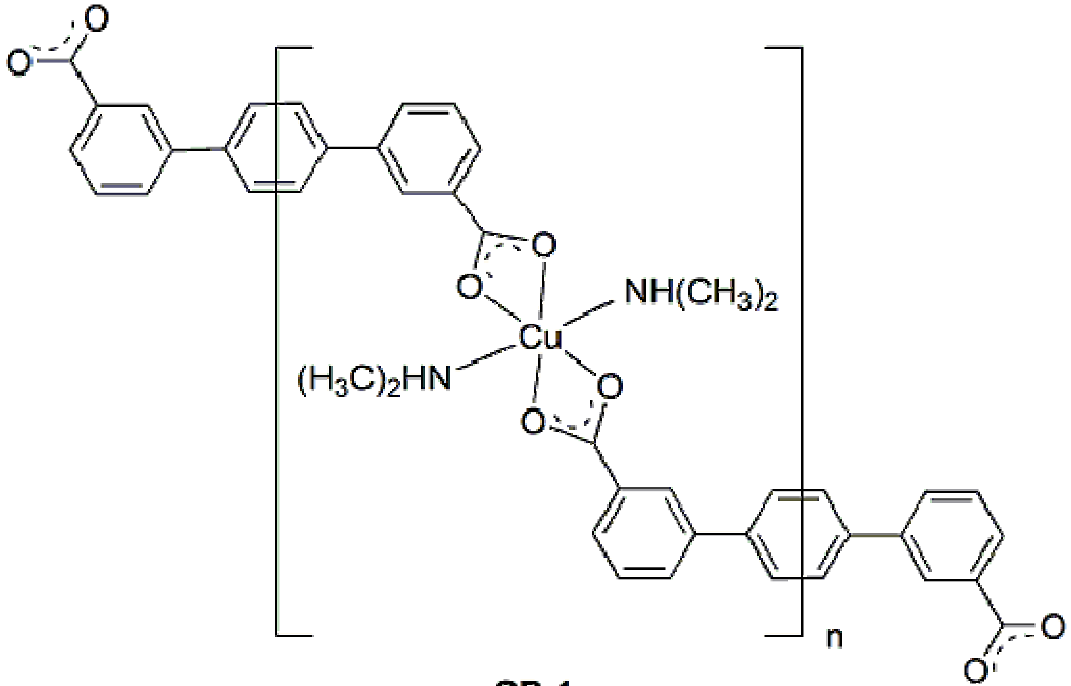
Cu^{II} Coordination Polymers Containing Terphenyl-3,3’-dicarboxylate Linker

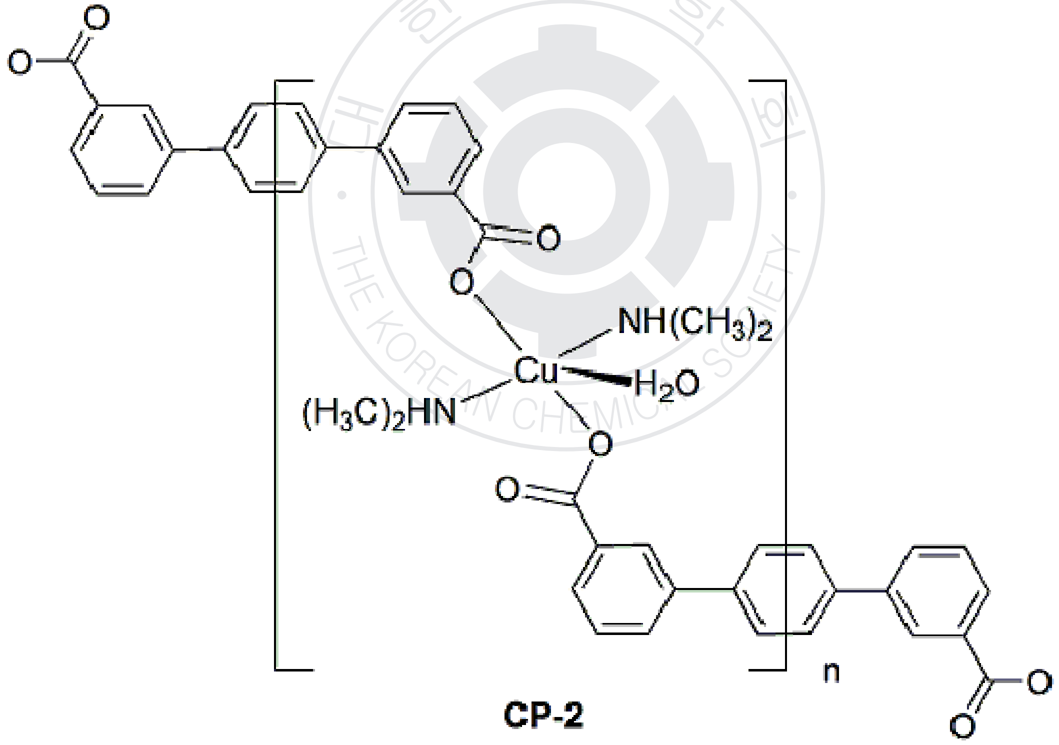
김현철 허성* 여철현[1] 김성진[2] 김영미[3,*]

한국외국어대학교 화학과 [1]연세대학교 화학과 [2]이화여자대학교 화학과 [3]이화여자대학교 화학-나노과학과

Two new one-dimensional Cu^{II} coordination polymers containing a C_{2h}-symmetric terphenyl-based dicarboxylate linker, terphenyl-3,3’-dicarboxylate, were obtained from different preparation methods: one reaction was performed in the presence of 1,4-diazabicyclo[2,2,2]octane as a potential pillar ligand, and the other was done in the absence of DABCO pillar.



CP-1



CP-2

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis of Copolymers Containing 1,1-Diisopropyl-3,4-diphenylsilolene and Disubstitutedsilylene along the Main Chain and their Applications to Lithium-ion Battery

정영민 민용기 박지영 이창섭 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-silolene and disubstituted silylene 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 $CDCl_3$. 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. In order to study the electrochemical properties of the synthesized materials, we also prepared a composite of the obtained polycarbosilanes with silicon nano powder, and examined the characteristics as a lithium-ion battery.

Acknowledgements : This research was partially supported financially by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO. 2015035858).

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Secondary Coordination Sphere: Biomimetic Zinc Complexes as a Model of Carbonic Anhydrase

정동현 조재홍*

대구경북과학기술원(DGIST) 신물질과학

The increase of atmospheric CO_2 causes serious environmental problems which should be overcome in the near future. For CO_2 fixation, we focus on the small biomimetic zinc-containing catalysts mimicking the carbonic anhydrase in terms of the first coordination sphere as well as the second coordination sphere for effective catalytic processes. Carbonic anhydrase (CA; carbonate hydro-lyase, EC 4.2.1.1) is a zinc-containing enzyme that catalyzes the reversible hydration of carbon dioxide: $CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$. The zinc center in the active site is coordinated by three N-histidines and one water molecule. Recently, researchers in chemistry and biology realized that the importance of the second coordination sphere on the active site of metalloenzymes, which performs critical role of enzymatic activity. Thus, we have controlled the second coordination sphere to be more hydrophobic by adding methyl group to aza-macrocycle ligands and investigated enzymatic activities by ESI-MS, stopped-flow spectrometry, and DFT calculation. In addition, the other variables are considered, where aimed to be has greater activity. For example, the metal ion effect is performed by changing zinc to other transition metals. The size of second coordination sphere is controlled by varying from 14-membered to 12-membered macrocyclic ligand to investigate ring-size effect. Lastly, basicity is controlled to confirm optimized catalytic conditions.

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Structural Diversities of Zn-bpe MOFs with Dicarboxylate Bridging Linkers

김현철 허성[*] 김성진[1] 김영미[2,*]

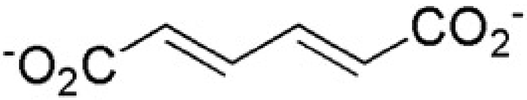
한국외국어대학교 화학과 [1]이화여자대학교 화학과 [2]이화여자대학교 나노바이오 기술연구소, 화학-나노과학과

A series of Zn-bpe (bpe = 1,2-bis(4-pyridyl)ethylene) metal-organic frameworks (MOFs) has been prepared using a mixed ligand system in the presence of ditopic alkane(alkene) dicarboxylate bridging ligands. All Zn-bpe MOFs were structurally characterized by single crystal X-ray analysis. The compound 1 with succinate bridging ligand exhibited a two-dimensional (2D) framework with binodal 5,6-connected net. Compared to 1, other Zn-bpe MOFs have three-dimensional (3D) framework structures. The compound 2 with fumarate bridging ligand displayed a 3-fold interpenetrated 4-connected net with a Schlafli symbol of 6^6 and the compound 3 with adipate bridging linker revealed a 3-fold interpenetrated 8-connected network topology. The structure of compound 4 with muconate bridging linker was a 4-fold interpenetrated 4-connected net with a Schlafli symbol of 6^6 . Interestingly, solvent-free compounds 2 and 4 contain large potential void volume. We investigated the gas sorption and adsorptive dye sorption properties of 2 and 4.

Succinate

Fumarate

Adipate



Muconate

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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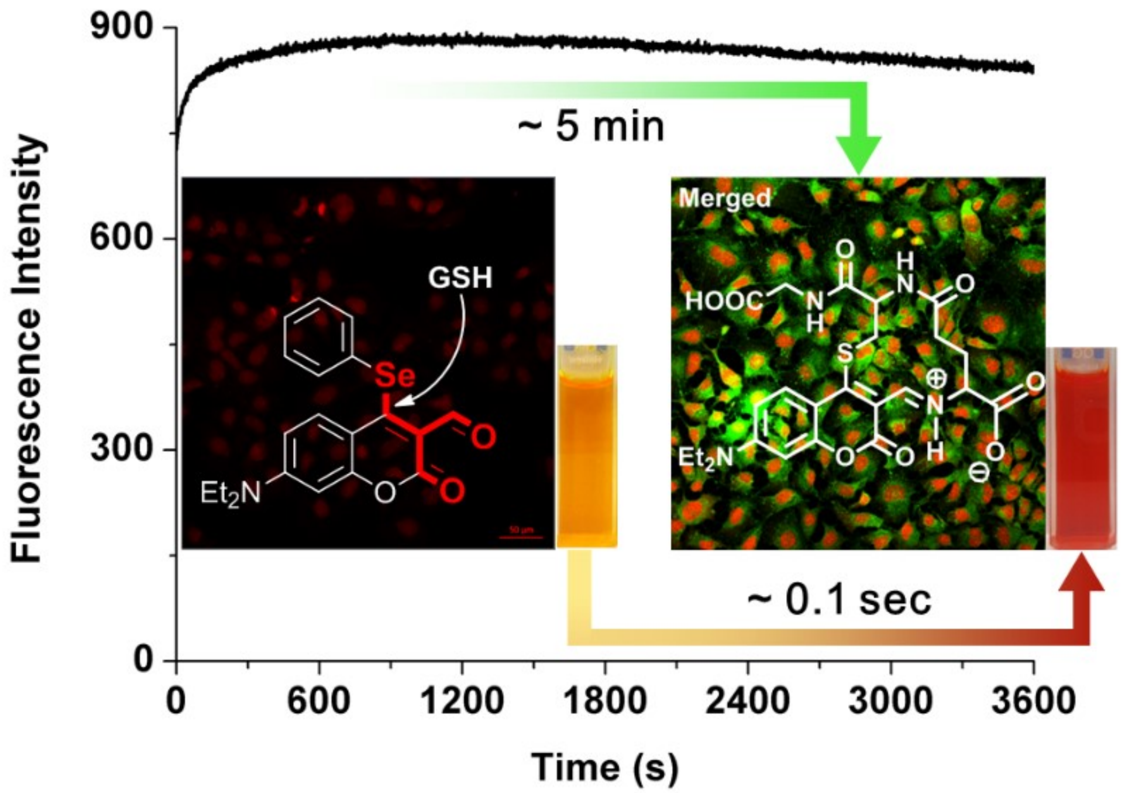
Exceptionally fast fluorescent GSH probing in live cells

D.G.Churchill* SANDIP MULAY 김영삼

한국과학기술원(KAIST) 화학과

Our laboratory is currently working on chemical synthesis intended for neurodegenerative disease research purposes. Three areas are currently being pursued: protein phosphorylation / phosphonylation; organoselenium chemistry; and MRI contrast agent technologies. In this poster presentation, we will be focused on organoselenium-/ organotellurium -based fluorescent probes. These systems also relate to the GPx enzymatic cycle. Recently, we have designed a probe platform that shows excellent selectivity to glutathione over closely related competing analytes such as cysteine and homocysteine.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600
900
Time (s)
0
600
1200
1800
2400
3000
3600
~ 5 min
~ 0.1 sec
GSH
Se
Et2N
O
O
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Merged
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Influence of Cation Mixing for the Thermoelectric Property in the $Ca_{11-x}Yb_xSb_{10}$ (x = 2, 5 and 9) Series

남근우 최웅진 유태수*

충북대학교 화학과

Three ternary antimonides compounds in the $Ca_{11-x}Yb_xSb_{10}$ (x = 2, 5 and 9) series have been synthesized by using the Sn metal-flux method, and batches of well grown block/plate-shaped single crystals were obtained. The isotypic crystal structure of title compounds were characterized by both powder and single crystal X-ray diffractions. All three compounds in the $Ca_{11-x}Yb_xSb_{10}$ (x = 2, 5 and 9) series adopted the $Ho_{11}Ge_{10}$-type structure, which included the body-centered tetragonal space group *I*4/*mmm* with Z = 4, and the lattice parameters were as follows: a = 11.94 - 11.99 Å and c = 17.21 - 17.26 Å. Chemical compositions including the atomic ratio between Ca and Yb of three compounds were verified by the energy dispersive X-ray spectroscopy (EDXS), and morphologies of well grown single-crystals were observed by the scanning emission microscope (SEM). The overall crystal structure can be described as an assembly of three different types of co-facial polyhedra formed by Ca/Yb and centered by isolated Sb atoms, and the three-dimensional (3-D) anionic skeletons consisting of the dumbbell- and square-shaped Sb atoms. More interestingly, the site-preference of Ca and Yb over four available cationic sites in the $Ca_{6.5}Yb_{4.5}Al_2Sb_6$ was studied for the first time for the $Ho_{11}Ge_{10}$-type phase by tight-binding linear muffin-tin orbital (TB-LMTO) method. Site- and bond energies were thoroughly analyze, and density of states (DOS) and crystal orbital Hamilton population (COHP) curves were also studied. Thermal gravimetric analysis (TGA) was measured to understand the thermal stability of three title compounds.

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장소: 대구 EXCO

발표코드: **INOR.P-103**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Various Ru-Ag heterometallic supramolecules based on stoichiometric control of multiple tectons via coordination-driven self-assembly

박유진 류지연 이민형[1,*] 이준승[*]

전남대학교 화학과 [1]울산대학교 화학과

Organometallic Ruthenium half-sandwich complexes and 5?(2-hydroxyphenyl)?1H?tetrazole($L\mathrm{H}_2$) have been used in the construction of supramolecular cages. The reaction of dimeric (*p*-cymene)RuCl_2 and $L\mathrm{H}_2$ in a ratio of 2:1 and 1:1 produced bridged Ru complexes by *L*H and Cl and two *L*H and methoxide respectively. Also, by controlling the reaction ratios, two types of rectangular supramolecules were formed in a ratio of 4:4 and 6:4 (Ru:*L*). The latter contained two ruthenocene units which have η^6 binding mode with half of *L* ligand. More interesting results were achieved when additional AgOTf was used. The reaction of (*p*-cymene)RuCl_2 : $L\mathrm{H}_2$: additional AgOTf in the ration of 6 : 6 : 18 and 6 : 6 : 20 resulted in the formation of unique two supramolecules having molecular ratio of 6 : 6 : 6 or 6 : 6 : 8 for Ru : *L* : Ag, which show cylindrical and double-cone shaped structures, respectively. They were characterized by ^{1}H-NMR, IR, ESI-MASS and their solid state structures were confirmed by X-ray crystallography.

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발표코드: **INOR.P-104**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Insulator to Ionic Conductor Transitions in Microporous Metal-Organic Frameworks

송유대 박경세[1] 윤민영*

가천대학교 글로벌캠퍼스 나노화학과 [1]군산대학교 화학과

Proton conducting materials have used in fuel cell, electrochromic (or electrochemical) sensors and electrochemical reactors. For better application, the conductivity should be tuned or controlled by external stimuli such as light, electric or magnetic field. However, most of the materials failed to demonstrate the conductivity control by the external stimuli. Recently, metal-organic frameworks (MOFs) and related porous materials have widely studied to control the proton conductivity using their modular nature and tunability. Here, we present a microporous metal-organic framework demonstrating humidity dependent conductivity change from insulator to superionic conductor. In low humidity, the MOFs behave like an insulator and the conductivity was detectable at ~ 60% RH, which was further changed to superionic conductor at > 90% RH. For better understanding of such a transition, vapor sorption of the MOFs was studied. Interestingly, three different vapor sorption states were found in the isotherms with a drastic vapor sorption increase; no vapor sorption, medium vapor sorption, and large vapor sorption. Thermogravimetric analysis (TGA) helps to estimate the adsorbed vapor amount and the vapor releasing temperature. Powder X-ray diffraction (PXRD) data demonstrates that the structure of MOFs is slightly changed by adsorption of water vapor. Therefore, we can conclude that the subtle changes in MOF structure by water vapor sorption induce a significant change in the proton conductivity. Details of our recent work will be presented.

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발표코드: **INOR.P-105**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cobalt-Ruthenium Bimetallic Supramolecules Having Different Shapes by Means of Lengths of Linker Units

류지연 박유진 박형련 이준승*

전남대학교 화학과

A cobalt metalloligand, [Tetrakis(4-pridyl)cyclopentadienone]cyclopentadienylcobalt, has been employed in [2 + 4] self-assembly with three di-ruthenium electron accepters, which have different linkers including oxalate, phenolate, naphthalate bridges, respectively. The constructions of three-dimensional supramolecular architectures were confirmed by ESI-MS, NMR spectroscopy, and X-ray crystallography. The solid-state structures revealed that the lengths of spacer in the acceptor units greatly influenced the molecular structures of these metallacages. From these [2 + 4] assemblies, a waterwheel-shaped, a tweezers-shaped and a butterfly-shaped architectures were selectively achieved.

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발표코드: **INOR.P-106**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Investigations of the hole-doping effect for the $Eu_{11-x}Li_xBi_{10-y}Sn_y$ (x = 0, 0.52; y = 0, 2) series

전범용 유태수*

충북대학교 화학과

The $Ho_{11}Ge_{10}$-type compounds having divalent cation, such as Eu and Yb, have been studied by researchers worldwide for thermoelectric material application. Given the particular physical properties including low thermal conductivity caused by a complex crystal structure and electrical resistivity, these compounds were regarded as as good candidates for effective thermoelectric materials. However, due to the coexistence of holes and electrons in the same compounds, Seebeck coefficients of these candidates were relatively poorer than the other thermoelectric materials having complex crystal structures. To figure out this intrinsic issue of title phase, we have attempted to introduce the hole-doping method for these compounds.Therefore, two novel ternary compounds, $Eu_{10.48(3)}Li_{0.52}Bi_{10}$ and $Eu_{11}Bi_8Sn_2$, have been synthesized by a typical high temperature reaction method using a Nb-ampule and characterized by both powder and single crystal X-ray diffractions. All of the title compounds were isotypic and crystallized in the tetragonal $Ho_{11}Ge_{10}$-type structure (space group $I4/mmm$, Pearson symbol $tI84$), and lattice parameters were a = 12.543 - 12.537 ? and c = 18.124 - 18.131 ?. The overall crystal structure can be described as a combination of the cage-shaped 3-dimentional (3D) anionic framework built by Bi or Sn and three different types of co-facial polyhedra formed by cations. Theoretical investigations using tight-binding linear muffin-tin orbital (TB-LMTO) method were also performed to understand overall electric structure including chemical bonding and the site-preference of cations. In particular, the observed cationic site-preference was explained by the comprehensive analyses based on the QVAL values of each atomic site.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-107**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multifunctional Metal/Carbon-Mesoporous Silica Composites

김다정 서원석*

서강대학교 화학과

The metal/carbon-mesoporous silica composites have been synthesized by a simple CVD method. The obtained nanocomposites possess superparamagnetism, high surface area and large pore volume with a mesoporous structure. We have also shown that the composites exhibited high chemical stability in acidic and basic aqueous media. The metal/carbon-silica composites can be used as a multifunctional adsorbent due to strong adsorption through hydrophobic interaction between organic dyes and graphitic carbon shell and selective binding of mercury ion using thiolated mesoporous silica. Additionally, because of the useful magnetic properties and unique mesoporous structure, the composites were applied as magnetically reusable adsorbent for fast, convenient, and highly efficient removal of organic dyes and heavy metal ion. Therefore, we expect that the composites may provide excellent promise for many applications such as environment, material science and so on.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **INOR.P-108**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Alloy Nanocrystals and Alloy/Graphitic Carbon Nanocrystals in Ordered Mesoporous Silica

홍용훈 서원석*

서강대학교 화학과

We have synthesized alloy nanocrystals and alloy/graphitic carbon nanocrystals by a chemical vapor deposition (CVD) method. The alloy nanocrystals are composed the alloy/core is stabilized by the uniform noble metal-rich/shell, and also alloy/graphtic carbon nanocrystals are composed of alloy/core and graphitic carbon/shell nanocrystals. The resulting nanocrystals were characterized by XRD, TEM, EDX, ICP-Mass, SAED pattern and Raman. Alloy nanocrystals are a promising catalyst for both ORR (Oxygen Reduction Reaction) and HER (Hydrogen Evolution Reaction). Also alloy/graphitic carbon nanocrystals are excellent magnetic materials which are expected to be utilized for ultra-high density magnetic recording media due to their superior coercivity.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Functionalization of Metal/Graphitic-Shell Nanocrystals

서유정 서원석*

서강대학교 화학과

We have synthesized metal/graphitic carbon shell (Metal/GC) nanocrystals by thermal decomposition of metal precursors in large pore silica and subsequent methane CVD. And then the metal/GC nanocrystals were covalently functionalized using the 1,3-dipolar cycloaddition of azomethine ylides generated by condensation of sarcosine (N-methylglycine) and glucose. The functionalized metal/GC nanocrystals are monodisperse and soluble in water due to hydrophilic functional groups. Moreover, the metal/GC nanocrystals are chemically stable against sonication and oxidation. The successful reaction was characterized by UV-vis spectroscopy, XRD, EDX, DLS, and TEM. Therefore, we expect the functionalized metal/GC nanocrystals to be useful for biomedical applications such as magnetic-resonance imaging contrast media.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal-organic framework gel of bis(tetrazole)-appended pyridine derivative with $CoBr_2$ as a chemosensor

이지하 박혜송 김채린 정종화*

경상대학교 화학과

We have demonstrated a rare example of a selective chemosensor for the detection of volatile gases containing chloride atom in the gel state. A tetrazole-appended ligand produced the metal-organic framework gel efficiently by the simple mixing with Co2+ ion. The metal-organic framework gel with CoBr2 showed a spherical structure. More interestingly, metal-organic framework gel with CoBr2 selectively recognized toxic gases such as HCl, SOCl2, (COCl)2, and COCl2 containing chloride atoms.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Morphogenesis of Graphene Domains on Copper Substrate using Chemical Vapor Deposition

정희경 강청 이진석*

숙명여자대학교 화학과

Graphene is a two-dimensional carbon material that has attracted great scientific and technological interest due to its intriguing physical properties and enormous potential for various applications. The industrial exploitation of chemical vapor deposition (CVD) graphene crucially depends on the ability to generate large-area sheet. During graphene growth pressure can be divided into low pressure (LP) and atmospheric pressure (AP). Commonly, the electric properties and device performance are strongly dependent on the size, shape, crystallinity, layer numbers, and edge structures of pristine graphene. The graphene syntheses using a Cu catalyst in APCVD processes at higher methane concentrations disclosed that the growth is not self-limiting. LPCVD is a striking contrast from previous experiment. Controlling these parameters of graphene in synthesis or post-synthesis manipulation is thus critical to achieve tunable properties and optimized device performance.Here, we synthesized graphene domains with four-folded, two-folded, and isotropic morphology by chemical vapor deposition (CVD) under low pressure. It was confirmed that the growth of graphene domains is governed by reaction pressure and temperature, as well as concentration of carbon precursor during the chemical vapor deposition (CVD) process. Also, we investigated their morphological change on different Cu lattices. Acknowledgment : This research was supported by Nano·Material Technology Development Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and Future Planning.(2009-0082580)

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발표코드: **INOR.P-112**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Applications of N-Heterocyclic Carbene Based MOFs

이현정 이재철 김용휘[1] 김기문 이은성*

포항공과대학교(POSTECH) 화학과 [1]기초과학연구원 복잡계자기조립연구단

Metal organic frameworks (MOFs) have attracted great interest due to their potential applications such as catalysis, gas storage, and separation of molecules. Since MOFs can be constructed with a variety of building units, they can be easily tuned for appropriate applications. N-heterocyclic carbenes (NHCs) have been emerging as organic linkers for supporting various transition metal catalysts in MOFs. However, there is a little study on intrinsic properties of free NHC in MOFs although N-heterocyclic carbenes (NHCs) are well-known to activate small molecules such as CO_2, CO, NH_3 and H_2 or even to stabilize main group radicals.Recently, we found that NHCs could stabilize nitric oxide (NO) radical in a solution phase to form stable NHC nitric oxide radicals.[1] To investigate sorption properties of various small gas molecules inside free NHC MOFs for potential gas separation, Several imidazolium MOFs have been prepared and attempted for the deprotonation of the imidazolium MOFs to access free NHC MOFs. The synthesis and applications of NHC MOFs will be presented.Reference(1) J. Park, H. Song, Y. Kim, B. Eun, Y. Kim, Y. Bae, D. S. Park, Y. M. Rhee, W. J. Kim, K. Kim, E. Lee, *J. Am. Chem. Soc.* 2015, 137, 4642.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-113**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Simple and Efficient Regeneration of Metal-Organic Frameworks via Acid-Base Treatment

한승완 나명수*

울산과학기술대학교(UNIST) 화학과

Simple and efficient regenerations of MOF-5 and HKUST-1 are demonstrated via acid-base treatment. The reactants are recovered simply dissolving the deteriorated MOFs using a strong acid. The pristine MOFs are regenerated in high yields by adjusting the solution pH either via in-situ base formation or via ex-situ base addition. The both regeneration protocols are environmentally benign and cost effective because the reactants in the deteriorated MOFs are recycled. Especially the ex-situ base addition protocol can be done in a cheap and environmentally friendly ethanol/water mixed solvent at ambient condition and is suitable for large scale batch regeneration owing to the simple procedure and short reaction time.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of Nickel Oxide Nanostructures with High Surface Area and Application for Urea Detection

MAIDUYHIEN 유효종*

한림대학교 화학과

In this presentation, we describe the synthetic procedure for the fabrication of uniform nanostructured nickel-based coordination polymer particles with multilayered morphologies (mL-NiCPPs) through a two-step heating process. To increase the surface area by reducing the size of mL-NiCPPs, pyridine and acetic acid were added as size modulators during the growth process. The resultant coordination polymer nanoparticles were then calcinated at a controlled temperature in order to produce nickel oxide nanostructures (mL-NiOs), which have a regular multilayered morphology and a high degree of crystallinity. Moreover, the mL-NiOs had a relatively high BET specific surface area (112 m^2/g) and a well-defined pore size (10 nm), hence exhibited significant potential for use in a variety of applications.The synthesized mL-NiOs were successfully deposited onto an indium tin oxide (ITO) using electrophoretic deposition. The prepared NiO/ITO electrodes were subsequently employed for both enzymatic and non-enzymatic urea detection. Both urea sensing systems exhibited high sensitivity towards urea (22.39 and 300 ?A mM^{-1} cm^{-2} for enzymatic and non-enzymatic, respectively) and a linear dependence of the current on the urea concentration with short response time. Furthermore, the influence of interferents, which simultaneously exist in human serum (e.g. glucose, uric acid, cholesterol), was investigated to assess the sensing performance of the electrodes.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-115**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Surface Engineered Doubly Open-Ended TiO2 Nanotubes For Highly Efficient Solar Water Splitting

최종민 박태호*

포항공과대학교(POSTECH) 화학공학과

We report a synergistic effect of flame and chemical reduction methods to maximize the efficiency of solar water splitting in transferred TiO2 nanotube (TNT) arrays on a transparent conducting oxide (TCO) substrate. The flame reduction method (>1000 °C) leads to few oxygen vacancies in the anatase TNT arrays, but it exhibits unique advantages for excellent interfacial characteristics between transferred TNT arrays and TCO substrates, which subsequently induce a cathodic on-set potential shift and sharp photocurrent evolution. By contrast, the employed chemical reduction method for TNT arrays/TCO gives rise to an abrupt increase in photocurrent density, which results from the efficient formation of oxygen vacancies in the anatase TiO2 phase, but a decrease in charge transport efficiency with increasing chemical reduction time. We show that flame reduction followed by chemical reduction could significantly improve the saturation photocurrent density and interfacial property of TNT arrays/TCO photoanodes simultaneously without mechanical fracture via the synergistic effects of coreducing methods.(Ref) Nano lett. 2015. DOI: 10.1021/acs.nanolett.5b01406

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-116**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Reactivity of N-heterocyclic Carbene Nitric Oxide Radicals

박준범 송하영 김영석 김용휘[1] 김기문 이은성*

포항공과대학교(POSTECH) 화학과 [1]기초과학연구원 복잡계자기조립연구단

N-heterocyclic carbenes (NHCs) are well-known to stabilize main group radicals and radical ions. Pioneered by the Bertrand group and other groups, phosphoryl, silyl, boryl and other organic radicals stabilized by NHCs have been isolated and characterized. A successful preparation of the radical compounds was explained by NHCs' π-acceptor character, which imparts remarkable stability because the significant portion of the spin density of the radicals resides on the carbene carbon. We found that NHCs could stabilize nitric oxide (NO) radical in a solution phase to form stable NHCNO radicals. Full characterization of the compounds including X-ray crystallography, EPR, UV-vis, and cyclic voltammetry will be presented in addition to the mechanistic studies and NO transfer experiments. This study clearly adds another important example of stable singlet carbenes acting as mimics for transition metal centers. Further studies on carbenes' reactivity with other small molecules will deepen our understanding of this interesting resemblance.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel probe for simple fluorometric detection of nerve agent simulant DECP in aqueous media

NGUYEN THI THUY TIEN

한국과학기술원(KAIST) Chemistry

A novel, water-based probe for simple and selective detection of the nerve agent simulant DECP was synthesized, using the 1, 8-napthalimide fluorogenic skeleton. The probe under basic condition shows a color change under UV light in the presence of DECP.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-118**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Crystallinity-dependent conductivity of multi-interactive molecular materials

이길령 Yumi Yakiyama[1] Masaki Kawano[*]

포항공과대학교(POSTECH) 첨단재료과학부 [1]Osaka University

Recently, we have successfully revealed the structure of efficient conduction state with nano-meter size water layer formed by multi-interactive molecule, tris(4-pyridyl)hexaazaphenalene (TPHAP) by ab initio XRPD analysis. The potassium salt of TPHAP showed high ion conductivity up to 3.4 x 10^{-3} S/cm by hydration. This conductivity was realized by the large water layer formation which was stabilized by multi-interactivity of TPHAP. Furthermore, the crystalline powders of ammonium and sodium salts showed close relationship between crystallinity and conductivity: crystalline powders were two orders higher conductivity than that of amorphous powder under humid condition. We revealed crystalline structure using X-ray technique.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **INOR.P-119**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Selective Growth of C_{70} Cube- and Tube-Shaped Crystals

김정아 박치범[1,*] 최희철[*]

포항공과대학교(POSTECH) 화학과, 기초과학연구원 CALDES [1]기초과학연구원 CALDES

Changing a crystal shape and a packing structure attracts interests beyond academic view point because it causes significant changes of the property observed from powder or solution phase. However, quiet limited cases were reported showing a significant crystallization change (*i.e.* crystals having different dimensions) without altering materials participating the reaction. Here in, we report facile crystallization control of C_{70} crystals from cube to tubes without replacing solvent. It was confirmed that crystal shape does not depend on supersaturation level but mesitylene ratio during the crystallization. Details about experiments and proposed mechanism of selective growth of C_{70} cube and tube will be discussed.

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Single Atom and Molecule Manipulation and Spectroscopy with a Scanning Tunneling Microscope

권태연 최희철*

포항공과대학교(POSTECH) 화학과, 기초과학연구원 CALDES

Progress of our new low temperature ultrahigh vacuum scanning tunneling microscope (STM) will be presented. Lateral manipulation of single magnetic atoms such as dysprosium and holmium on the Ag(100) and Ag(110) surfaces was carried out using an STM tip. Single inorganic molecules such as fluorinated copper phthalocyanine ($F_{16}CuPC$) on the silver surfaces were detected using STM spectroscopy and were manipulated. We are also developing a new scheme to implement a tuning fork style atomic force microscope (AFM) capability as well as STM routines. Some of our key instrument concepts such as an exchangeable low temperature preamplifier will be presented. This AFM function will enable studying elementary chemical reactions involving single atoms and single molecules not only on conducting surfaces, but also on insulating surfaces. This capability of tuning fork AFM together with STM manipulation and spectroscopy routines are important to realize “angstrom-chemistry” of single atoms and single molecules.

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Improvement of the Structural Stability of SiGe Alloy Nanowire Anode by Finely Controlling the Si Surface Segregation

김형기 박치범[1] 김정아 이민경 최희철*

포항공과대학교(POSTECH) 화학과, 기초과학연구원 CALDES [1]기초과학연구원 CALDES

SiGe nanowire (NW) is the attractive anode material for lithium ion battery because of its high energy density. However, it suffers from the mechanical stress due to tremendous volume change during the charging/discharging process, which results in pulverization of anode material. To improve the structural stability of anode material, we propose new SiGe nanoarchitecture (Type-G SiGe NW) with highly populated Si at the surface where tardy lithium diffusion in Si induces the formation of unlithiated part as structural support frame. Type G-SiGe NWs are easily prepared by simple thermal annealing the SiGe NW with uniform distribution of Si (Type U-SiGe NW) in hydrogen environment. Resulting Type G-SiGe NW exhibits high reversible capacity (> 1031 mA·h·g^{-1}), and long cycle life (400 cycles) with high capacity retention (89 %) at 0.2 C. The mechanism of Si segregation at the surface and further electrochemical characterization of SiGe NW will be discussed in detail.

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Solid State Conversion of Anthracene Disks to Anthraquinone Disk by Photoreaction

이민경 박치범[1] 최희철[*]

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The organic materials have been widely studied for optoelectronic device applications such as organic display, laser, and organic field effect transistors. Recently, controlling molecular arrangement in organic single crystal is gathering great attention since it is one of the most important factor for modulation of the electrical and optical properties. So, many researches have studied polymorph single crystal in solution phase by solvent molecules effect.Here, we present anthraquinone disk was synthetized from anthracene disks through photooxidation of anthracene molecules in ambient condition. Upon ultraviolet (> 300 nm) light illumination in the presence of oxygen, the anthracene with monoclinic structure rearrange to the anthraquione wire with orthorhombic structure. The photoluminescence property shows definite difference between anthracene disk and anthraquinone disk which is also different with that of anthraquionoe powder. The anthraquinone disk presents red photoluminescence which is attributed to the changed molecular arrangement.

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Large-scale growth of two-dimensional transition metal dichalcogenides atomic layers using surface-alloy-mediated chemical vapor deposition

송인택 박치범[1] 최희철*

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Transition metal dichalcogenides (TMD) atomic layers have been one of the most intriguing materials for researchers in recent years. While the bulk is just an indirect gap semiconductor, their two-dimensional nanosheets are direct-gap semiconductors with fascinating applicability to nanoelectronics. The real application of these materials require the achievement of uniformly large-scale material for mass production. Herein, we demonstrated growth of MoS_2 atomic layers, a well-known TMD, by using Au substrate, on which volatile Mo precursors form Mo-Au surface alloy, an atomically thin reservoir of Mo. Treatment of the surface alloy with sulfur-containing precursors further convert it into atomic layers of MoS_2. A number of methods, including Raman spectroscopy and transmission electron microscopy, have confirmed the formation of atomic layers. In addition, for the first time, patterned growth of the atomic layers was achieved by using pre-patterned gold film. We further demonstrated the growth of WS_2 atomic layers as well.

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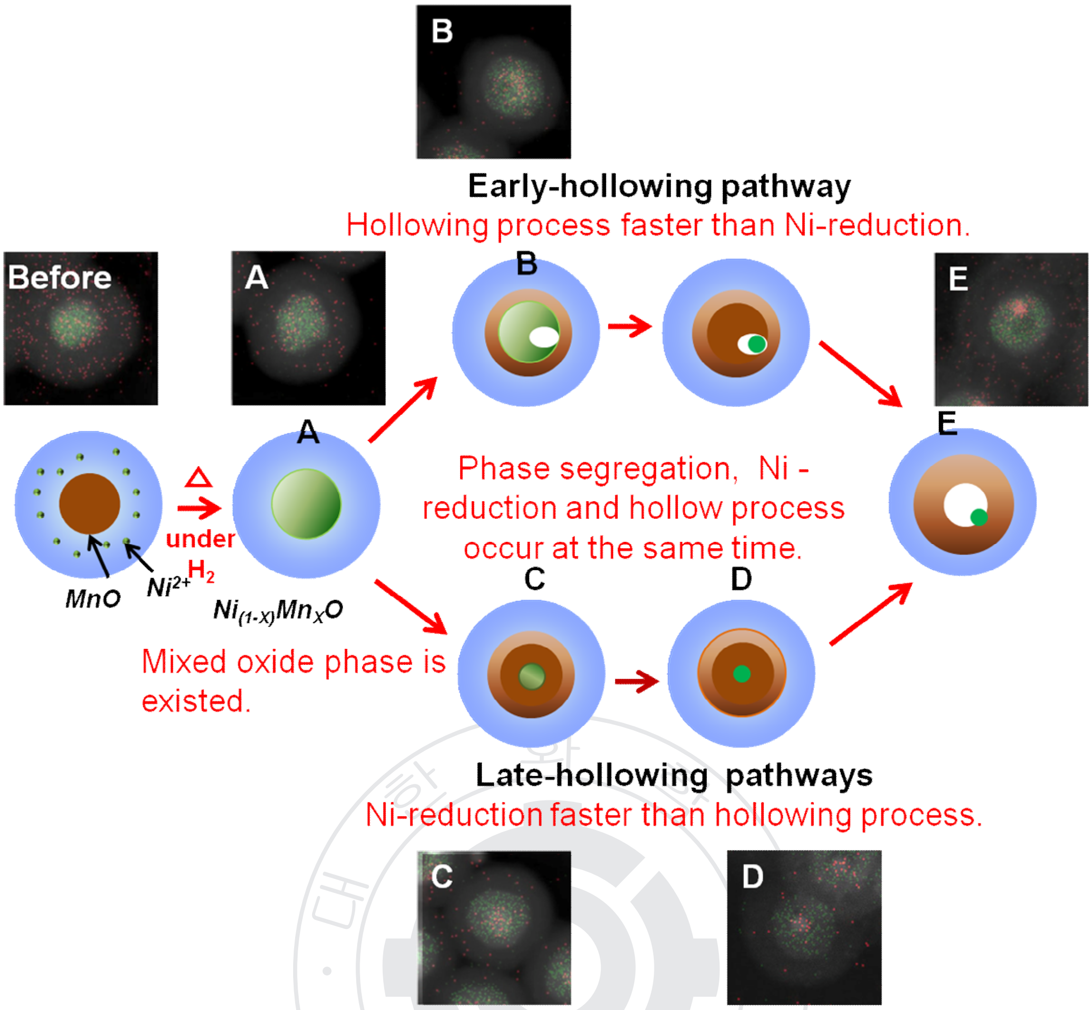
Mechanistic Insight into the Yolk@Shell Transformation of MnO@Silica Nanospheres Incorporating Ni^{2+} ions: the Solid-State Route toward a Colloidal Hollow Nanoreactor

김진구 이인수*

포항공과대학교(POSTECH) 화학과

As an effort to develop a simple and versatile synthetic strategy that contributes the evolution of hollow nanostructures with increasing complexity and functionality, this research was devoted to study the hollow transformation within a nano-sized solid matrix. Through an in-depth investigation of a hollowing process of MnO nanocrystal confined within a Ni^{2+} incorporating silica nanosphere, we could explain a very distinctive transformation pathway that produces the yolk@shell nanostructure with a single Ni nanocrystal inside a silicate nanoshell. It was revealed that the yolk@shell structure was developed by the mechanism combining different processes, including the formation of a $(Ni_{0.1}Mn_{0.9})O$ mixed-metal oxide and subsequent segregation of the reduced Ni. Furthermore, this study also devised a protocol to exploit the solid-state-synthesized powder for fabricating a colloidal hollow nanoreactor that can selectively catalyze the reduction of nitroarenes and be recycled via the magnetic process.


B
Early-hollowing pathway
Hollowing process faster than Ni-reduction.
Before
A
B
E
A
E
Phase segregation, Ni - reduction and hollow process occur at the same time.
△
under H_2
MnO
Ni^{2+}
$Ni_{(1-x)}Mn_xO$
Mixed oxide phase is existed.
C
D
Late-hollowing pathways
Ni-reduction faster than hollowing process.
C
D

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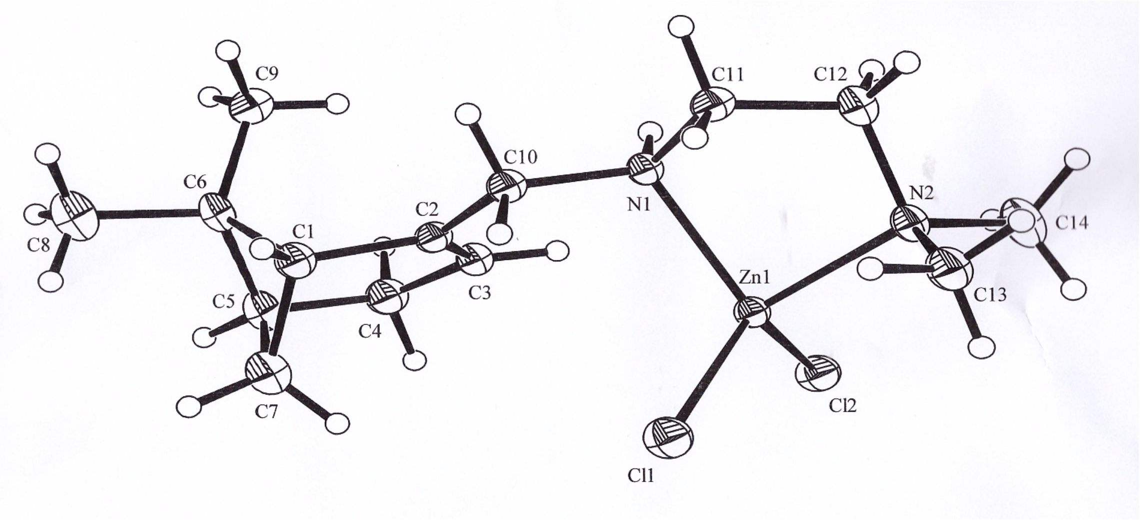
Synthesis of copper(II) and zinc(II) complexes bearing N^1,N^1-dimethyl-N^2-(((*1R*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl)ethane-1,2-diamine and their application to *rac*-Lactide polymerization

천민경 정종화*

경북대학교 화학과

Novel dichloro copper(II) and zinc(II) complexes of N^1,N^1-dimethyl-N^2-(((*1R*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl)ethane-1,2-diamine ligands were synthesised and characterised by X-ray diffraction. The alkoxide derivatives of the well characterized two complexes were assessed for ring opening polymerization (ROP) of *rac*-Lactide. The active catalyst species were generated by treating the complexes with 2 equivalent $LiOCHMe_2$. Furthermore, the heterotactic polylactide with Pr up to 84 % can be obtained by using the initiator of the complex bearing N^1,N^1-dimethyl-N^2-(((*1R*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl)ethane-1,2-diamine in CH_2Cl_2 at room temperature. The stereoselectivity and molecular weight of the polymer was determined by 1H-NMR spectra, and GPC.


C9
C6
C8
C1
C5
C7
C2
C4
C3
C10
N1
C11
C12
N2
C14
C13
Zn1
Cl2
Cl1

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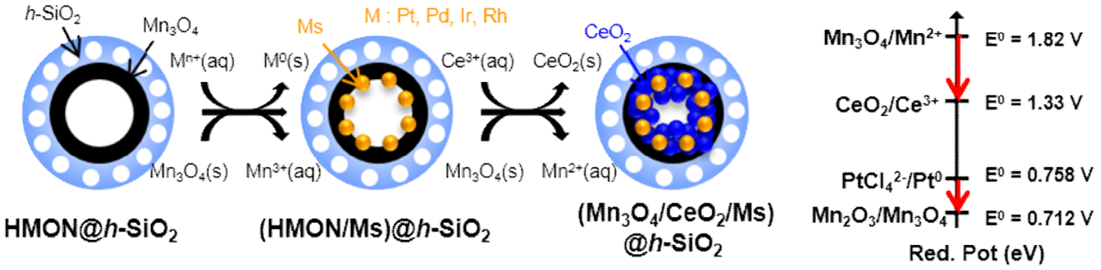
Post-synthetic Modulation of Catalytic Interface inside Hollow Nanoreactor: Exploitation of Bidirectional Performance of Mixed-valent Mn3O4 Phase in Galvanic Replacement Reaction

이동규 이인수*

포항공과대학교(POSTECH) 화학과

This research intended to develop the post-synthetic method of diversifying and modulating catalytic interface inside the hollow nanoreactor by replacing the pre-loaded catalyst-supporting layer with a more active and synergistic support material such as CeO2. This study discovered the bidirectional performance of a mixed-valent Mn3O4 nanoparticle in the galvanic replacement process, which templates both of reduction of noble metal ions and oxidation of Ce3+ ions, therefore generating noble metal/CeO2 nanocomposites. Moreover, by applying the explored process to the pre-synthesized hollow silica nanoreactor, the catalyst-immobilizing Mn3O4 layer inside the cavity could be exchanged with CeO2 while preserving tiny size and well-dispersed state of supported catalysts, which allowed for the introduction of noble-metal/CeO2 interface exerting the synergistic performance in catalyzing the aerobic oxidation.



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Position Controlled Growth of C_{60} Single Crystals for Superconducting Devices

이진호 박치범[1] 최희철*

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It is important issue to place organic single crystals at the desired position on a substrate not only for optoelectronic applications but also for fundamental studies. To achieve this goal, researchers have recently developed some methods to control the position of organic crystals. However, most of them are inefficient or unsuitable to fabricate optoelectronic devices. Here, we present a simple but efficient method to grow morphologically well-defined fullerene single crystals on specific position of solid substrates, which enables extended study on unique physical properties, especially on superconductivity. By patterning C_{60} seeds and using solvent vapor annealing (SVA) process, we successfully fabricate the C_{60} single crystal devices on the bottom contact electrodes. This allows us to monitor the change in Raman signal and conductivity simultaneously during alkali metal doping. The temperature-dependent resistivity results confirms that the alkali metal doped fullerene single crystal is superconducting with higher critical temperature (T_C) than that of polycrystalline thin film devices and it is metallic above critical temperature. These results provide promising approach for the discovery of new organic superconductor as well as practical applications such as organic field effect transistor.

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Novel properties in alkali metal intercalated triphenylene

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Since the first discovery of the superconductivity in potassium doped picene, numerous types of alkali metal intercalated polycyclic aromatic hydrocarbons (PAHs) have attracted significant interests to reach higher critical temperature. Notably, potassium doped 1,2:8,9-dibenzopentacene shows critical temperature up to 33 K, which is higher than former charge transfer type superconductors. For organic superconductors, alkali or alkali-earth metals are generally injected to organic molecules to provide additional electrons. However, the experimental limits according to this injection procedure make it hard to induce homogeneous doping and tolerate oxygen and moisture. In addition, the small size of crystallites can cause low shielding fraction and poor reproducibility.Thus in this work, to overcome these drawbacks, we made an effort to produce homogeneous alkali-metal-doped samples by making pellets. We chose triphenlyene as a target PAH molecule. These samples are annealed in a vacuumed glass chamber at various temperatures and time. The color of the annealed sample is changed into black, and we measured magnetic susceptibility and hysteresis to check the superconductivity. Also we tried to confirm whether the black powder conserves the former structure.

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Novel crystallization of organic molecules mediated by solvent shell formation using solute-solvent interaction in binary solvent system

박요환 최희철*

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Solution-phase crystallization has been widely studied so far, because it enables to control diverse parameters of growth. Among various solution-phase crystallization methods, liquid-liquid interfacial precipitation (LLIP) is especially useful to control the local environment of the solutes, because it introduces an anti-solvent that decreases the solubility of the solutes. However, LLIP cannot fully control the environment around the nucleation seeds, because the range of the anti-solvents is limited and the initial solution is homogeneous. To this end, we introduce a novel method that can control the local environment of solutes in binary solvent mixture system by forming shells of specific chemical species around the nucleation seeds.As a proof of concept, we chose metalloporphyrin derivatives as the target solute molecule, because they are difficult to be crystallized without the use of external ligand or metal ion auxiliaries despite their wide applications in dyes, catalysts, and photodynamic therapy. Therefore, the preparation of metalloporphyrin crystals, or the direct self-assembly of metalloporphyrin into coordination polymers, bears great importance. In this presentation, we show the crystallization of zinc-tetra(4-pyridyl)porphyrin (ZnTPyP), where their aromatic macrocycle ring with well-defined π-conjuated system and various functional groups can effectively interact with solvent molecules. Based on this method, we prepared cube-shaped single crystals of ZnTPyP, and we expect that this method can be generalized to other molecules.

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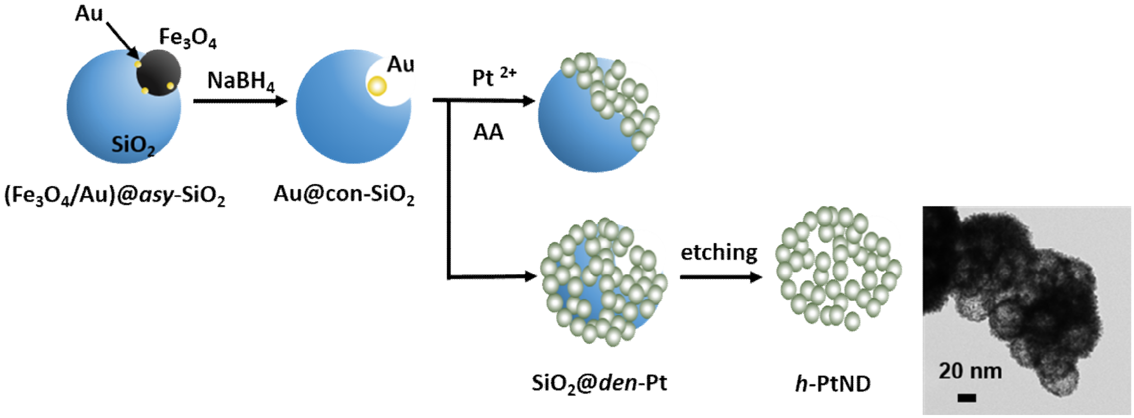
Asymmetric Silica Encapsulation toward Colloidal Janus Nanoparticles: Concave Nanoreactor for Templating the Synthesis of Hollow Dendritic Pt Nanoshell

김다운 이인수[1,*]

포항공과대학교 화학과 [1]포항공과대학교(POSTECH) 화학과

The silica coating strategy has provided synthetic methodologies to render colloidal inorganic nanoparticles. Before this study, nanoparticles having concentric core-shell structure such as Au@SiO2, Ag@SiO2 and Fe3O4@SiO2 were synthesized. However recently, synthetic methodologies of colloidal asymmetric Janus nanoparticles have been suggested applying reverse microemulsion strategy using organosilane reagent with amine functional group. The Janus nanoparticles including Fe3O4 and Au asymmetrically silica deposited were found to leave a concave silica nanosphere with single Au nanoparticle inside the hole, Au@con-SiO2, in a continued reductive dissolution step. In particular, the Au@con-SiO2 nanoreactor was used as a template to synthesize Au@asy-SiO2, Pd@asy-SiO2 and Pt hollow dendritic nanoshell which has much potential usefulness as an electrocatalyst. The Pt hollow nanoshell was successfully isolated in a ligand-free system and exhibited enhanced electrocatalytic activities in oxygen reduction reaction (ORR).



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Light-induced Synthesis and Patterning of Covalent Organic Frameworks (COFs) with Unique Morphology

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Covalent organic frameworks (COFs) are crystalline organic building block, which are linked by covalent bond between light elements. Since the first report on COFs in 2005 they have been widely studied as potential next-generation materials for gas storage and chemical catalysts because of their high thermal stability and stable porosity. In addition, they were further expected as superior two-dimensional nanomaterials which shows remarkable charge transfer and separation properties across π-conjugated layers. In spite of these advantages of COFs, however, the current solvothermal synthesis procedure has limitations such as long synthesis time (2~7 days) and high reaction temperature (90~120 ºC).Herein, we have successfully synthesized COF-5 by using light irradiation. Light-induced method significantly reduces reaction time down to a few hours at room temperature, which is dramatically milder condition than that of conventional solvothermal method (3 days, 90 ºC). Moreover, their homogenous sea-urchin-type morphology increases the surface area and the CO2 adsorption/desorption ability, which are, to the best of our knowledge, one of the highest among previously reported COF-5. Also, as an application perspective, we have succeeded in patterning the COF-5 into various geometry on a SiO2 substrate at the desired positions, exploiting the unique advantages of light as the energy source.

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Symmetry Reduction through Shape Transformation Involved in Seed Mediated Synthesis of Large 2D Bi_2Se_3

Mukul Pradhan 최희철[1,*]

기초과학연구원 CALDES [1]포항공과대학교(POSTECH) 화학과, 기초과학연구원 CALDES

We report symmetry reduction phenomenon through shape transformation of circular to hexagonal disc involved in a seed mediated synthesis of large 2D Bi_2Se_3. However, previously reported Bi_2Se_3 nanostructures are limited to hexagonal nanoplates of small lateral diameter (~1-5 ?m lateral diameter). In this study, a simple and reliable method for the growth of large (~20-50 ?m lateral diameter and 10-15 nm thickness) circular as well as hexagonal disk of Bi_2Se_3 is reported in presence of ethylenediaminetetraacetic acid (EDTA). EDTA acts as a complexing agent for the bismuth precursor. During the growth process, small circular disk with higher symmetry gradually increases its size and finally converted to hexagonal disk having lower symmetry and then further growth is stopped. We can synthesize 2D Bi_2Se_3 with single grained as well as multiple grained crystals with stacked spirals by controlling the nucleation and growth process. We have characterized thoroughly the morphology and crystal structures of the synthesized new shapes and we have discussed the possible growth mechanisms in the context of control over surface chemistry and the nucleation stage. Raman spectroscopic analysis as well as AFM studies shows that the synthesized Bi_2Se_3 hexagonal disks are composed of 10-15 quintuple-layers. At the best of our knowledge this is the first in situ gradual addition methodology in presence of complexed precursor as well as face selective capping for slow over growth of seed for large 2D crystal synthesis.

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The microwave-assisted synthesis of Covalent organic framework with micro- and mesopores for CO_2 capture

강동원 이종현 홍창섭*

고려대학교 화학과

We designed two covalent organic framework compounds, $C_8H_5O_2$ (1) and, Meso-1. Compounds 1 and Meso-1 were synthesized via microwave method. Meso-1, which has micropore and mesopore was prepared via the same synthesis process of 1 except for polymer F-127($H(OCH_2CH_2)_x(OCH_2C(CH_3)CH)_y(OCH_2CH_2)_zOH$). These compounds were characterized by element analysis, infrared spectroscopy, thermogravimetric analysis and sorption. We confirmed formation of the mesopore in Meso-1 via pore size distribution. Also, the amount of carbon dioxide uptake was measured and these heat of CO_2 adsorption enthalpy was investigated. Detailed synthesis condition and sorption properties will be given in the presentation.

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Synthesis, crystal structures and physical properties of a dysprosium based framework

이종현 강동원 홍창섭*

고려대학교 화학과

We have synthesized a two-dimensional coordination polymer $Dy_2(DSBDC)_{1.5}(DEF)_5$ (1) ($DSBDC^{2-}$=2,5-disulfo-1,4-benzenedicarboxylate) using a solvothermal reaction of $Dy(NO_3)_3$? $6H_2O$ and H_2DMBDC(2,5-dimercapto-1,4-benzenedicarboxylic acid) as a organic liker in DEF solvent. Thiol groups in ligand oxidized to sulfonic acid groups during the reaction. Compound 1 crystallizes in the triclinic system with the space group P-1. It contains two Dy^{3+} ion, 1.5 DSBDC ligands and five DEF molecules. One Dy^{3+} ion is coordinated by eight oxygen atoms from five DSBDC ligand and two oxygen atoms from DEF and the other Dy^{3+} ion is bridged by nine oxygen atoms from seven DSBDC ligand and two oxygen atoms from DEF. Compound 1 was characterized by elemental analysis, IR, PXRD and single crystal X-ray diffraction. Detailed structures and other measurements will be given in the presentation.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-135**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Asymmetric Silica Encapsulation toward Colloidal Janus Nanoparticles; Concave Nanoreactor

구정훈 이인수[1,*]

포항공과대학교 화학과 [1]포항공과대학교(POSTECH) 화학과

A novel reverse microemulsion strategy was developed for the asymmetric silica encapsulation of metal-oxide nanoparticles, by exploiting the self-catalytic growth of amino-silane-containing silica occurring at a single surface site. This strategy produced various colloidal Janus nanoparticles, including Au/Fe3O4@asy-SiO2, which was further converted to Au-containing concave silica nanosphere, Au@con-SiO2, by reductive Fe3O4 dissolution. Employment of Au@con-SiO2 as a metal-growing nanoreactor allowed the templated-synthesis of a hollow dendritic Pt nanoshell.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Asymmetric Silica Encapsulation toward Colloidal Janus Nanoparticles: Concave Nanoreactor

구정훈 이인수*

포항공과대학교(POSTECH) 화학과

A novel reverse microemulsion strategy was developed for the asymmetric silica encapsulation of metal-oxide nanoparticles, by exploiting the self-catalytic growth of amino-silane-containing silica occurring at a single surface site. This strategy produced various colloidal Janus nanoparticles, including Au/Fe3O4@asy-SiO2, which was further converted to Au-containing concave silica nanosphere, Au@con-SiO2, by reductive Fe3O4 dissolution. Employment of Au@con-SiO2 as a metal-growing nanoreactor allowed the templated-synthesis of a hollow dendritic Pt nanoshell.

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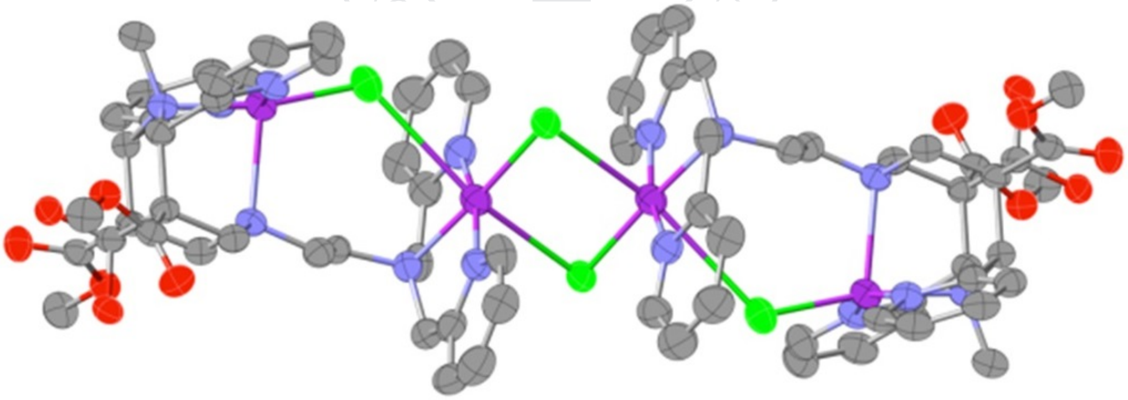
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multinuclear complexes with nitrogen and oxygen donor atoms

박상석 최순일 고성신 조정환 김양*

고신대학교 화학신소재학과

A bispidine-style ligand involving four pyridine-N and three aliphatic-N donor atoms forms a bimetallic species with $CuCl_2$ in which all seven N-donors are bound and which aggregates in the crystal through chloride bridging. The magnetism of this solid can be interpreted in terms of a relatively strong ferromagnetic coupling of Cu(II) centres in different binuclear units and rather weak antiferromagnetic coupling within the units. The geometry and dimensions of chloride bridges in the two cases are quite different.



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발표코드: **INOR.P-138**
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Facial Synthesis of Pt/NaY zeolite @MOFs with Gas Sorption Properties

임대운 이희주[1] 최용남* 조인화

한국원자력연구원 중성자과학연구부 [1]서강대학교 물리학과

Metal-organic frameworks (MOFs) including exceptional porosity, large surface area, and uniform micro pore have been attractive with a considerable attention because their various potential applications such as such as gas storage and separation, sensor, heterogeneous catalysis, proton conduction, and fabrication of nanoparticles. Although they are a good candidate in a various applications, for a practical application, their physicochemical property should be improved. Synthesis of nano composite composed of MOF and one or more materials is considered as one of the strategies. However, it is challenge to combine two or three components as a single platform. Therefore synthesis of a new type of composite will receive substantial attentions from various research fields. Herein we try to synthesize the unprecedented nano composite material for enhancement of heat of H_2 adsorption. These composite integrate the advantageous properties of Pt nanoparticles, zeolite and MOFs. We expected that the composite will be fascinating as a hydrogen storage materials or heterogeneous catalyst.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Ordering in Vanadium-Iron-Hydrogen system observed by in situ neutron diffraction measurement

조인화 이희주[1] 최용남*

한국원자력연구원 중성자과학연구부 [1]서강대학교 물리학과

In situ neutron diffraction patterns of V_3Fe alloys were measured at RT - 400C under D_2 3 bar to observe an accelerated ordering in the vanadium-iron alloys by the hydrogen admission. Thanks to the neutron's peculiar scattering properties by atoms, vanadium and iron are identified successfully while x-rays can hardly differentiate one atom from its adjacent atoms such as V from Fe. A new satellite peak appeared at 350 C following a simple thermal expansion of the initial structure (BCC) where V and Fe atoms are randomly occupied the same position. In addition, the appearance of this peak depends on the existence of hydrogen reversibly at 350 C. We tried to match the new phase to the expected ordered structure, A15 [1], and the results were quite acceptable. X-ray diffraction patterns of the sample and additionally prepared ex situ samples were also analyzed for complementary information.[1] J. Bloch et al., Phys. Rev. Lett. 108 (2012) 215503

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Nickel Nitrosyl Complexes Supported by a PEP ligand

곽진성 이윤호*

한국과학기술원(KAIST) 화학과

The reactivity of transition metal nitrosyl complexes is of particular interest in our research. This is due in part to the extensive roles of nitric oxide (NO) in biology, which involves an integral part of immune response, vasodilatation, and neurotransmission. Recent researches have revealed that reactive nitrogen species (RNS) might be generated from the interaction of NO with various reactive oxygen species (ROS) mediated by transition metal ions in biological systems. Our investigation has focused on the chemistry of metal nitrosyl in particular with nickel. To date, structurally characterized nickel nitrosyl complexes reported in literature feature only an Enemark-Feltham configuration of $\{Ni(NO)\}^{10}$. Despite this lack of diversity, recent works have shown that nickel nitrosyl complexes can exhibit a diverse range of reactivity such as dissociation, disproportionation, and reduction.Recently we have synthesized dinuclear nickel dinitrogen complexes $\{(PP^{R}P)Ni\}_2(?\text{-}N_2)$ with tridentate $PP^{R}P$ ligands; $PP^{R}P = P(R)(2\text{-}P\textit{i}Pr_2\text{-}C_6H_4)_2$, (R = Ph and Me), well-characterized by various physical methods such as NMR and IR spectroscopies as well as X-ray crystallography. A series of 4-coordinate nickel nitrosyl complexes $[(PP^{R}P)Ni(NO)][BF_4]$ were prepared by the reaction of dinuclear nickel N_2 complexes with nitrosonium ion ($NOBF_4$). A neutral paramagnetic nickel nitrosyl species $(PP^{R}P)Ni(NO)$ featuring an unusual $\{Ni(NO)\}^{11}$ configuration was chemically prepared by the chemical reduction of $[(PP^{R}P)Ni(NO)][BF_4]$. As closely analogous complexes, square planar 4-coordinate nickel nitrosyl complexes (PNP)Ni(NO) with a tridentate PNP^- ligand; ($PNP^- = N[2\text{-}P\ \textit{i}Pr_2\text{-}4\text{-}Me\text{-}C_6H_3]_2^-$) was also prepared by oxygen atom transfer reaction. A series of these nickel nitrosyl complexes were characterized by various spectroscopic techniques. Details of nickel nitrosyl species will be presented especially describing their structural parameters and electronic character.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mesoporous Silica Spheres Embedded with Metal/Graphitic Shell Nanoparticles and Pt Nanocatalysts

김다정 서원석*

서강대학교 화학과

We have developed a highly stable and magnetically recyclable nanocatalyst system for alkene hydrogenation. The materials are composed of mesoporous silica spheres (MSS) embedded with FeCo/graphitic shell (FeCo/GC) magnetic nanoparticles and Pt nanocatalysts (Pt-FeCo/GC@MSS). The Pt-FeCo/GC@MSS exhibit superparamagnetism at room temperature and show type IV isotherm typical for mesoporous silica, ensuring a large enough inner space to undergo catalytic reactions. We have shown that Pt-FeCo/GC@MSS readily convert cyclohexene to cyclohexane as a only product and can be seperated very quickly by an external magnetic field after the catalytic reaction. We have demonstrated that the recycled Pt-FeCo/GC@MSS can be reused further for the same hydrogenation reaction at least four times without loss of the initial catalytic activity.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Fluorescent differentiation of Cu+ and Cu2+ in acetonitrile solvent via non-innocent mechanism

하용황 D.G.Churchill[1,*]

중원대학교 의약바이오학과 [1]한국과학기술원(KAIST) 화학과

A novel Schiff base probe (N,N′?bis(N?dimethylcarbamoyl?salicyl?2?imine)carbohydrazone) was synthesized and investigated for chemosensing purposes. Strongly selective ‘Turn?ON’ fluorescence signals were found for Cu2+ at 345 nm (85?fold) and for Al3+ at 445 nm (771?fold). Biothiols (L?cysteine, homocysteine, glutathione, N?acetyl cysteine) showed partial reversibility for Cu2+ fluorescence. Cu+, in the presence of Al3+, presented strong fluorescence at 360 nm (32?fold), likely occurring from H+ generated by Al3+ hydrolysis. H+ generated by Al3+ highly enables Cu+ fluorescence signaling based on proposed redox non?innocence. Reliability of Cu+ probing in this system was reasonable by verification via EPR analysis and lifetime measurements, which were collected under inert and ambient conditions. This probe is novel for Cu+ chemosensing in terms of having no soft donor atoms typical for such probes and serves as the first discriminator of mono? and divalent copper by a fluorescence ‘turn?ON’ signal via non-innocent mechanism.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Reactivity of *N*-heterocyclic carbenes (NHCs) with TCNE

송하영 박준범 김영석 김용휘[1] 배대영 김기문 이은성*

포항공과대학교(POSTECH) 화학과 [1]기초과학연구원 복잡계자기조립연구단

ABSTRACT

One-electron oxidation of *N*-heterocyclic carbenes (NHCs) to afford NHC radical cations, $NHC^{\cdot+}$, is highly challenging due to intrinsic instablility of the cations. Previous attempts to react NHCs with one-electron oxidants such as tetracyanoethylene (TCNE) formed dication $[NHC\text{-}NHC]^{2+}$, which was proposed to be formed through dimerization of $NHC^{\cdot+}$. [1] To avoid such dimerization, more sterically hindered NHC such as 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (IPr) was used for one-electron oxidation with TCNE. Surprisingly, one-electron oxidation reaction of *I*Pr with TCNE yields two distinct products, a direct adduct of TCNE to IPr and a heterocyclic compound formed from one *I*Pr and two TCNEs, depending on the reaction conditions. More detailed study will be presented including theoretical calculations to understand such reactivities.

REFERENCES

[1] Ramnial, T.; McKenzie, I.; Gorodetsky, B.; Tsang, E. M. W.; Clyburne, J. A. C. *Chem. Comm*. 2004, 1054.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis of Bulky *Ortho*-Substituted Triphenol Amines via Reductive Amination

배대영 이은성*

포항공과대학교(POSTECH) 화학과

Aminotrisphenolate transition metal complexes, which adopt a trigonal bipyramidal geometry dominantly, have been studied for efficient catalytic reactions such as C-C bond formation, polymerization, and selective enantiomeric epoxidation of alkene. For the past decade, aminotrisphenolate ligands have been upgraded aiming at novel reactivity by modification of the steric hindrance and electronic properties. Although there are several examples of *ortho*-substituted triphenol amine ligands, synthesis of highly sterically demanding *ortho*-substituted aminotrisphenol is still a challenge because there are only limited examples. We designed aminotrisphenolate ligand *ortho*-substituted with 2,4,6-triisopropylphenyl (TRIP) and successfully prepared the ligand by reductive amination. The ligand is also investigated for complexation with various transition metal ions. Detailed synthetic route for the ligand and transition metal complexes will be presented.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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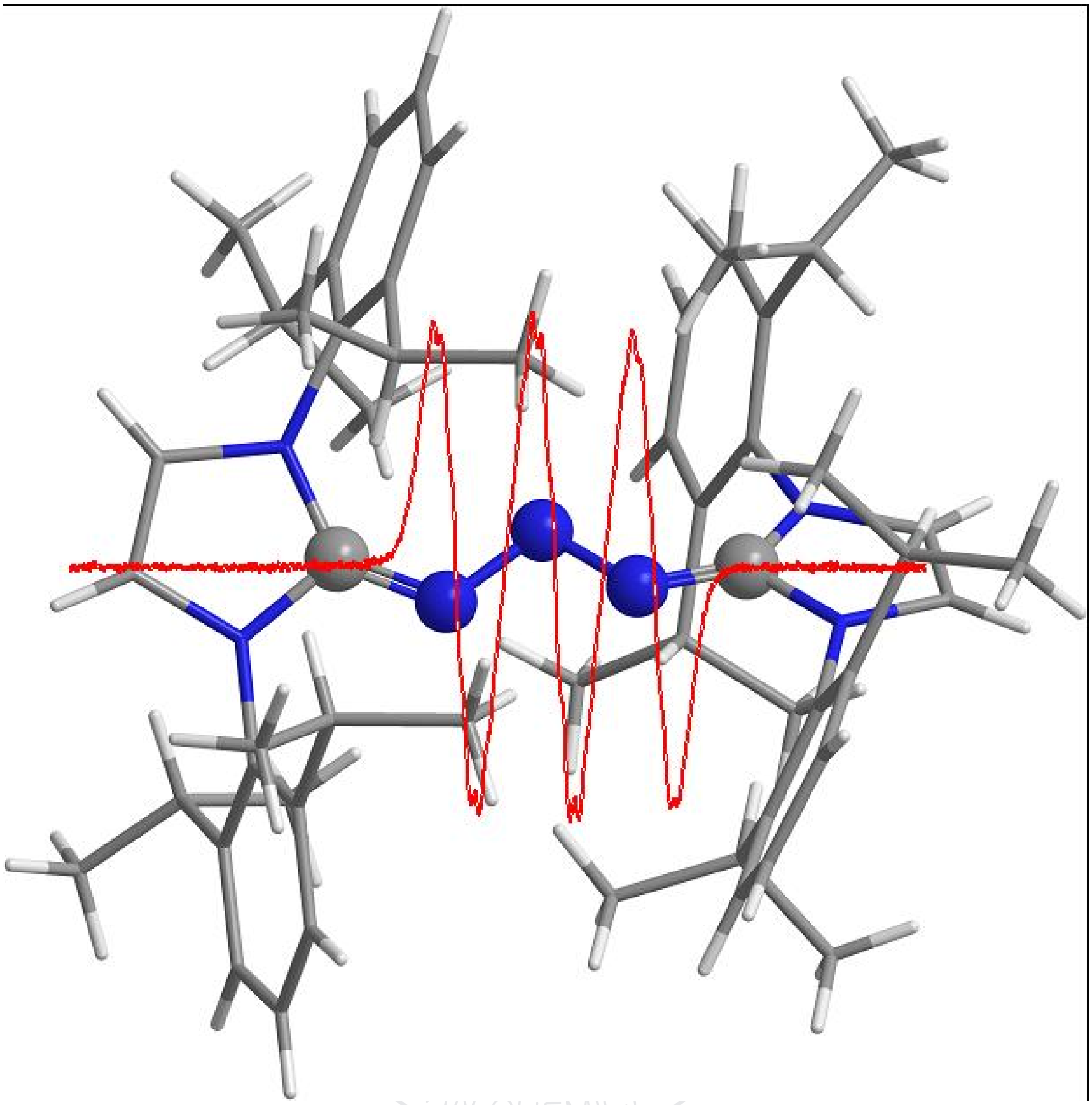
발표종류: 포스터, 발표일시: 목 11:00~12:30

An *N*-Heterocyclic Carbene Stabilized Triazenyl Radical

백지수 이은성*

포항공과대학교(POSTECH) 화학과

Radicals play important roles in chemical and biological reactions. However, certain radical species are unstable and highly reactive due to the unpaired electron. One of the general methods for stabilizing the radicals is to delocalize the unpaired electron by *N*-heterocyclic carbenes (NHCs). For instances, the Bertrand group has demonstrated successfully a phosphinyl radical stabilized by imidazolin-2-iminato. However, a triazenyl radical, an analogue of the phosphinyl radical, has not been demonstrated to date. Herein, we report synthesis of the triazenyl radical stabilized by 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (*I*Pr). The radical, *I*Pr_2N_3, was fully characterized by single-crystal X-ray analysis and electron paramagnetic resonance (EPR) spectroscopy in addition to hydrogen-atom abstraction reactivity.



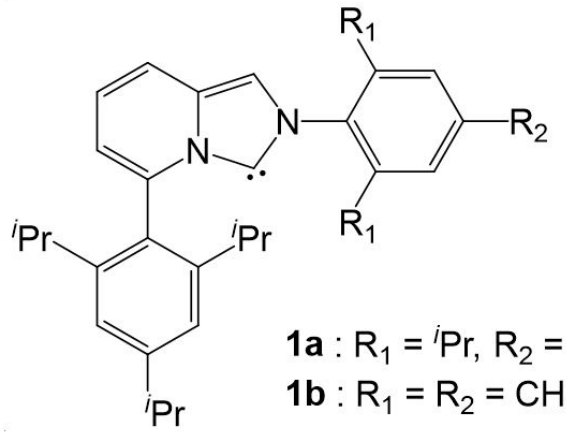
일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **INOR.P-146**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Efficient Synthesis of Bulky *N*-Heterocyclic Carbene Ligands for Coinage Metal Complexes

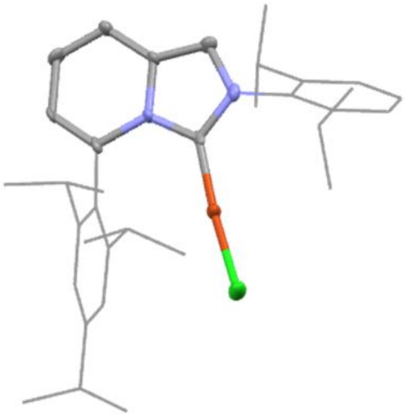
김영석 김용휘[1] 김기문 이은성*

포항공과대학교(POSTECH) 화학과 [1]기초과학연구원 복잡계자기조립연구단

N-heterocyclic carbenes (NHCs) have been drawing great attention for its excellent roles in catalysis. For past two decades, a variety of NHCs have been developed by not only adjusting electronic and steric properties but also by replacing one nitrogen atom of imidazole ring with carbon atom or sulfur atom. Especially, the steric factor is important because it enhances regio? or stereoselectivity of various reactions and promotes reactivity of certain reactions by stabilizing low-valent intermediates.[1]However, synthesis of bulky NHC usually requires some harsh reaction conditions and the multiple reaction steps to afford low chemical yields.[2] Therefore, a facile and efficient synthetic route to bulky NHC is highly desired.Here we report the the synthesis of bulky NHC ligands 1a and 1b with imidazo[1,5-*a*]pyridin-3-ylidene moiety, and their coinage metal complexes. The bulky NHCs were synthesized in four steps with approximately 40% of overall yield depending on the substituents. More interestingly, the method does not require harsh reaction conditions or any chromatographic purification process, which is sustainable for large scale synthesis.[3]Copper(I), silver(I), and gold(I) complexes were synthesized and fully characterized by NMR and single crystal X-ray analysis. The percent buried volume[4] for copper(I) complex is 55.5%, which indicates the high steric effect (compared to commonly used IPr and IMes with %V_{Bur} = 44.5 and 36.5 respectively).Reference[1] Christmann U.; Vilar R. *Angew. Chem. Int. Ed.* 2005, *44*, 366-374.[2] Dierick, S.; Dewez, D. F.; Mark?, I. E. *Organometallics* 2014, *33*, 677?683.[3] Espina, M.; Rivilla, I.; Conde, A.; D?az-Requejo, M. M.; P?rez, P. J.; ?lvarez, E.; Fern?ndez, R.; Lassaletta, J. M. *Organometallics* 2015, *34*, 1328?1338.[4] Calculated via SambVca with following parameters: Radius of sphere = 3.5 ?; Distance from sphere 2.0 ?; Mesh step 0.5 ?; H atoms omitted.



1a : R$_1$ = ^{i}Pr, R$_2$ = H
1b : R$_1$ = R$_2$ = CH$_3$



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발표종류: 포스터, 발표일시: 금 13:00~14:30

Kinetic Study of Solvolysis of Diphenylthiophosphinyl Chloride

고한중* 강석진

전주교육대학교 과학교육과

Rate of solvolysis of diphenylthiophosphinyl chloride in ethanol, methanol, and aqueous binary mixtures incorporating ethanol, methanol, acetone, 2,2,2-trifluoroethanol (TFE) or 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) are reported. The 29 solvents gave a reasonably precise extended Grunwald-Winstein equation plot, correlation coefficient (R) of 0.933, which improved to 0.983 when the four TFE-ethanol points were excluded. The sensitivities (l = 1.00 and m = 0.64) were similar to those obtained for dimethyl phosphorochloridate and phosphorochloridothionate and diphenylphosphinyl chloride. As with the previously studied solvolyses, an SN2 pathway is proposed for the solvolyses of diphenylthiophosphinyl chloride.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Correlation of the Rates of Solvolyses of Benzhydryl halide Using an Extended Grunwald-Winstein Equation

고한중

전주교육대학교 과학교육과

Rates of solvolyses of benzhydryl chloride (1) and benzhydryl bromide (2) in ethanol, methanol, and aqueous binary mixtures incorporating ethanol, methanol, 2,2,2-trifluoroethanol (TFE) and acetone are reported. Solvolyses were also carried out in TFE-ethanol mixtures. Application of the extended Grunwald-Winstein equation led to l value of 1.19 (1), 1.29 (2) and m value of 1.00 (1), 0.77 (2), correlation coefficient of 0.965 (1) and 0.970 (2). Sensitivities (l = 1.19 (1), 1.29 (2) and m = 1.00 (1), 0.77 (2)) were similar to those obtained for several previously studied solvolyses, in which an SN2 pathway is proposed for the solvolyses of benzhydryl halides.

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Eco-friendly fabrication of Ag@SiO_2@Ag sandwich nanostructures

이재원 장두전*

서울대학교 화학부

Nanoscale noble-metals have attracted significant attention from researchers in diverse fields of study because of their unusual optical properties as well as novel chemical properties. Especially, silver nanoparticles stand out from various types of noble-metal nanostructures due to their superior performance in a range of applications involving localized surface plasmon resonances, catalysis, SERS, and biosensing. Thus, extensive efforts have been devoted to the investigation of silver-based nanocomposites to achieve high catalytic performances and utilization efficiencies. Recently, we have shown that Ag@SiO_2@Ag sandwich nanostructures with highly enhanced catalytic performances have been fabricated facilely and eco-friendly by just irradiating 355 nm laser pulses only to Ag@SiO_2@Ag-seed nanoparticles for 30 min; silver seeds adsorbed on the silica surfaces have grown up to larger silver nanoparticles via the photochemical reduction of dissolved silver ions to form silver shells. The catalytic activity of the laser-fabricated sandwich nanostructures for the degradation reaction of rhodamine B in the presence of KBH_4 has been observed to be higher five times than that of the unirradiated nanoparticles. The sandwich nanostructures can be further transformed into hollow SiO_2@Ag nanostructures with irradiation of laser pulses for additional 30 min. Our laser-induced fabrication method of silver-based nanocatalysts can be regarded as a new approach of green chemistry because it does not require any reducing agents nor any surface-treatment processes.

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Fabrication of Hierarchical Hollow Cu_2O-CuO Composites with Well-Designed Structrues to Enhance Their Catalytic Performances

최다연 장두전*

서울대학교 화학부

Industrial wastewater is one of the most serious environmental pollutants and is predicted to become a major threat to the ecosystem. To degrade pollutants in the wastewater, many researchers have paid attention to develop catalysts having efficient performances with unique structures. Among different structures of materials, those with 3-D structures with well-designed structures have been extensively explored to enhance their catalytic performances. High catalytic activity can be attributed to the large surface areas, high surface-to-volume ratios, and sufficient surface active sites of the materials. Here, hierarchical hollow Cu_2O-CuO composite microstructures with numerous nanometer-sized sheet-like nanostructures distributed on the surfaces and the edges have been fabricated using pristine Cu_2O cubes as templates by an oxidation etching process. By controlling the concentration of OH^-, various structures have been synthesized and their catalytic performances have been tested. Hierarchical hollow cubes exhibit the highest catalytic activity among our prepared catalysts, especially 17.3 times higher than pristine cubes. The high catalytic performances of the hierarchical hollow cubes have been attributed mainly to their large specific surface areas, which make good contact with the organic dye molecules. Overall, our as-prepared Cu_2O-CuO composite structures without having any high-cost noble metals have outstanding catalytic properties for organic-dye degradation.

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Fabrication and Photocatalytic Activity of ZnS Nanobelts with Graphene Quantum Dots

함수호 김연호 장두전*

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Hybrid nanostructures combining inorganic materials and graphene have shown great potential for the environmentally friendly treatment of effluents. Herein, graphene quantum dots (GQDs)-decorated ZnS nanobelts have been synthesized via a facile hydrothermal method. The electrostatic attraction of two materials and the thermal reduction of graphene are main driving forces to fabricate well-defined composite nanostructures. GQDs in GQD/ZnS nanocomposites have been found to exist discretely and uniformly on the surfaces of ZnS nanobelts. The photocatalytic activity of GQD/ZnS nanocomposites has been found to be highest at a GQD/ZnS mass ratio of 8×10^{-4}. The photocatalytic rate constant (0.0046 min^{-1}) of GQD/ZnS nanocomposites having the optimized GQD content in the photodegradation reaction of rhodamine B has been found to be 14 times higher than that of commercially available ZnS powder. Embedded GQDs introduce additional visible-light response and serve as electron collectors and transporters to block electron-hole recombination efficiently, enhancing the photocatalytic performances of ZnS nanobelts immensely.

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Observing fusion pore dynamics by host-guest FRET pair based single-vesicle content-mixing assay

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Fluorescence-based single-vesicle fusion assays provide a?powerful method for studying mechanisms underlying complex biological processes of SNARE (soluble N-ethylmaleimide-sensitive factor attachment protein receptor)-mediated vesicle fusion and neurotrasmitter release. A?crucial element of these assays is the ability of the fluorescent probe(s) to reliably detect key intermediate events of fusion pore opening and content release/mixing. Here, we report a new, reliable and efficient single-vesicle content-mixing assay using a high affinity, fluorophore tagged host-guest pair, cucurbit[7]uril-Cy3 and adamantane-Cy5 as a FRET pair. The power of these probes is demonstrated by the first successful in vitro observation of reversible flickering dynamics of the fusion pore during neuronal-SNARE mediated vesicle fusion. We further discover that Ca2+ accelerates fusion pore opening after docking and helps pore dilation during the first pore opening but has no effect on the re-opening of fusion pore during reversible fusion pore flickering.

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Correlation of the Rates of Solvolysis of Electron-Rich Sulfonyl Chloride Using the Linear Free Energy Relationship

김연학 구인선* 최호준 고한중[1]

경상대학교 화학교육과 [1]전주교육대학교 과학교육과

The rates of solvolysis of 1,4-benzodioxan-6-sulfonyl chloride (BDSC) have investigated at 25.0℃ in water, CH_3OD, and in aqueous binary mixtures of acetone, ethanol, methanol, and 2,2,2-trifluoroethanol. The original Grunwald-Winstein plot of first-order rate constants for the solvolytic reaction of BDSC with Y_{Cl} shows marked dispersions into separated lines for various aqueous mixtures. With use of the extended Grunwald-Winstein equation, the l and m values obtained are 1.19 and 0.64 respectively for the solvolyses of BDSC. From the *l* and *m* values, the KSIE of 1.49 and 1.59 in methanol and 50% aqueous methanol, and activation parameters($\Delta H\neq$, $\Delta S\neq$), it is proposed that the solvolysis of BDSC proceed through S_N2 mechanism rather than though ionization mechanism.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Water proton relaxivities of Succinic acid, Glutaric acid and Terephtalic acid coated ultrasmall gadolinium oxide nanoparticles

tirusew tegafaw 이강호*

경북대학교 화학과

In the past few years, much effort have been made on investigation of several ligands which is water soluble, biocompatible and can give better water proton relaxation. It is important to know that ligand size can affect the invivo MRI images. Alternative approach is needed to increase the signal intensity of mri contrasting agents. In this work we used different water soluble and biocompatible ligand for the surface coating. The ligands used in this work are succinic acid, glutaric acid and terephtalic acid. The structural, morphological, magnetic properties, and their application are studied .The goal of this work is to examine the effect of the surface coating of gadolinium oxide nanoparticles on the longitudinal relaxivity (r1) in aqueous suspensions.

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Iodine compound coated gadolinium oxide nanoparticles for MRI-CT dual imaging

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경북대학교 chemistry [1]경북대학교 화학과

Gadolinium (Gd) is a powerful element useful for magnetic resonance imaging (MRI), X-ray computed tomography (CT), and neutron capture therapy for cancers. The surface modified gadolinium oxide nanoparticles has a higher relaxation rate compared to currently commercialized MRI contrast agent. The performance of nanoparticles for biomedical applications is highly dependent on the nature and quality of surface coating materials. In this study,the coating of iodine compound on the surface of gadolinium oxide nanoparticles were confirmed by FT-IR, TEM, XRD, TGA and MRI instrument. These analyses also demonstrated the strong attachment of iodine compound on the surface of gadolinium oxide, forming a protective layer on the nanoparticles. The relaxometric properties, cytotoxicity and the MRI signal of iodine coated gadolinium oxide nanoparticles were examined. In vivo T1 MR and CT images of mice were also acquired, supporting that the GNP is a potential dual imaging agent.

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Intrinsic conformations of L-β-homotyrosine studied by REMPI spectroscopy and TD-DFT Calculation

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아주대학교 화학과

L-β-homotyrosine (HTyr) is a β-amino acid where its amino group and residue are attached to the β-carbon of its carboxyl group, thus having one more CH2 group than tyrosine (Tyr). β-amino acids are generally regarded as promising tools in medicinal chemistry due to their biological activity and biological stability, therefore their conformations are of great interest. HTyr was desorbed from its HCl salt by a nanosecond 1064 nm laser and cooled by a supersonic expansion, and UV absorption of cold isolated HTyr was measured by resonance-enhanced multiphoton ionization (REMPI) spectroscopy. Though HTyr and Tyr share the same phenol chromophore, they show different vibronic progressions in REMPI spectra, presumably due to different distribution of conformers and different Franck-Condon activity. In order to elucidate the conformations of HTyr and to explain the difference between HTyr and Tyr, quantum mechanical calculations were performed. Stable conformations of HTyr were first searched for by molecular dynamics (MD) calculation with AMBER* force field in MacroModel, resulting in 85 stable conformations below 50kJ/mol. The candidate conformations found by MD were further optimized at M05-2X/6-31G** level of theory in Gaussian 09, and 16 conformations were found below 5.5 kJ/mol. The lowest electronically excited state of each HTyr conformer was optimized by time-dependent density functional theory (TD-DFT) at TD-M05-2X/6-31G**, and electronic spectra of the stable conformers were obtained by Franck-Condon simulation using the optimized ground and excited state geometries. Adiabatic transition energy and Franck-Condon simulation were used to tentatively explain the REMPI spectrum of HTyr. UV-UV hole-burning spectroscopy and resonant ion dip IR spectroscopy will be applied to reveal the intrinsic conformational structure of HTyr.

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Monitoring of Brownian Motion of Microspheres as a Colloid in Confined Water at Various Temperatures

윤병집

강릉원주대학교 화학과

The Brownian motions of polystyrene microspheres of size 1um are monitored with inverted phase contrast microscope. The microspheres are dissolved as a colloid in water confined in narrow two cover slips departed about 30um, and the temperature of the water media was controled and maintained from 6 to 40 C. The focus position to be captured varies with temperature change because the compartment of cell varies slightly with temperature however the change is not negligible in a microscopic level. Thus the focus position needs to adjusted, so we made it possible with Z-motor automatically. We developed several ways of calculating the defusion coefficient and the other important parameters. The defusion coefficients are observed with temperature change and with the distance from the surface of glass cover slip. We found that the surface effects affect to a quite long distance as of several micrometers while the usual theoretical calculations show the surface effect to only several nanometer range and also this is the range to be treated as possible in computer simulations. The anomalous behavior from the analyses of Brownian motion will be presented and explained.

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Fluorescein modified Gadolinium Oxide Nanoparticles as MRI-FI dual-Image

MiaoXu 이강호*

경북대학교 화학과

We accomplished the synthesis of fluorescein surface-modified gadolinium oxide nanoparticles in buffer solution. The surface-modified nanoparticles were characterized by using XRD, PL, FT-IR, HRTEM, TGA, MRI instrument and SQUID magnetometer. The nanoparticles were monodisperse with diameter ~1.5 nm. These nanoparticles showed fluorescence at ~ 524 nm and enhanced relaxivity. So it can be used as a dual MRI-FI imaging probe.

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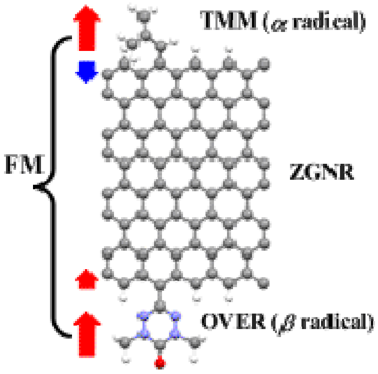
Designing Ferromagnetic Graphene Nanoribbons: Edge Termination with Stable Organic Radicals

조대흠 남연식 SHIHU 이진용*

성균관대학교 화학과

The intramolecular magnetic exchange coupling of edge terminated zigzag graphene nanoribbon (ZGNR) was studied with density functional theory calculations employing PBE functional. We investigated the magnetic behaviors of pristine zigzag graphene nanoribbon with 8 zigzag chains (8-ZGNR) and 8-ZGNRs terminated with trimethylenemethane (TMM) and 6-oxoverdazyl (OVER) radicals, i.e., TMM-ZGNR-TMM (TZT), OVER-ZGNR-OVER (OZO), and TMM-ZGNR-OVER (TZO) on its edges. As expected from the spin alternation rule and a classification scheme for radicals and couplers, only ZGNR terminated with different group radicals, combination of syn- and anti-radicals, on each edge (TZO) had a ferromagnetic (high-spin) ground state with an energy gap of 39 meV/supercell (462.68 K, 321.57 cm-1) relative to the low-spin state. The strong preference of high-spin state over low-spin state allows the TZO to be utilized as a possible room temperature pure organic ferromagnet. On the other hand, TZT and OZO were found to have an antiferromagnetic (low-spin) ground state with magnetic coupling weaker than that of inter-edge antiferromagnetic superexchange of pristine 8-ZGNR. This strongly supports the validity and applicability of the spin alternation rule and the classification scheme for radicals and couplers to rationally design ferromagnetically coupled graphene nanoribbon based materials.


TMM (α radical)
FM
ZGNR
OVER (β radical)

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Tautomeric Behaviors of Histidine in Structure Properties and Aggregation Mechanism of Amyloid β-peptide (1-40)

SHIHU 조대흠 남연식 이진용*

성균관대학교 화학과

As a result of pH effects, different histidine protonation states were considered as an important factor influencing structure properties and aggregation mechanisms of amyloid β-peptide (Aβ peptide) monomer, which is associated with the pathogenesis of Alzheimer's disease (AD). Understanding mechanisms affected by different free neutral states of histidine (Hie or Hid) is great challenge because distinguish them is difficult in physiological environment. Here, replica exchange molecular dynamics simulation was implemented to elucidate the changes of structure and aggregation properties upon variously neutral His states. Our results show that Hie6-Hie13-Hie14 (EEE), Hie6-Hid13-Hie14 (EDE), and Hid6-Hie13-Hid14 (DED) are in intrinsic random property with significant structural diversities. Meanwhile, sheet dominated conformations can be found in Hid6-Hid13-Hie14 (DDE) and Hid6-Hid13-Hid14 (DDD). Further results display that, DDE dimer is considered as an amorphous aggregation agent. However, DDD displays significantly ordered formation with parallel β-sheet between recognition units, implying the generation of regulated aggregates. This work is helpful to understand the fundamental role of deprotonated state of His in aggregation, which could be useful for further development of new drugs to inhibit Aβ aggregation.

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Energy flow and bond dissociation of vibrationally excited 2-Chlorotoluene in collisions with H_2, Cl_2 and HCl

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전남대학교 화학교육과 [1]Dept. of Chem. University of Nevada

Energy flow and C-H_{methyl} and C-Cl bond dissociations in vibrationally excited 2-Chlorotoluene(2CT) in the collision with H_2, Cl_2 and HCl have been studied by use of classical trajectory procedures. The energy lost by the vibrationally excited 2CT upon collision is not large and it increases slowly with increasing total vibrational energy content between 5,000 and 45,000 cm^{-1}. Intermolecular energy transfer occurs via both of V-T and V-V transfers. Both of V-T and V-V transfers increase as the total vibrational energy of toluene increases. The overall extent of energy loss is greater in $2CT+H_2$ than that in $2CT+Cl_2$ and 2CT+HCl. The different efficiency of the energy transfer pathways in three collisions is mainly due to the near-resonant condition between the vibration of incident molecule and C-H or C-Cl vibration. When the total energy content ET of 2CT is sufficiently high, either C-H or C-Cl bond can dissociate. Collision-induced dissociation of C-H_{methyl} and C-Cl bonds occurs when highly excited 2CT (55,000-70,400cm^{-1}) interacts with the ground-state H_2/Cl_2/HCl. Dissociation probabilities are low (10^{-5}~10^{-2}) but increase exponentially with rising vibrational excitation. Intramolecular energy flow between the excited C-H and C-Cl bonds occurring on a subpicosecond timescale is responsible for the bond dissociation.

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Kinetic Study on Nucleophilic Displacement Reactions of Phenyl Y-Substituted Phenyl Carbonates with 1,8-Diazabicyclo[5.4.0]undec-7-ene: Effects of Amine Nature on Reaction Mechanism

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Second-order rate constants (k_N) for the nucleophilic displacement reactions of phenyl Y-substituted phenyl carbonates (7a-7l) with 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) in 80 mol % H_2O/20 mol % DMSO at 25.0 ± 0.1 ^oC have been measured spectrophotometrically. The Brønsted-type plot for the reactions of 7a-7l with DBU is linear with β_{lg} = ?0.48, indicating that the reactions proceed through a concerted mechanism, which is in contrast to the stepwise mechanism reported previously for the corresponding reactions with ethylamine (a primary amine) and piperidine (a secondary amine). The Hammett plots correlated with $\sigma^?$ and σ^o constants exhibit many scattered points. In contrast, the Yukawa-Tsuno plot results in an excellent linear correlation with ρ_Y = 1.28 and r = 0.54, implying that a negative charge develops partially on the O atom of the leaving group in the transition state. The bulky DBU is less reactive than the primary and secondary amines toward substrates possessing a weakly basic leaving group. It has been concluded that steric hindrance exerted by DBU in the plausible intermediate ($T^{\pm}$) forces the reactions to proceed through a concerted mechanism because expulsion of the leaving group from $T^{\pm}$ could reduce the steric hindrance.

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Dynamics of highly polydisperse colloidal liquids and its implications to protein diffusion in cytoplasms

황지예 김정민 성봉준*

서강대학교 화학과

Recent single molecule experiments revealed that protein diffusion in dormant cells should be slow, heterogeneous and even non-ergodic. Such anomalous diffusion behaviors of proteins would also affect biological functions of proteins such as biological reactivity. Glasses (where the system is cooled so quickly below the freezing temperature that molecules are not crystalized but amorphous) may serve as systematic model systems to investigate such anomalous diffusion. However, most glasses that have been investigated extensively are binary mixtures of molecules of similar size. Considering that cell cytoplasms consist of proteins that differ significantly in size, it is of academic significance to investigate and understand the dynamics of highly polydisperse (in size) glasses. We perform Langevin dynamics simulations of a mixture of colloids with large size polydispersity and find that the size polydispersity affects the particle diffusion in qualitative ways. Highly polydisperse colloidal system is dynamically heterogeneous, which is the characteristic features of glass forming liquids and cytoplasms in dormant cells. We also find that the dynamics changes qualitatively at the kinetic glass transition point. More interestingly, dynamic decoupling and multistep glass transition are observed depending on the size of colloid. In this talk, we will also discuss how the size polydispersity and anomalous diffusion may influence the protein diffusion in cell cytoplasms.

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그래핀 옥사이드(Graphene Oxide)의 응용성 증대를 위한 시간분해능 분광기를 이용한 전자전이 특성 연구

김창호[*] 이홍순[1] 정세채[2,*]

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우수한 전기적인/구조적인 장점을 가지는 Graphene 과 비교하여 Graphene oxide 의 광학적인 가장 큰 특징은 밴드갭이 존재하여 가시광선부터 근적외선의 범위에 결쳐서 광범위한 형광을 발생하며 Graphene 은 밴드갭을 가지지 않아 형광을 발생하지 않는 특징을 가진다. 또한 Graphene 에 대해서 고비용이 들어가는 CVD 생성 하는 방법보다 graphene oxide sheets 로부터 Graphene 을 만들 수 있는 방법으로 저비용으로 만들 수 있는 장점을 가진다. 이런 Graphene oxide 의 장점과 응용성을 증대시키기 위해서는 광학적 특성 및 전자전이에 대한 이해의 폭을 넓히는 것이 필수적이다. 따라서 우리 연구팀은 펨토초 레이저 시스템의 시간분해능 분광기를 통하여 Graphene oxide 의 전자전이에 대한 특성 연구를 수행하였다. 이 실험을 통해서 기존 연구해온 Graphene oxide 의 형광 기원에 대한 기본연구를 보완하였고 또한 이 실험결과는 Graphene oxide 의 응용성 증대을 위한 기반이 될 것이다.

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Structural roles of guide RNAs in the nuclease activity of Cas9 endonuclease

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The type II CRISPR-Cas system, composed of the Cas9 endonuclease and two guide RNAs (gRNA; tracrRNA and crRNA), works for bacterial adaptive immunity against invading viruses and plasmids. Here we report the structural roles of the two guide RNAs in the CRISPR-Cas9 endonuclease system, studied by pseudo-ensemble and single-molecule fluorescence assays. The tracrRNA plays an important role on catalytically active Cas9-gRNA complex formation step. It leads Cas9 preferentially toward a folding pathway for nuclease activity over other pathways leading to deactivated structures. After the Cas9-gRNA complex binds the target DNA, the crRNA structure with respect to the target DNA shows repetitive transitions between two distinct structures. This dynamic, crRNA-related conformational change controls the nuclease activity of Cas9 by allowing the DNA cleavage reaction in only one of the two intermediate structures.

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A molecular dynamics simulation study on a single nanoparticle in freestanding polymer thin films

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Adding nanoparticles to polymer films may change glass transition temperature, which should influence the viscosity and dynamic properties of polymers. However, the dynamic behaviors of both nanoparticles and polymers still remain unclear at a molecular level. In this work, therefore, we aim to get some useful insights by employing computer simulations and coarse-grained models for freestanding polymer thin films and nanoparticles. We systematically investigate how the nanoparticle is spatially located within the freestanding polymer film. We find that depending on the size of the nanoparticle the spatial distribution of the nanoparticle changes qualitatively. When the nanoparticle size is large enough, the nanoparticle stays at the center of the polymer film. For small nanoparticles, however, the nanoparticle is located at the surface of polymer films. Interesting is that such a change in nanoparticle position occurs suddenly at a critical nanoparticle size. By calculating the Helmholtz free energy, we find that as the nanoparticle size decreases, the free energy surface changes qualitatively: a single energy minimum exists at the film center for large nanoparticles but two energy minima appear for small nanoparticles. Because there is a significant difference in the local viscosity of polymer films between the film center and film surface, the dynamics of nanoparticles is also affected by the nanoparticle size and location.

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A molecular simulation study on non-equilibrium kinetics of polymer translocation process into a strong confinement

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The translocation of a viral DNA into a small capsid is a critical step in viral infection. Because the number of conformations of the DNA should be decreased significantly inside the capsid, the entropic cost during the translocation process should be extremely large. A motor protein located at the capsid mouth, therefore, is required to force the DNA to translocate into the capsid. A recent experiment study (Proc. Natl. Acad. Sci. U. S. A., 111, 8349 (2014)) showed that the DNA underwent non-equilibrium conformational change depending on how the motor protein was stalled and restarted. In this study, we perform Langevin dynamics simulations along with coarse-grained models for the DNA, the capsids, and the motor protein. We control the force size and the stall period of the motor protein, and investigate how the DNA would be packaged into the capsid. Our simulations show that depending on the capsid size and the stall period, the initial stage of packaging would be very heterogeneous, i.e., the fraction of being packaged inside the capsid is sensitive to the initial condition of simulations. And we also construct a contact map for the DNA in order to investigate the conformational dynamics during and after the translocation process.

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Anomalous diffusion mechanism of cancer cells: A cellular heterogeneity and persistence movement

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The diffusion mechanism of cancer cells is crucial to understanding cancer metastasis, yet its diffusion mechanism remains unclear. We present a study on the anomalous diffusion mechanism of A549 cancer cells. We obtain and analyze the trajectories of A549 cancer cells by employing the video microscopy. In the case of A549 cancer cells, the mean square displacement is linear with time like Brownian particles but the van Hove correlation function is non-Gaussian. It is well known that such a “seemingly Fickian diffusion but non-Gaussian” dynamics in colloidal systems is caused by the kinetic arrest of particles due to the obstruction of neighbor particles. A549 cancer cells also show the heterogeneous and seemingly Fickian diffusion but non-Gaussian dynamics despite the low cell density, which suggests that not the kinetic arrest but a certain biological origin should be responsible. Through the angular distribution function of A549 cancer cells, we reveal that A549 cancer cells show not only persistence movement but also anti-correlation persistence movement at short time scales. By incorporating cellular heterogeneity and persistence into simple numerical simulation, we could reproduce the mean square displacement and the displacement distribution of A549 cancer cells.

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Formation of Ordered Self-Assembled Monolayers of Octaneselenocyanates on Au(111): Immersion Time and Temperature Effect

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Self-assembled monolayers (SAMs) of alkanethiols on metal surfaces have been constantly studied for nanotechnology. In the recent decades, selenium-based SAMs have gotten into the spotlight because they have enough potential alternatives to thiols which have a disadvantage during the SAM formation in solution that produce the oxidized compounds. Alkylselenocyanates will be one of useful precursors for preparation of SAMs because they are chemically quite stable in solution. However, there have been no literatures concerning the formation and structure of SAMs on Au(111) by octaneselnocyanates (C8SeCN) from various SAM preparation conditions. In this study, we examine the surface structure and electrochemical behaviors of SAMs formed by C8SeCN as a function of immersion time, solution temperature, and concentration using scanning tunneling microscopy (STM), cyclic voltammetry, and contact angle (CA) measurement. In this study, we found that highly ordered C8Se SAMs can be obtained from short immersion time and an elevated solution temperature.

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Comparative Study of Structure and Growth Process of 4-Fluorobenzenethiolate and 4-Fluorobenzeneselenolate Self-Assembled Monolayers on Au(111): Headgeoup Effect

성시천 강훈구 한슬기 한명수[1] 박희건 한진욱 노재근*

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Self-assembled monolayers (SAMs) of aromatic thiols have drawn much attention due to their interesting electrical property. Among them, fluorine-terminated compounds are especially useful in molecular electronics because of the ability to enhance the charge carrier injection rate by lowering the injection barrier height. This property considerably improves electronic device performance, but monolayer structure and molecular orientation are critical factors also. In this study, we examined 4-fluorobenzenethiolate (4-FBS) and 4-fluorobenzeneselenolate (4-FBSe) SAM samples from 4-fluorobenzenethiol and bis(4-fluorophenyl)diselenide on Au(111) to understand headgroup effect on the formation and structure of SAMs using scanning tunneling microscopy (STM), cyclic voltammetry (CV), reductive desorption (RD), contact angle (CA), X-ray photoelectron spectroscopy (XPS) and thermal desorption spectroscopy (TDS). STM observation showed 4-FBSe SAMs on Au(111) mainly have disordered multilayer structure, while 4-FBS SAMs have highly ordered surface structure.

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Molecular Self-Assembly and Adsorption Structure of Triphenylphosphine on Au(111) Surface

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Molecular-self-Assembly techniques on metal surfaces provide a powerful means for the fabrication of functionalized molecular films that can be applied for a variety of applications in nanotechnology and biotechnology. It is very important to understand the surface structure and characteristic of molecular films because they significantly affect the physical and chemical properties of films. Triphenylphosphine (TPP) is a well-known capping agent for synthesizing metal nanoparticle or quantum dots. Especially, phosphine-encapsulated AuNPs are extensively studied for examining their plasmonic behaviors by a number of notable groups. Recently, some of the surface chemists reported that phosphine-derivatives on Au (111) in ultrahigh vacuum (UHV) system led to the formation of ordered self-assembled monolayer (SAM). However, there have been no literatures regarding the surface structure and characteristic of molecular films on Au(111) surfaces formed by adsorption of TPP molecules. Therefore, in this research, we examined surface structure and electrochemical behavior of TPP layers using scanning tunneling microscopy (STM) and cyclic voltammetry. STM imaging reveals that TPP molecular films have a disordered phase containing many defects.

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A study of magnetic and water proton relaxivity properties of HA modified Gd_2O_3 Nanoparticles

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경북대학교 화학과

It was great interest in nanobiology and medicine that nanoparticles with high biocompatibility and stability, low toxicity, diversification of imaging modality, and specificity of targeting to desired organs or cells. In this poster, I synthesized HA which can be used for cancer cell targeting modified gadolinium oxide nanoparticles which were synthesised in triethylene glycol as a cancer cell targeting MRI contrast agent. It was characterized with XRD, ICP-MS, TGA, FT-IR, TEM and MRI instrument. These nanoparticles have targeted the cancer cell. Hence, it can be used as a cancer diagnose MR imaging contrast agent.

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Theoretical Study for The Mechanism of Acetic Acid Synthesis from Carbon and Methane on Zn-ZSM-5 Zeolite Model System

박예은 김용호*

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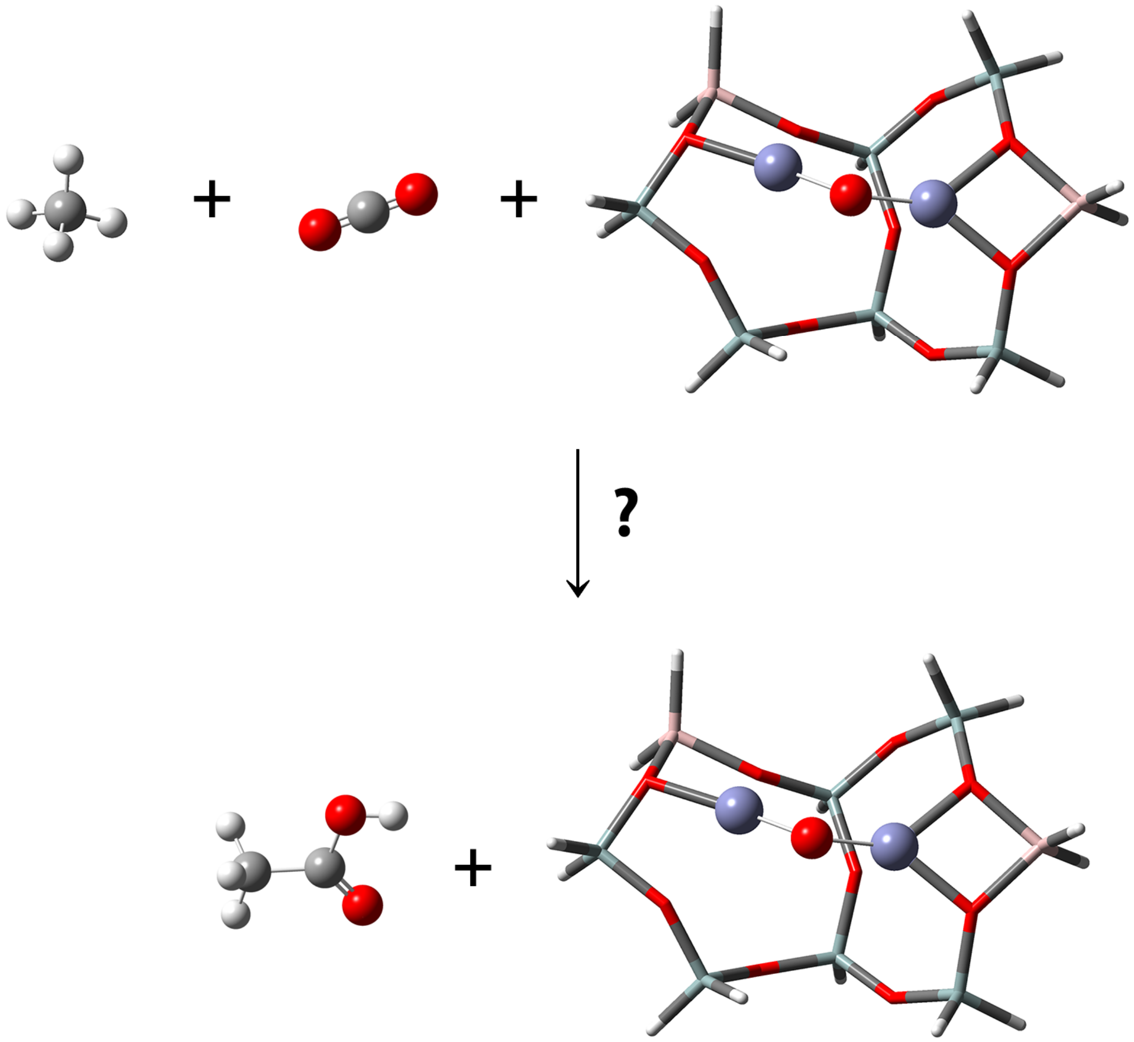
It is a well known fact that Methane and Carbon cause greenhouse effect and co-conversion of methane and carbon dioxide into valuable products is one of the most important subjects in Chemistry. Though the direct synthesis of acetic acid from CH_4 and CO_2 has been examined theoretically and experimentally both, almost nothing was known for the possible mechanisms so far. Recently, several research groups succeeded in achieving important facts about methane activation on metal-exchanged zeolites, and based on the facts a study proposed a possible mechanism of the co-conversion of CH_4 and CO_2 on a zinc-modified H-ZSM-5 zeolite. However, the proposed mechanism was only from solid-state C and H MAS NMR spectroscopic study, so there is still not any exact mechanism as well as theoretical study. In this study, we built a two-ringed $Al_2Si_6O_9H_{14}$ cluster model system with dizinc cluster center to represent zinc modified H-ZSM-5 zeolite and we discovered other possible mechanisms for the synthesis of acetic acid from CH_4 and CO_2 on the zeolite. They are new and different from the one proposed earlier. We will show you our theoretical study for the mechanisms with geometries and energies along the reaction process in detail.



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Pulsed Laser Ablation Synthesis of Graphitized Carbon-Encapsulated Palladium Core-Shell Nanospheres for Catalytic Reduction of Nitrobenzene to Aniline

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Graphitized carbon-encapsulated palladium (Pd) core-shell nanospheres were produced via pulsed laser ablation of a solid Pd foil target submerged in acetonitrile. The microstructural features and optical properties of these nanospheres were characterized via high resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and UV-visible spectroscopy. Microstructural analysis indicated that the core-shell nanostructures consisted of single-crystalline cubic metallic Pd spheres that serve as the core material, over which graphitized carbon was anchored as a heterogeneous shell. The absorbance spectrum of the synthesized nanostructures exhibited a broad (absorption) band at 264 nm; this band corresponded to the typical inter-band transition of a metallic system and resulted possibly from the absorbance of the ionic Pd^{2+}. The catalytic properties of the Pd and Pd@C core-shell nanostructures were investigated using the reduction of nitrobenzene to aniline by an excess amount of $NaBH_4$ in an aqueous solution at room temperature, as a model reaction. Also the mechanism of this reaction was determined using LC-MS analysis. Owing to the graphitized carbon-layered structure, the resulting Pd@C nanostructures exhibited higher conversion efficiencies than their bare Pd counterparts. In fact, the layered structure provided access to the surface of the Pd nanostructures for the hydrogenation reaction, owing to the synergistic effect between graphitized carbon and the nanostructures. Their unique structure and excellent catalytic performance render Pd@C core-shell nanostructures highly promising candidates for catalysis applications.

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Time-Resolved Ru K-edge X-ray Absorption Spectroscopy (XAS) study on the metal-to-ligand charge-transfer (MLCT) states of $Ru(bpy)_2(dppp2)_2^+$

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Time-Resolved X-ray Absorption Spectroscopy (TR-XAFS) is a special tool to investigate molecular dynamics. It also has become possible to observe the transient chemical reactions on fundamental timescale. Ru-based polypyridyl complexes are used in various fields as solar energy conversion, artificial photosynthetic systems and optical sensing. Metal-to-ligand charge-transfer (MLCT) process plays most important role in these devices for solar energy conversion. Specially, complexes of $Ru(bpy)_2(dppp2)_2^+$, where dppp2 = pyrido[2’,3’:5,6]pyrazino[2,3-f][1,10]phenanthroline, are known to process two low-lying 3MLCT excited states in fast equilibrium. In this TR-XAFS study, all measurements were performed using the fluorescence XAFS method on the undulator beamline, NW14A, at the PF-AR To study their coordination and electronic structure form EXAFS, we had an experiment with $Ru(bpy)_2(dppp2)_2^+$ in acetonitrile. The results from visible (400 nm) excitation indicate that electrostatic interaction between the oxidized Ru atom and the reduced dppp2 ligand is the dominant factor affecting the Ru?N bond contraction. To interpret transient x-ray spectra, we performed the FEFF simulation with time-dependent density functional theory (TD-DFT) calculations. This study provides the detailed understanding of the electronic structure for the ultrafast transient ^{3}MLCT state of transition Ru complex.

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Photophysical Investigation of a *meso*-Tetra(Arylethynyl)porphyrin derivative in Neutral and Diacid Form

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Meso-arylethynylporphyrin is a new class of porphyrins in which intervening ethynyl moieties connect aryl groups to the porphyrin macrocycle. Unlike typical *meso*-arylporphyrins such as tetraphenylporphyrins (TPPs), the presence of the ethynyl spacer allows for a coplanar geometry between the porphyrin macrocycle and the peripheral substituents, resulting in highly expanded π-conjugation. Such modification results in substantially altered photophysical properties compared to nominal TPPs, that is, considerable red shifts of the B and Q band regions and the enhanced oscillator strengths of the Q bands. Owing to their unique photophysical properties induced by expanded π-conjugation, *meso*-arylethynyl porphyrins are used in a variety of applications including artificial photosynthetic systems, nonlinear optical materials, and optoelectronic systems. However, in the case of free-base arylethynyl porphyrins, fundamental photophysical and physicochemical studies are limited to only a few examples despite their unique functionality. We report herein, the photophysical properties for the *meso*-tetra(hexylphenylethynyl)porphyrin and the corresponding *meso*-tetraarylporphyrin (TPP) have been studied via electronic and absorption and emission spectroscopy. In addition, the photophysical properties of diacid forms are also investigated to correlate them with the degree of structural distortion upon protonation because the arylethynyl porphyrins are expected to be *less* distorted upon diacid formation relative to TPPs.

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Green Synthesis of the Reduced Graphene Oxide-CuI Quasi-Shell-Core Nanocomposite : toward photocatalytic activity for organic dye removal

최지하 devulapalliamaranathareddy ISLAMMOHAMMADJAHURUL 김태규*

부산대학교 화학과

Surfactant-free, reduced graphene oxide (RGO)-CuI quasi-shell?core nanocomposites were successfully synthesized using ultra-sonication assisted chemical method at room temperature. The morphologies, structures and optical properties of the CuI and CuI-RGO nanocomposites were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Fourier-transformed infrared spectroscopy (FTIR), UV-visible diffuse reflectance spectroscopy (DRS/UV-Vis), and photoluminescence (PL) spectroscopy. Morphological and structural analyses indicated that the CuI-RGO core?shell nanocomposites comprise single-crystalline face-centered cubic phase CuI nanostructures, coated with a thin RGO quasi-shell. Photocatalysis experiments revealed that the as-synthesized CuI-RGO nanocomposites exhibit remarkably enhanced photocatalytic activities and stabilities for photo degradation of Rhodamine-B (RhB) organic dye under simulated solar light irradiation. The photo degradation ability is strongly affected by the concentration of RGO in the nanocomposites; the highest photodegradation rate was obtained at a graphene loading content of 2 mg·mL-1 nanocomposite. The remarkable photocatalytic performance of the CuI-RGO nanocomposites mainly originates from their unique adsorption and electron-accepting and electron-transporting properties of RGO. The present work provides a novel green synthetic route to producing CuI-RGO nanocomposites without toxic solvents or reducing agents, thereby providing highly efficient and stable solar light-induced RGO-CuI quasi-shell?core nanocomposites for organic dye photo degradation in water.

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Single-step Peptide Backbone Dissociations in FRIPS by Higher-energy Collisional Activations of Q-TOF and Orbitrap Mass Spectrometers

오한빈

서강대학교 화학과

TEMPO-assisted free radical initiated peptide sequencing (TEMPO-FRIPS) is a method using TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl) as a radical initiator to sequence peptide by collision-activated dissociation. Peptides of interest were conjugated with o-TEMPO-Bz-C(O)-NHS at the position of the N-terminus for TEMPO-FRIPS application. Here, two step collisional activations are needed to be implemented for FRIPS analysis by ion-trap instrument, that is, MS3 is required, since FRIPS can yield peptide backbone dissociations with two collisional activations; one for the radical generation (?Bz-C(O)-peptides) and the other for peptide backbone dissociations. So, in order to reduce a collisional activation step, we used instruments such as Q-TOF and orbitrap that can apply higher-collisional activation. When higher-collisional activation was applied to o-TEMPO-Bz-C(O)-peptide, not only homolytic cleavage in the bond between benzyl carbon and oxygen of the TEMPO group but also peptide backbone fragmentations occurred. Consequently, peptide sequencing was possible in a single-step FRIPS in the positive-ion mode.

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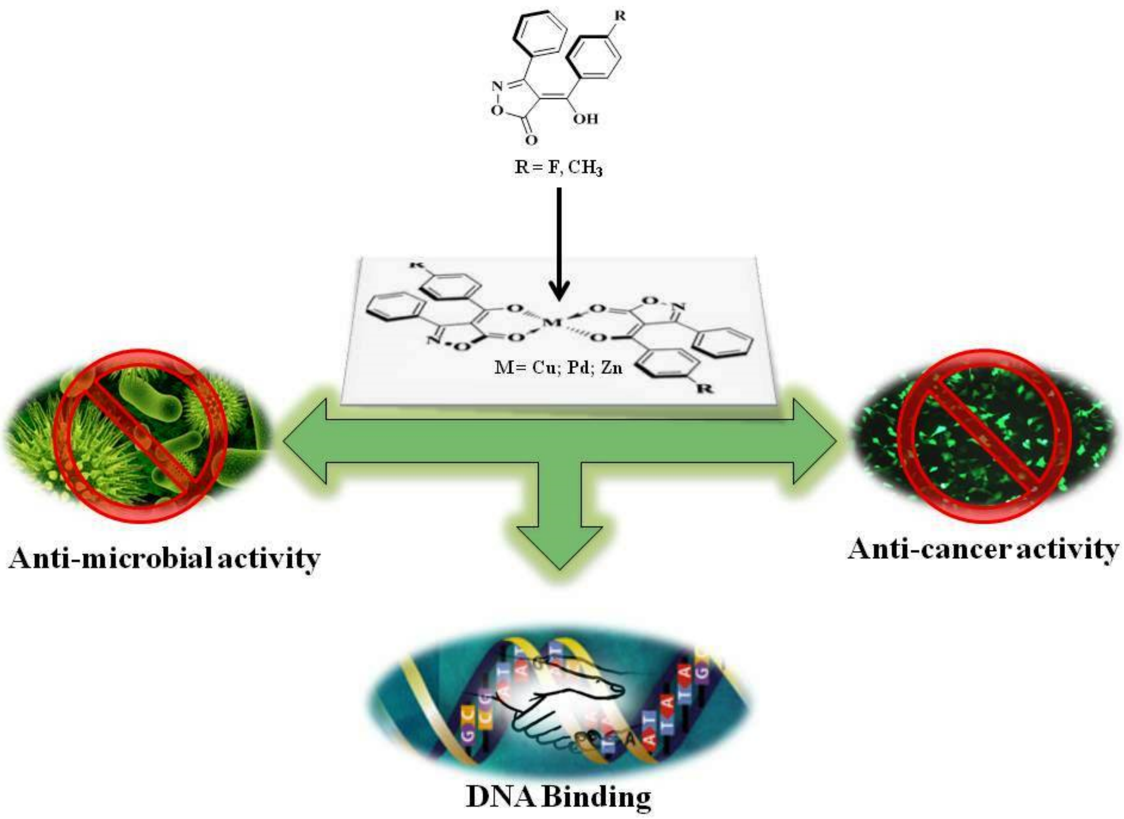
Synthesis, crystal structure, antitumor activity and DNA binding studies of complexes of copper, zinc and palladium with monobasic bidentate β-diketonate ligands

MAHIMALURUJAGADEESH 김태규*

부산대학교 화학과

Three pairs of novel neutral mononuclear β-diketonate complexes of copper(II), zinc(II) and palladium(II) are synthesized from two different monobasic O^O donor ligands, 3-phenyl-4-fluorobenzolyl-5-isoxazolone (HL1) and 3-phenyl-4-touoyl-5-isxoazolone (HL2) respectively. All the compounds are characterized by using FT-IR, ESI/FAB mass, 1H-NMR, UV-visible, thermogravimetric analysis. The free ligand HL1 and the copper(II) complex, Cu(L2)2 are unambiguously characterized by single crystal X-ray diffraction studies. The free ligand HL1 has adopted orthorhombic crystal system with P2(1) space group and the unit cell parameters are: a = 8.1552(3)?, b = 10.1169(4)?, c = 17.0819(6)?, and α = β = γ = 90°. The crystal structure of the complex, Cu(L2)2 is monoclinic with P2(1)/c space group with the unit cell parameters are: a = 10.2571(2)?, b = 16.2640(3)?, c = 20.1717(3)?, and α = 90, β = 99.56 and γ = 90° . The crystal structure of the copper complex has shown a distorted octahedral geometry where, the z-axis is occupied by two solvent methanols. The epr spectra of both the complexes display a strong axial signal with g|| ? 2.2 and g⊥ ? 2.0 suggests the square planar geometry around the copper(II) ion. Anticancer activity studies of the complexes have revealed their potential towards inhibiting the growth of human breast cancer cell lines, MDA-MB-231. The palladium complexes of both the ligands are found to be more active in exhibiting apoptosis. Moreover, the complexes of fluoro-substituted ligand are better antimicrobial agents than the methyl substituted ligand containing complexes.


R
N
O
O
OH
R = F, CH3
R
O
M
O
N
M= Cu; Pd; Zn
R
Anti-microbial activity
Anti-cancer activity
DNA Binding

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Self-cleaning and anti-reflective properties of ZnO@TiO$_2$ core/shell nano-rod grown on ITO glass by using hybrid method

유정열 김재욱* 김종규*

단국대학교 화학과

The high-quality ZnO/TiO$_2$ core/shell nano-rod arrays were grown on indium-tin oxide(ITO) glass substates by hybrid method. Synthesis of the ZnO nano-rod arrays glass substate was used sol-gel method and synthesis of the ZnO@TiO$_2$ core/shell nano-rod arrays glass was used hydrothermal method. Structural and elemental chemical composition analysis of the sample was carried out using field emission scanning electron microscopy(FE-SEM) and energy-dispersive X-ray spectroscopy(EDX). For chemical stability test, the sample was immersed into pH 0~14 aqueous solutions for 30 min and then rinsed with distilled water, ethanol and acetone. The optical transmission was monitored with UV-Vis spectrophotometer(UV-Vis). The photocatalytic activity of the sample was evaluated through the decolorization of rhodamin B(RhB) in aqueous solution as a model pollutant under UV light irradiation with UV-Vis. The transparency analysis of the sample was carried out for evaluated anti-reflective properties using UV-Vis.

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Red to Ultraviolet Emission Tuning of Two Dimensional Gallium Sulfide/Selenide

정찬수 박정희* 박기동[1] 오진영 임형순[1] 강홍석[2]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자 [2]전주대학교 나노신소재공학과

Graphene-like two-dimensional (2D) nanostructures have attracted significant attention because of their unique quantum confinement effect at the 2D limit. Multilayer nanosheets of GaS-GaSe alloy are found to have a band gap (E_g) of 2.0-2.5 eV that linearly tunes the emission in red-to-green. However, the epitaxial growth of monolayers produces a drastic increase in this E_g to 3.3-3.4 eV, which blue-shifts the emission to the UV region. First-principles calculations predict that the E_g of these GaS and GaSe monolayers should be 3.325 and 3.001 eV, respectively. As the number of layers is increased to three, both the direct/indirect E_g decrease significantly; the indirect E_g approaches that of the multilayers. Oxygen adsorption can cause the direct/indirect E_g of GaS to converge, resulting in monolayers with a strong emission. This wide E_g tuning over the visible-to-UV range could provide an insight for the realization of full-colored flexible and transparent light emitters and displays.

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Nickel diselenide as superior bifunctional electrocatalyst for water splitting

곽인혜 박정희* 정찬수 임형순[1] 박기동[1] 박충효

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Catalysts for the oxygen and hydrogen evolution reactions are central to key renewable-energy technologies including fuel cells and water splitting. Despite tremendous effort, the development of oxygen electrode catalysts with high activity at low cost remains a great challenge. In this study, we report unique method for the synthesis of metal selenide for an efficient electrocatalytic oxygen evolution reaction (OER). They are synthesized using photo-induced cation exchange reaction of germanium selenide nanocrystals (NC) in aqueous solution. The $NiSe_2$ exhibits superior catalytic power not only for the OER, but also for HER. In situ raman spectroscopy provides an evidence for the formation of metal peroxide M-OOH, which are suggested as the three electron oxidation intermediate of OER.

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Defective III-VI Semiconductor Ga_2S_3 Nanowires

박기동 박정희[1,*] 정찬수[1] 임형순 오진영[1] 곽인혜[1] 박충효[1] 임영록[1] 권익선

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

Semiconductor nanowires (NWs) have attracted considerable attention because they can be used as well-defined 1-dimensional (1D) building blocks of future nanodevices with unique optical and electrical properties using bottom up approaches. Ga_2S_3 is a typical representative of III-VI chalcogenide semiconductor, which has a defective zinc blende-like structure in which one third of the cationic sites are vacant. Interest in the III?VI defect semiconductors has increased as they are promising materials for using in optoelectronic devices. Here, we synthesized Ga_2S_3 NWs via catalyst-assisted thermally vapor transport method under vapor-liquid-solid mechanism. The NWs consisted of monoclinic phase which is known as the most stable phase. Ga_2S_3 NWs exhibited strong defect-likely broad emission at 2.08 eV and low intensity blue emission at 2.87 eV which corresponds to near band edge transition. We demonstrated that the present NWs are useful in a wide range of potential applications as photodetectors.

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Comparative Bending Deformation of GaP and GaAs Nanowires Using Raman Spectroscopy

임형순 박기동 정찬수[1] 박정희[1,*]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

GaP and GaAs NWs were synthesized using the chemical vapor transport method. The growth direction of NWs was controlled to be [111] and [112]. The GaP NWs consisted of twinned superlattice structures domains which is perpendicular or parallel to the growth direction. Raman scattering spectroscopy is one of most straightforward technique that have been broadly utilized to estimate the strain in semiconductors. Raman scattering spectroscopy is one of most straightforward technique that have been broadly utilized to estimate the strain in semiconductors. We report on the first Raman investigations of strain in individual NW that were bent by the mechanical buckling processes of poly(dimethylsilioxane) that transform the initially straight NWs into wavy shapes via releasing pre-strain. Raman spectra were collected along the bent wires and strain broadened phonon lines were observed insections of the wire with large curvature. We correlate the peak broaden ing and shift of the Raman spectra to the measured strain of the twinned structure NWs is higher than that of the single-crystalline ones.

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Composition Tuned Organometal Trihalide Perovskite Colloidal Nanocrystals via Reversible Halide Exchange Reaction

김덕환 박정희* 박기동[1]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

n recent years, methylammonium lead halide perovskites ($MAPbX_3$, X = Cl, Br, I) have attracted tremendous interest because of their outstanding photovoltaic performance, approaching a photoconversion efficiency of 19%. Previous studies have reported that these perovskites exhibit a large absorption coefficient over a broad spectral range, high charge carrier mobility, small exciton binding energy, and long exciton diffusion length. Herein, we report a remarkable finding of reversible halide-exchange reactions of $MAPbX_3$, which facilitates the synthesis of a series of mixed halide perovskites. The synthesis of $MAPbBr_3?_3Cl_3$ and $MAPbBr_3?_xI_3$ NCs was achieved by the halide exchange reaction of $MAPbBr_3$ with MACl and MAI, respectively, in an isopropyl alcohol solution, demonstrating full-range band gap tuning over a wide range (1.6?3 eV). We also fabricated photodetector devices using composition-tuned nanocrystals for investigation of photoconversion efficiency. Among the two mixed halide perovskite series, those with I-rich composition (x = 2), where a sole tetragonal phase exists without the incorporation of a cubic phase, exhibited the highest photoconversion efficiency. The $CH_3NH_3PbX_3$ nanocrystals with different composition may be of future use in the construction of high performance solar cells and light-emitting devices.

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Iron Phosphide Nanowires for Hydrogen Evolution Reaction

<u>손창용</u> 박정희* 박기동[1] 정찬수 박충효 곽인혜

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Production of molecular hydrogen by the electrochemical reduction of water is an important component of several developing clean-energy technologies. The hydrogen evolution reaction constitutes half of the water-splitting reaction. Currently, platinum is the best known hydrogen evolution catalyst with only small overpotentials and high reaction rates, but the scarcity and high cost may limit its widespread technological use. Recently, transition metal phosphides, including Ni2P, CoP, and FeP, have been identified as promising hydrogen evolution reaction electrocatalysts. Herein, we synthesized vertically iron phosphide nanowire arrays using a unique gas-phase anion exchange reaction of pre-grown Fe2O3 nanowires with phosphine gas. This method provides many benefits including no extra fabrication process, high yield, short reaction time, and excellent reproducibility. Their electrocatalytic performance was tested for hydrogen evolution reaction, showing an excellent catalytic activity and stability.

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The electrical properties of chalcogenide nanostructures studied by conductive atomic force microscopy

이정아 임영록 정찬수 임형순[1] 박기동[1] 박정희*

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Electronic transport properties of chalcogenide nanostructure devices were studied by a conductive atomic force microscopy (C-AFM). In this work, the chalcogenide nanostructures were synthesized by chemical vapor deposition and their crystal structure were determined from X-ray diffraction, scanning electron microscopy and transmission electron microscopy. For the device fabrication with a sandwiched structure of PtIr tip/Pt-coated nanostructure/Au, the alignment of the nanostructure between patterned Au electrodes was accomplished by dielectrophoresis. The electrical contacts between the nanostructures and Au electrodes were formed by focused ion beam assisted Pt deposition. During the C-AFM based measurement, PtIr tip and Au electrode were used as a movable top electrode and bottom electrode, respectively. The electrical characteristics of each devices were measured at room temperature and in air. The resistive switching behaviors obtained from the devices were analyzed in the aspect of a space-charge limited current conduction mechanism and schottky contact behaviors.

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Defect Engineering of MoS_2 Nanosheets for Hydrogen Evolution Reaction

권익선 정찬수[1] 곽인혜[1] 오진영[1] 박정희[1,*]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

Hydrogen energy is an ideal, clean and efficient secondary energy resource. Although some noble metals such as platinum and palladium are well-known for their superior electrocatalytic property in the hydrogen evolution reation (HER) in an acidic medium and commonly used as electrocatalysts in the applications, large-scale application of them is limited due to their high prices and global low availabilities. Therefore, extensive research efforts have been devoted to the development of non-platinum electrocatalysts for HER. Recent theoretical and experimental work has highlighted the promise of MoS_2 as potentially low cost catalysts for hydrogen evolution. Here, we show that the formation of catalytically active surface defects leading to improve the catalytic activity. We achieve this by designing a reaction strategy using a controlled pH and mixed solvent, thus realizing the defect modulation. With the merits of the defect-induced additional active edge sites, the defect-rich MoS_2 ultrathin nanosheets exhibit excellent HER activity, which demonstrates the best integrated electrocatalytic performance. Finally, This study successfully demonstrates that introducing defect site to ultrathin MoS_2 nanosheets is feasible by a facile mixed solvent strategy and pH-dependent control route and these may open up a potential pathway for designing more efficient MoS_2-related catalysts for HER.

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Ta_3N_5 Photoanode for Overall Water Splitting under Visible Light Irradiation

김영운 박정희[1,*] 정찬수[1] 임형순[2] 박기동[2] 오진영[1] 박충효[1] 곽인혜[1]

호서대학교 그린에너지공학과 [1]고려대학교 소재화학과 [2]고려대학교 미세소자공학협동/마이크로소자

Photoelectrochemical (PEC) water splitting is a promising approach to direct conversion of solar energy into storable hydrogen fuel that could act as a green energy carrier. Tantalum nitride (Ta_3N_5) is a promising semiconductor photocatalyst for solar water splitting because it has band edge potentials capable of producing hydrogen and oxygen from water under visible light ($\lambda < 590$ nm). Herein, we developed unique synthesis method for high-yield Ta_3N_5 nanoparticles by combining a sol-gel method and a gas phase substitution reaction. We analyzed the electronic structure by transmission electron microscopy, electron-energy loss spectroscopy, and X-ray diffraction, and synchrotron X-ray absorption and photoelectron spectroscopy. The photoanodes for water splitting were fabricated on conducting support, which forms effective contacts, afforded a significant increase in the photocurrent and water splitting. The photoelectrochemical cells with these photoanodes show excellent visible-light-driven photocatalytic performance and stability for water splitting.

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Synthesis of transition-metal doped $SrTiO_3$ nanocubes and the photocatalytic efficiency for water splitting reaction

오진영 박정희* 김영운[1] 김덕환 곽인혜 박기동[2] 임형순[2] 정찬수

고려대학교 소재화학과 [1]호서대학교 그린에너지공학과 [2]고려대학교 미세소자공학협동/마이크로소자

Photocatalytic reaction with visible light have many various and important application such as water splitting reaction and carbon dioxide reduction reaction. Transition-metal (Mn, Fe, Co, Ni, Cu) doped $SrTiO_3$ nanocubes (average size = 30 nm) have been synthesized by hydrothermal reaction method. The morphology, composition, and crystal structure were investigated by transmission electron microscopy(TEM), X-ray diffraction pattern(XRD), and UV-visible spectroscopy. We investigated the photocatalytic efficiency of photoanodes for water splitting reaction. We found that the Co-doped $SrTiO_3$ photoanodes show the highest efficiency,

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Metal encapsulated N-doped Nanodiamond As Highly Efficient Electrocatalysts for Hydrogen Evolution Reaction

박충효 서재민 곽인혜 손창용 권익선[1] 박정희[*]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Large-scale practical application of fuel cells will be difficult to realize if the expensive platinum-based electrocatalysts cannot be replaced by other efficient, low-cost, and stable electrodes. Here we report the catalytic ability of metal nanocrystal-N-doped graphitized onion-like nanodiamond (NC-NGND) hybrid nanostructures for oxygen reduction reaction. They were prepared by laser induced reaction of metal precursor (Pt, Pd, Ag, Au, Cu etc.) and nanodiamonds in ethanol, and were sybsequently doped with the N atoms by the thermal annealing under NH_3 gas. The metal NC-NGND hybrid nanostructures exhibits low overpotential and high activity for hydrogen evolution reaction (HER), which is credited to their unique electronic structures of NGND and selectivity of metal nanocrystals. The finding may lead to a new strategy to develop cost-effective electrocatalysts with superior efficiency for CO_2 reduction Reaction.

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Phase evolution of ZnSe nanowires

김예진 임형순[1] 박기동[1] 정찬수 오진영 손창용 박정희*

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Phase control of compound semiconductor offers the advantages of band gap tunability, controlled conduction band gap offsets, and localized defect energy levels, which are critical for achieving high photoconversion efficiencies in photovoltaic cells. ZnSe, a typical II-VI compound semiconductor, nanowires have been synthesized by chemical vapor deposition. Phase evolution from zinc-blende phase to wurtizite phase were successfully achieved by controlling the growth conditions such as temperature and pressure. In contrast to their bulk counterparts (mostly in cubic zinc blende (ZB) phase), the hexagonal wurtzite (WZ) structure is the most striking feature. They contain stacking faults such as twins due to the coexisting WZ-ZB phase. Moreover, the growth direction of the zinc-blende phase nanowires has been controlled using the Au and Ni nanoparticle catalysts; [111] for Au and [112] for Ni. Raman and photoluminescence were collected along the NWs, and correlated with the twinned structure as well as the growth direction.

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Comparative Cycling Performance of Zn_2GeO_4 and Zn_2SnO_4 Nanowires as Anodes of Lithium - and Sodium Ion Batteries

임영록 정찬수 임형순[1] 박기동[1] 박정희[*]

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High-yield zinc germanium oxide (Zn_2GeO_4) and zinc tin oxide(Zn_2SnO_4) nanowires were synthesized using a hydrothermal method. We investigated the electrochemical properties of these Zn_2GeO_4 and Zn_2SnO_4 nanowires as anode materials of lithium ion battery and sodium ion battery. The Zn_2GeO_4 and Zn_2SnO_4 nanowires showed excellent cycling performance of the lithium ion battery, with a maximum capacity of 1021 mAh/g and 692 mAh/g after 50 cycles, respectively, with a high Coulomb efficiency of 98 %. For the first time, we examined the cycling performance of Zn_2GeO_4 and Zn_2SnO_4 nanowires for sodium ion batteries. The maximum capacity is 168 mAh/g and 139 mAh/g after 50 cycles, respectively, with a high Coulomb efficiency of 97 %. These nanowires are expected as promising electrode materials for the development of high-performance lithium ion batteries as well as sodium ion batteries.

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Synthesis of iron nitride Nanoparticle and their application as catalysts for water splitting

서재민 곽인혜 임영록 박충효 권익선[1] 박기동[1] 박정희*

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Employing a low-cost and highly efficient electrocatalyst to replace Pt-based catalysts for water splitting hydrogen evolution reaction (HER) has attracted increasing interest in renewable energy research. Herein we report the synthesis of Fe_2N and Fe_4N nanoparticles that can efficiently electrocatalyze the HER with activities close to that of Pt and function well under acidic medium. We synthesized these nanoparticles by annealing the iron nanoparticles under a stream of NH_3. We report excellent HER catalytic activity and their durability in acid or alkaline medium. Therefore Fe_2N and Fe_4N might serve as a promising new class of non-noble metal catalysts for practical HER.?

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Adsorptive removal of indole from model fuel using an amino groups functionalized metal-organic frameworks via hydrogen bond formation

서필원 정성화*

경북대학교 화학과

Fossil fuel contains different types of nitrogen-containing compounds (NCCs) which are composed of basic materials such as quinoline (QUI) and neutral materials such as indole (IND). Because of the negative effect of NCCs on the environment and catalyst stability, NCCs should be removed from fuels. The NCCs can be removed by various methods including adsorption. Compared with basic NCCs, neutral NCCs are more difficult to remove through adsorption due to their less affinity towards adsorbents. In this report, adsorption of IND (as one of the representative neutral NCCs) was studied over the metal-organic frameworks (MOFs), UiO-66 and UiO-66-NH2, which contain terephthalate and amino-terephthalate linkers, respectively. In spite of the reduced porosity of UiO-66-NH2, the adsorption capacity of IND was improved upto 46% when compared with pristine UiO-66. Therefore, the additional amino group in the MOF imparts extra adsorption capability on the MOF. For a detailed investigation, adsorption of other NCCs such as QUI, pyrrole, and methylpyrrole was studied. The improved adsorption of IND over amino-functionalized MOFs could be attributed to the improved interaction of IND with the MOF via H-bonding because of the -NH2 group. In addition to this remarkable improvement in IND adsorption, UiO-66-NH2 could be regenerated several times for the adsorption of IND by simple solvent washing. Additionally, it can be concluded that these types of modification be applied for the removal of those less active materials which are not so easy to remove by other means.

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Highly Capable Photocatalytic Activity of CeO2-AgI nanocomposite Photocatalyst through Z-scheme Photocatalytic Mechanism under Sun-light Irradiation

ISLAMMOHAMMADJAHURUL 김태규[*]

부산대학교 화학과

A highly-efficient solar-light driven Z-scheme CeO2-AgI nanocomposite photocatalyst were fabricated by simple precipitation process and characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction spectroscopy (XRD), Fourier-transform infrared spectroscopy (FTIR) and UV-Vis diffuse reflectance spectroscopy. Under the solar-light irradiation, CeO2-AgI nanocomposite photocatalyst exhibits the higher photocatalytic performance than pure AgI and CeO2 for the degradation of RhB dye. Among the nanocomposite photocatalysts, CeO2-AgI with 20 wt % of CeO2 demonstrated the highest phtocatalytic activity for the degradation of RhB dye. The kinetic constant of photocatalytic degradation of RhB for CeO2-AgI is 3.3 times and 25.7 times higher than that of pure AgI and CeO2. The X-ray photoelectron spectroscopy (XPS) results revealed that CeO2-AgI nanocomposite contain oxygen vacancies which play an important key role for the photocatalytic performance. The composite photocatalyst shows good stability. In addition, ˙O2- and ˙OH play the major role for the degradation of RhB, revealed by the different scavenger’s experiments. The mechanism for the enhancement of photocatalytic performance of CeO2-AgI nanocomposite is proposed to the efficient separation of photogenerated electron-hole pairs through a Z-scheme system, where oxygen vacancy states also play an important role. The photoluminescence result is highly supported as an evidence of the Z-scheme mechanism of the nanocomposite photocatalyst.

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A simple combination of analytic functions for non-adiabatic coupling terms, and its use in the constructions of diabatic potential energy surfaces

안희선 백경구*

강릉원주대학교 화학과

In order to study chemical dynamics involving multi-electronic states, by using the quantum wave-packet propagation method,[1] the construction of the diabatic potential energy surfaces (PESs) and the coupling term between them is an essential premise. One of the most rigorous procedures for the construction is the use of the non-adiabatic coupling terms (NACTs) in the path integral for the mixing angle.[2] However, the computation of the NACTs by ab-initio methods is very expensive and often exhibits singularities at near the conical intersections. As the model functions for the ab-initio NACTs, the use of the Lorentzian function or a linear combination of the hyperbolic secant functions was suggested earlier,[4] but the functions do not decay fast enough. Moreover, the method has too many parameters to be extended to multi-dimensional systems. In order to overcome the above problems, we propose a simple combination of analytic functions to ensure qualitatively proper behavior of the mixing angle.[3] The performance of our analytic function is examined with respect to various systems, such as LiF,[4] FHCl,[5] H_2S[2] and NH_3Cl.[6]

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대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Adsorption and removal of methylchlorophenoxypropionic acid with a metal-organic framework

서여송 정성화*

경북대학교 화학과

Adsorptive and removal of methylchlorophenoxypropionic acid (MCPP) using metal-organic frameworks (MOF), namely Zr-benzenedicarboxylate (UiO-66), were investigated for the first time to determine the applicability of MOFs in the removal of hazardous herbicides and pesticides from contaminated water. Compared with activated carbon, UiO-66 has a very high adsorption rate (kinetic constant ~ 30 times that of activated carbon). This rapid adsorption is remarkable because the pore size of UiO-66 is smaller than that of activated carbon. Moreover, the adsorption capacity of UiO-66 is higher than that of activated carbon especially at low MCPP concentrations (~7.5 times at 1 ppm of MCPP). These rapid and high uptakes by UiO-66 suggest that there is a special mechanism for interactions between MCPP and UiO-66. Additionally, the adsorbent can be reused for adsorptive removal by washing the spent adsorbent with a simple solvent. MOFs such as UiO-66 are therefore potential adsorbents for use in the adsorptive removal of MCPP from contaminated water. An adsorption mechanism could be suggested based on the effects of pH on the zeta potential of the adsorbent and on adsorption performances. Both electrostatic and π-π interactions might be important for the adsorption and removal of MCPP by UiO-66.

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Aqueous phase adsorptive removal of organoarsenic compounds with three different analogous metal-organic frameworks

전종원 정성화*

경북대학교 화학과

Adsorptive removal of the two typical organoarsenic compounds, p-Arsanilic acid (ASA) and roxarsone (ROX), from water onto metal organic frameworks (MOFs) have been studied for the first time. Iron-benzenetricarboxylate (Fe-BTC), a MOF also known as MIL-100-Fe showed much higher competence for ASA and ROX removal as compared with activated carbon, zeolite (HY), goethite, and other MOFs. The kinetics of ASA and ROX adsorption over MIL-100-Fe was quite faster than that over activated carbon. Moreover, the used MIL-100-Fe could be recycled by simple washing with acidic ethanol. Therefore, it was resolute that a MOF such as MIL-100-Fe can be used to remove organoarsenic compounds from spent water because of its high adsorption capacity, rapid adsorption, and ready regeneration. Interestingly, the porosity of the MOFs was not an important factor in the adsorption of organoarsenic compounds. Moreover, among analogous MIL-100s (MIL-100-Fe, MIL-100-Al or MIL-100-Cr), MIL-100-Fe was able to effectively remove the organoarsenic compounds. This selective and high adsorption over MIL-100-Fe, different from other analogous MIL-100s, could be explained (through calculations) by the facile desorption of water from MIL-100-Fe as well as large (absolute value) replacement energy (difference between the adsorption energies of the organoarsenic compounds and water) exhibited by MIL-100-Fe. The surface charge of the MOFs, FTIR results, calculations, and the reactivation results lead us to put forward a conceivable adsorption/desorption mechanism.

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Remarkable adsorptive removal of thiophenics from fuel with a metal-organic framework supported with ionic liquids

Nazmul Abedin Khan 정성화*

경북대학교 화학과

Thiophenics are naturally occurring sulfur containing species in fossil fuel. There is a extensive command to reduce the content of sulfur-containing compounds in fuels like diesel and gasoline to a low level to prevent air pollution and deactivation of catalysts. Ionic liquid (IL)-supported metal-organic framework (MOF) was firstly demonstrated for the beneficial utilization of acidic IL in adsorptive desulfurization. For that, 1-butyl-3-methylimidazolium chloride (a typical IL) was introduced to one of the widely studied MOFs, MIL-101 (chromium-benzenedicarboxylate) 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. The adsorption of bulky dibenzothiophene (DBT) with the same adsorbent showed the similar trend where IL/MIL-101 adsorbed larger amounts of DBT for the whole adsorption times compared to virgin MIL-101, confirming again that the supported ILs can be effective sites for the adsorption of various organosulfur compounds.

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Preparation of a composite, graphite oxide/metal-organic framework (MIL-101) and its application in adsorptive denitrogenation and desulfurization of model fuels

imteaz ahmed 정성화*

경북대학교 화학과

Metal-organic frameworks (MOFs) are known for their high functionality and improved porosity. To improve the functionality of a porous MOF, MIL-101 (Cr-benzenedicarboxylate), it was composed with graphite oxide (GO) to obtain GO/MIL-101 composites. Accelerated synthesis was obtained upon adding the GO content to the MOF precursor during the formation of the composite. Additionally, the surface properties also improved in the composite compared with the pristine MOF. The surface area of the composites increased remarkably in the presence of a small amount of GO (

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Efficient removal of phthalic acid and diethyl phthalate from water over the zeolitic imidazolate framework ZIF-8

Biswa Nath Bhadra 정성화*

경북대학교 화학과

The removal of phthalic acid (H2-PA) and diethyl phthalate (DEP) from aqueous solutions, a typical ZIF material, zinc-methylimidazolate framework-8 (ZIF-8) has been used via adsorption. The adsorption capability of the ZIF-8 for H2-PA was superior to that of a commercial activated carbon or other typical metal-organic frameworks (MOFs). The remarkable adsorption with ZIF-8 suggests no favorable effect of the surface area and pore volume of the adsorbents but favored by a specific interaction (electrostatic interaction) between the positively charged surface of ZIF-8 and the negatively charged PA anions. In addition, other encouraging contribution in the adsorption of H2-PA is acid-base interactions, based on the adsorptive performances of pristine and amino-functionalized MOFs and adsorption over ZIF-8 at acidic condition (pH=3.5). On the other hand, the DEP removal capacity onto ZIF-8 was not efficient, probably due to the little charge of DEP in a water solution. The used ZIF-8 was very easily reusable just by simple washing with methanol.

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Quantum wave-packet propagation study of a pre-dissociating state: The S_1 and T_1 states of dichlorine monoxide isomers, ClOCl and OClCl

문자연 안희선 백경구*

강릉원주대학교 화학과

Dichlorine monoxide is one of many halogen oxides playing a key role in the ozone depletion mechanism in the stratosphere, and its detail photo-dissociation mechanism is still under active studies. Especially, the stability and spectroscopic properties of the first excited singlet S_1 and the lowest triplet state T_1, as well as the isomerization related to the S_1 and T_1, are still under disputes. The molecular structure and spectroscopic properties of two isomers of dichlorine monoxide (Cl-O-Cl and O-Cl-Cl) in S_0, S_1, and T_1 states were studied by various ab initio and DFT methods. Their potential energy surfaces (PESs) were also constructed in two- and three-dimensional spaces by using MRCI method. Then the photo-absorption spectra to the excited states are simulated by applying the quantum wave-packet propagation (QWP) method. It will be shown that the fine structure of a photo-absorption spectrum to a pre-dissociating state can be disclosed by QWP method.

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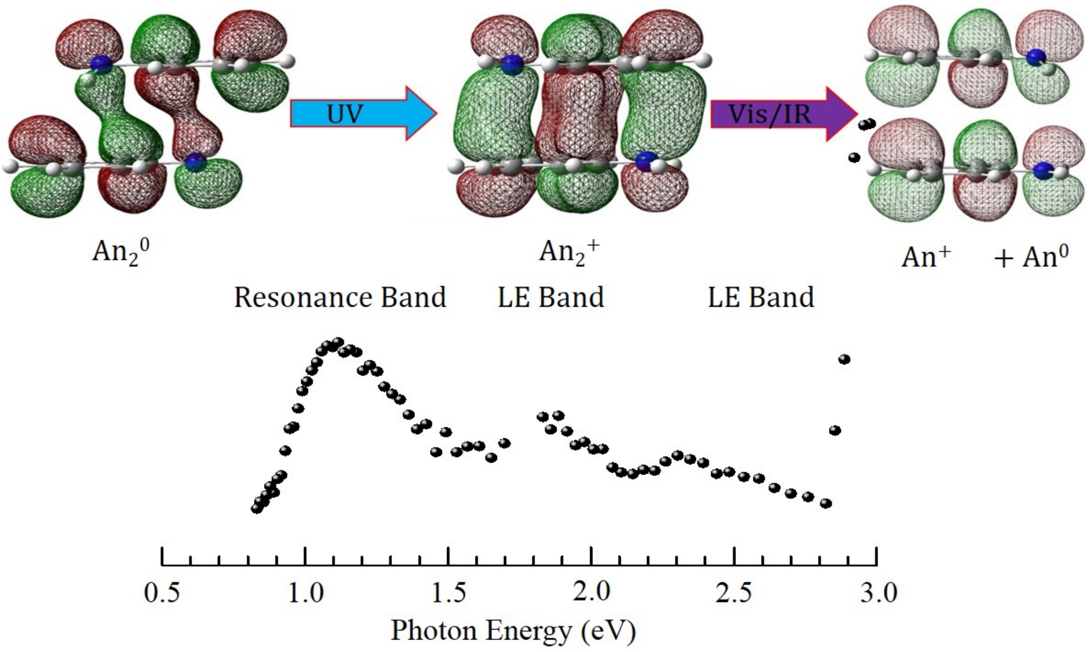
Charge Resonance Structure of Aniline Dimer Cation

<u>Madhusudan Roy</u> 김국기 송재규* 박승민*

경희대학교 화학과

Molecular structure of aniline dimer cation has been investigated with infrared spectroscopy coupled with tandem time of flight mass analyzer. Mass-selected aniline dimer cation was dissociated by irradiation of photons ranging from visible to near infrared (420-1500 nm). An intense absorption band was observed around 1.12 eV (1110 nm) in the photodissociation action spectrum, which was assigned as charge resonance (CR) interaction band for aniline dimer cation. Two other bands observed around 1.9 eV (650 nm) and >3.0 eV ($^2A_2$ <-- X^2B_1 and B^2B_1 <-- X^2B_1) transition band of locally excited An^+ in An_2^+, respectively. In the infrared spectrum, two broad and intense absorption bands were observed around 3190 and 3420 cm^{-1}, which were assigned as combination band of symmetric and antisymmetric NH_2 stretching of aniline, respectively. Density functional theory calculation at the theory level of M06-2X/ 6-311++G(2d) and B3LYP/cc-pVTZ methods suggested a “head to tail” type stacked CR structure for An_2^+, which is stabilized by at least 800 or 300 cm^{-1} compared to other possible isomers for the two methods respectively, and the theoretical and experimental infrared spectra matched quite well. Besides, the basis set super position error (BSSE) corrected binding energy derived from counterpoise calculation also proved that the interaction energy is maximum in the CR structure.


UV
Vis/IR
An_2^0
An_2^+
$An^+ + An^0$
Resonance Band
LE Band
LE Band
0.5
1.0
1.5
2.0
2.5
3.0
Photon Energy (eV)

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Distance and Wavelength Dependent Fluorescence of Gold Nanoclusters Adsorbed to Ag@SiO2 Nanocomposites

김준기 장두전*

서울대학교 화학부

Plasmonic nanoparticles can significantly interact with closed fluorophore, resulting in surface plasmon-enhanced fluorescence or fluorescence quenching. This coupling is dependent upon distance between the fluorophore and the plasmonic surface, and the degree of spectral overlap between the fluorophore's emission band and the surface plasmon resonance band (SPR) of nanoparticles. Fluorescent metal nanoclusters, especially gold nanoclusters (NCs), have stimulated extensive interest because of their remarkable optical properties. However, only a few studies have been reported on the interaction of noble metal nanoparticles with Au NCs. We have demonstrated a novel method for the preparation of a fluorescent complex by combining a Ag core and protein-templated Au NCs. Biomolecules, such as Bovine Serum Albumin (BSA), have been utilized for the synthesis of Au NCs by simple wet chemistry. A thickness-variable silica shell prepared by the Stober method is placed between the plasmonic Ag core and Au NCs to play a role as a spacer. To understand the spectral overlap, we have prepared blue-emitting small Au8 NCs and red-emitting big Au25 NCs. Then, the spectra and the kinetic profiles of the fluorescence of Au NCs adsorbed to Ag@SiO2 nanocomposites have been investigated systematically with variation of space distances, excitation wavelengths, and cluster sizes.

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Comprehensive Studies on the Stable Conformers of Arginine in Aqueous Solution: A Theoretical Study

김창곤 박병호 권영민[1] 손창국[2] 김찬경[*]

인하대학교 화학과 [1]인하대학교 화학화공공학융합학과 화학전공 [2]전남대학교 화학교육과

Arginine is one of the most interesting amino acids because it is able to form a stable zwitterion species in the gas phase due to its extremely basic guanidine side chain (-$(CH_2)_3$-NHC-(NH_2)NH). Therefore arginine has been the subject of many intensive experimental and theoretical studies, but most theoretical works have focused on the stable conformers in the gas phase. Moreover, very little theoretical work has been done for transformations between these conformers. In this work, various conformers of arginine and transition structures for the interconversions among these conformers were studied theoretically at the MP2/6-311+G(d,p) level of theory in the gas phase and in aqueous solution. For studies in aqueous solution, the structures have re-optimized by use of the conductor-like polarizable continuum model (CPCM) with the PAULING cavity model. The energetics were then refined using the CCSD(T)/6-311+G(d,p) level on geometries optimized at the MP2 level. All calculations were performed with Int(grid=ultrafine) option by using the Gaussian-09 program.

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Theoretical Studies on Front-side Nucleophilic Substitution Reactions between Pyridines and Isothiocyano Benzene Sulphonates

Adhikary Keshab Kumar 박병호 김찬경*

인하대학교 화학과

The reaction mechanism on the pyridinolysis ($X-C_5H_4N$) of isothiocyano benzene sulphonates [$(Y-C_6H_4O)S(=O)_2(NCS)$] in acetonitrile is investigated computationally using the CPCM approach at the B3LYP/6-311+G(d,p) level of theory. In the front-side attack, the nucleophile pyridine approaches the substrate from the side syn to leaving group (?NCS). Experimentally, nucleophilic substitution to the sulfur center could proceed through two different mechanisms - concerted or stepwise. The concerted mechanism may involve front- or back-side approach of the nucleophile. In the stepwise mechanism, the mechanism can be either associative or dissociative depending on the rate-determining step. Our present studies show that the substitution reaction is a single step reaction involving a trigonal bi-pyramidal penta-coordinated (TBP-5C) transition state. In this work, we focused on the front-side attack of the nucleophile. The reaction mechanism will be discussed in terms of Hammett constants, ρ_X, ρ_Y, and ρ_{XY} and the Br?nsted β_X values. In addition, the steric effects between the nucleophile and the substrate will be examined in detail.

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The effects of ablation condition on the formation of gold nanoparticles by laser ablation in liquid

권혜진 김국기 송재규 박승민*

경희대학교 화학과

Gold nanoparticles were synthesized by laser (Nd: YAG, λ = 1064 nm) ablation of a gold target immersed in NaCl, NaBr and NaI solutions. The sruface plasmon absorption peak was measured by UV-Vis spectrophotometer to investigate the spectral change depending on the wide range of concentration and duration of the ablation. Transmission electron microscopy (TEM) used to observe the size change of nanoparticles according to the ablation condition, and X-ray photoelectron spectroscopy (XPS) results were analyzed to find out the mechanism of gold nanoparitlces growth in the electrolyte solutions.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of omniphobic polytetrafluoroethylene (PTFE) using SiO_2 nanoparticles and fluoroalkylsilane

박기정 정명근 김보라 김승연 김대한 박은지 한상욱 이주하 김일희 김영독*

성균관대학교 화학과

The omniphobic thin films on polytetrafluoroethylene (PTFE) were prepared with surface modification with SiO_2 nanoparticles and trichloro(1H, 1H, 2H, 2H-perfluorooctyl)silane (FOTS). Two different methods, dip-coating and molecular vapor deposition (MVD), for the FOTS-coating were provided to the PTFE surface modification with water and hexadecane contact angles exceeding 150 ^{o} and 90 ^{o}, respectively. On the other hand, the omniphobic PTFE film showed a gas-permeability for CO_2 and dimethylmethylphosphonate (DMMP), indicating that the omniphobic PTFE film can play a role as gas sensor shielding layers that allow selective permeation of gas from gas/liquid mixtures.

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Application of polydimethylsiloxane (PDMS)-coated TiO_2 as MALDI matrix for detecting dimethyl methylphosphonate (DMMP)

한상욱 박은지 정명근 김대한 이주하 김보라 김승연 박기정 김일회 김영독*

성균관대학교 화학과

In this work, TiO_2 nanoparticle was used as matrix for dimethyl methylphosphonate (DMMP) detection in matrix assisted laser desorption ionization mass spectroscopy (MALDI-MS) and its efficiency was compared with that of polydimethylsiloxane (PDMS)-coated TiO_2 nanoparticle. Two sampling methods, dried droplet and thin-layer method were used for each matrix and the efficiency of the matrices was determined in terms of DMMP signal intensity in MALDI-MS. The DMMP signal was significantly increased by using PDMS-coated TiO_2 instead of bare TiO_2 in both sampling methods. FT-IR result verified that the enhancement of DMMP signal upon PDMS coating is the result of weaker interaction between DMMP molecule and the PDMS-covered surface than that with bare TiO_2. A weaker interaction between DMMP and matrix can facilitate desorption of DMMP from the matrix surface in the MALDI process, yielding a higher sensitivity to DMMP in the MALDI-MS.

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Room temperature CO oxidation catalyzed by NiO nanoparticles on mesoporous SiO_2 prepared by atomic layer deposition

김일희 정명근 한상욱 김대한 박기정 김보라 김승연 이주하 박은지 김영독*

성균관대학교 화학과

NiO nanoparticles supported on mesoporous SiO_2 were prepared by atomic layer deposition (ALD), and the fabricated samples were annealed at four different temperatures (300, 450, 600, and 750 ^oC). Size of NiO nanoparticles on the surface of annealed samples was smaller than ~ 2 nm up to annealing temperature of 600 ^oC, whereas that of 750 ^oC-annealed sample became bigger as ~ 30 nm due to agglomeration. Among the four samples annealed at different temperatures, 450 ^oC-annealed sample showed the highest catalytic activity for CO oxidation at room temperature. Also the 450 ^oC-annealed catalyst showed the highest resistance toward deactivation, maintaining 60% of the initial catalytic activity for CO oxidation after 680 minutes. Moreover, after additional annealing at 450 ^oC, catalytic activity of the 450 ^oC-annealed catalyst deactivated after CO oxidation experiment was fully recovered. These results suggest that ALD followed by annealing is promising strategy to fabricate highly active and stable catalysts consisting of nanoparticles incorporated in the mesopores of a high-surface area support.

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Thickness-Dependent Native Strain in Few-Layer Graphene Visualized by Raman Spectroscopy

김수진 류순민*

포항공과대학교(POSTECH) 화학과

Since graphene, a representative 2-dimensional crystal, has an extreme surface-to-volume ratio, its various material properties are known to be susceptible to molecular interaction with environment. Recently it was shown that single-layer graphene exhibits native lattice strain induced by van der Waals interaction (vdW) with the underlying substrates. In this work, we report the Raman spectroscopy study on the native strain induced by the vdW interactions of mechanically exfoliated few-layer graphene with supporting silica substrates. Using freestanding graphene as a strain-free reference, we quantified the resulting strain with a precision of 0.01% and found that its standard deviation is much smaller than that of single-layer graphene (SLG) and decreases as increasing the number of layers finally reaching the detection limit for the thickness of ~30 layers. The spatially resolved strain maps revealed that the native strain is randomly distributed and that both of compression and expansion are also randomly generated. This work demonstrated that Raman spectroscopy can serve as a highly sensitive strain metrology tool for graphene samples in a wide range of thickness and can be extended to other 2-dimensional crystal systems.

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Compact instrumentation of a GC for real time analysis of VOC mixtures in air

유동욱 이재원[1] 오준식[2] 박창준[3] 안상정[4] 정광우*

원광대학교 화학과 [1]원광대학교 바이오나노화학 [2]원광대학교 생명나노화학부 [3]한국표준과학연구원(KRISS) 첨단장비기술센터 [4]한국표준과학연구원(KRISS) 첨단측정장비센터

We report the instrumentation of a portable GC system that was capable of performing real-time analysis of organic mixture vapors. This system consists of a preconcentrator/injector, a capillary column with at-column heater configuration and a photo ionization detector (PID). Through the compact design of fluidic system, this fully functional GC measured 15(l)×15(w)×15(h) cm and the weight was less than 2 kg. This system employs ambient air as a carrier gas and is powered by either a 24 V DC adapter or batteries. The analytical cycle including sampling, separation and cooling required only 10 min. We demonstrated the high sensitivity and selectivity of this device. The results indicate that the portable GC-PID module is expected to be used for a wide range of applications, particularly for in situ environmental monitoring, chemical processes, and regulation of contaminant emission.

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Design, fabrication, and performance of microfabricated columns for gas chromatography

이재원 유동욱[1] 오준식[2] 박창준[3] 안상정[4] 정광우[1,*]

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This study presents several aspects of etched-silicon/glass microfabricated channels that affect their performance as micro-gas chromatographic (GC) separation columns, including the consistency of stationary phase deposition, deactivation of surface-adsorption sites on the microcolumn walls, and the stability of the stationary phase following repeated thermal cycling. Convolved square-spiral microcolumns 3-m long with cross sections of 300 mm×300 mm consisting of deep-reactive-ion-etched (DRIE) Si with anodically bonded Pyrex caps are used. Microcolumnis is filled with a sol solution of appropriate composition, and sol-gel reactions are allowed to go on inside the capillary for a controlled period, typically 15-60 min. Using split-flow injection, theoretical plates are measured and a mixture of volatile organic vapors can be separated on a 3-m PDMS-coated column in less than 5 min. Results demonstrate that a high separation efficiently micro gas chromatography (GC) column can used to construct a portable rapid GC system.

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Effect of TiO_2-shell on the catalytic stability of Ni catalyst for CO_2 reforming of CH_4 reaction

김대한 정명근 박은지 한상욱 이주하 김보라 김승연 박기정 김일희 김영독*

성균관대학교 화학과

Bare and TiO_2-coated Ni particles were used as catalysts for the CO_2 reforming of CH_4 (CRM) reaction at 800 ℃ and TiO_2 layers with two different thicknesses were prepared by atomic layer deposition (ALD). We focused on the deactivation mechanism of various catalysts upon long-term operation. All of the catalysts showed a decrease in the catalytic activity as a function of the reaction time for 160 h, and the TiO_2-coated Ni showed a less pronounced decrease in the catalytic activity in comparison to that of the bare Ni catalyst. The graphitic carbon layers that formed on the Ni particles during the reaction were suggested to be responsible for the deactivation and the additional TiO_2 layer facilitated the formation of separate carbon filaments rather than the graphitic layer on the Ni, reducing the possibility that the active Ni sites of catalyst would be covered and poisoned by the deposited carbon layers. The fabrication of core-shell structures of metal and oxide by ALD can be a useful approach for the synthesis of heterogeneous catalysts, for which not only high activity, but also enhanced stability at an elevated temperature, is required.

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Photodegradation study of OLED by combined optical imaging system

배소현 강주연 민경석[1] 손정배 김경우[2] 권장혁[2] 김성근[*]

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학부 [2]경희대학교 정보디스플레이학과

Extended operation of organic light-emitting diodes (OLEDs) results in materials degradation. To investigate the degradation mechanism of an iridium doped OLED device, we introduced photo-induced degradation to mimic the operational damage of OLEDs. We measured the spectra and photoluminescence (PL) lifetime of host and dopant materials after light irradiation. As the photoinduced damage progressed, both PL intensity and lifetime of the dopant material decreased, but no remarkable change was observed in the corresponding properties of the host material. Our results suggest that photo irradiation mainly causes a direct damage to the iridium dopant and its micro-environment.

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Inactivation of Pathogenic Bacteria By Photo induced Reactive Oxygen Species Generated from Photo Functional polymer

정승진 왕강균 황정욱 허일 김봉진 김용록*

연세대학교 화학과

Reactive oxygen species (ROS) have been a long time subject in chemical, environmental, and bio-medical science due to its strong reactivity and selectivity, and their involvements with metabolism of cell and organs[1]. They have many applications such as photodynamic cancer therapy, decontamination of blood product, water disinfectant, drug delivery system, and stereo-selective synthesis of drug in life science area[2]. Therefore, the investigation for the photosensitizers with a high efficiency of ROS generation is in a great demand[3].In this study, we report inactivation effect of pathogenic bacteria using the photofunctional polymer. The photofunctional polymer (PFP) that is the polymer embedded with a photosensitizer is fabricated by a simple solvent swell-encapsulation-shrink method. Reactive oxygen species(ROS) generation from PFP is confirmed with photocatalysis experiment. Singlet oxygen generation from PFP is directly confirmed with time and wavelength resolved phosphorescence spectroscopy. The photodynamic inactivation (PDI) effect of the photofunctional polymer is evaluated for various pathogenic of bacteria.Reference1. Ogilby, P. R. Chem. Soc. Rev. 2010, 39, 3181.2. Choudhary, S.; Nouri, K.; Elsaie, M. L. Lasers Med. Sci. 2009, 24, 971.3. Wang, K.-K.; Choi, K.-H.; Shin, H.-W.; Kim, B.-J.; Im, J.-E.; Oh, S.-L.; Park, N.-S.; Jung, M.; Oh, J.-B.; Lee, M.-J.; Kim, H.-K.; Kim, Y.-R. Chem. Phys. Lett. 2009, 482, 81.

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Thermal Generation of Two-Dimensional Oxides and Oxidative Etching in Atomically Thin MoS_2

류예진 류순민*

포항공과대학교(POSTECH) 화학과

Atomically thin planar crystals may reveal novel knowledge on chemical reactions occurring in such a low dimensional space. In this regard, thermal oxidation of MoS_2, the first-isolated semiconducting 2-dimensional crystal, was investigated to resolve the recent controversial observations of its oxidative etching and growth of planar Mo oxides. Single and few-layer MoS_2 samples were prepared by mechanically exfoliating bulk MoS_2 crystals on to SiO_2/Si substrates. To characterize the changes in morphology, vibrational and electronic structures, Raman and photoluminescence (PL) spectroscopies were used with atomic force microscopy. Thermal oxidation was carried out in a quartz tube furnace open to the ambient air in the temperature range of 320 ~ 370 °C. At a lower temperature, the edges of MoS_2 flakes were oxidized and etched away whereas the remaining area was found to be structurally intact but generate strong PL. At a higher temperature, the top surfaces of the samples were uniformly oxidized and converted into highly flat oxides rather than being etched. We will discuss branching between etching and oxide growth, thickness-dependence of the reactions and the origin of PL enhancement.

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Simulated NMR order parameters in proteins with knowledge-based potentials

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It is rather paradoxical that a protein interacts with high selectivity in spite of its floppy side-chains. For this reason, the dynamics of protein side-chains is worth studying to understand protein-protein and protein-chemical interactions and their corresponding protein function. In this study, we proposed a computational method to predict order parameters in a protein: a simulated annealing (SA) protocol using target energy functions based on a knowledge-based Statistical Torsion Angle Potential (STAP). The side-chain motions of methyl carbons were primarily investigated, and their order parameters (S2) were evaluated and compared with experimental values. We predicted $\chi1$ and $\chi2$ order parameters for six target proteins. Our method was compared with other computational methods (i.e., ANN, TADBP, and flexible backbone model) and showed comparable results to the flexible backbone model. The SA protocol using STAP was successfully applied to exposed residues. For example, protein L, which has many exposed residues, has a low RMSD value of 0.038 and a high correlation coefficient of 0.7. The present computational method based on knowledge-based potentials can be used to characterize the $\chi1$ and $\chi2$ conformations of side-chain residues to further our understanding of side-chain mobility.

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Antitumor Response by Dendritic Cells Manipulated with Photo-induced Intracellular Reactive Oxygen Species

신언필 정승진 허일 김봉진 LIJING 송유진 김용록*

연세대학교 화학과

Reactive oxygen species (ROS) play an important role in intracellular signaling as second messengers[1,2]. However, studying the role of ROS in physiological redox signaling has not been performed due to the technical difficulties in manipulating ROS generation within cells[3]. Here, we manipulate two inert factors, a photosensitizer and light, to have the fine control on the generation of intracellular ROS and to understand their specific role in activating dendritic cells (DCs). Photo-switchable generation of ROS is capable of studying the effect of ROS to the DCs. A transient intracellular ROS surge can activate DCs from immature to mature and potentially enhances migration abilities of DCs *in vitro* and *in vivo*, but exogenous H_2O_2 does not work. Further, mice immunized by intracellular ROS-stimulated DCs show the enhancement of tumor antigen specific T-cell responses, delayed tumor growth and therefore better survival of mice than the control. Therefore, this novel approach could provide a valuable tool for studying the role of ROS in cancer immunotherapy and vaccine research. This work was collaborated with Prof. Nam-Hyuk Cho, Department of Microbiology and Immunology, Seoul National University Medical Research Center.References1. Paul D. Ray, Bo-Wen H., Yoshiaki T., Cellular Signalling, 2012, 24, 981-990.2. Groeger G., Quiney C., Cotter TG., Antioxidants & Redox Signalling, 2009, 11, 2655-26713. Jaquet V., Scapozza L., Clark RA., Krause KH, Lambeth JD., Antioxidants & Redox Signalling, 2009, 11, 2535-2552

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Photothermal effect of gold nanoparticles on titanium dioxide catalysis

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서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Titanium dioxide (TiO_2) is one of the most widely used photocatalyst materials in a variety of applications including photoelectrochemical conversion, water and air purification, solar energy conversion, and environmental remedies. Because of its nontoxicity, high photocatalytic efficiency and chemical stability, TiO_2 is a highly promising photocatalyst material. To enhance the photocatalytic activity of TiO_2, synthesis of various types of noble metal-containing TiO_2 nanoparticles has been carried out along with studies on their properties through a number of well-defined photocatalytic reaction systems. Since electron transfer is known to be the major source of TiO_2 photocatalysis enhancement, little attention has been given to the photothermal effect of noble metal on the TiO_2. In this work, we investigated the photothermal effect of gold on TiO_2 photocatalysis and its kinetics with various spectroscopic methods.

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The Kinetic Isotope Effect as a Probe of Spin Crossover in the C-H Activation of Methane by the FeO^+ Cation

Mai Khanh Binh 김용호*

경희대학교 응용화학과

Two-state reactivity (TSR) is often used to explain the reaction of transition-metal?oxo reagents in the bare form or in the complex form. The evidence of the TSR model typically comes from quantum-mechanical calculations for energy profiles with a spin crossover in the rate-limiting step. To prove the TSR concept, kinetic profiles for C-H activation by the FeO^+ cation were explored. A direct dynamics approach was used to generate potential energy surfaces of the sextet and quartet H-transfers and rate constants and kinetic isotope effects (KIEs) were calculated using variational transition-state theory including multidimensional tunneling. The minimum energy crossing point with very large spin?orbit coupling matrix element was very close to the intrinsic reaction paths of both sextet and quartet H-transfers. Excellent agreement with experiments were obtained when the sextet reactant and quartet transition state were used with a spin crossover, which strongly support the TSR model.

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Exciton dynamics in electro- and photo-luminescence of organic light-emitting diodes

강주연 배소현 민경석[1] 손정배 김경우[2] 권장혁[2] 김성근*

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학부 [2]경희대학교 정보디스플레이학과

We carried out a comparative study of electro-luminescence (EL) and photo-luminescence (PL) of organic light-emitting diodes (OLEDs) to understand their operating mechanism, especially regarding what is known as “efficiency roll-off” at high brightness levels. EL and PL generate excitons through different processes. In EL, an electrical potential applied to the device separates electron and hole, which then combine to form a singlet or triplet exciton. In PL, only singlet exciton is generated since the light excites the ground state molecule directly through optically allowed transitions. Decay dynamics of excitons formed in different ways were investigated by time-resolved luminescence measurements. The polaron formed in the EL can quench the exciton, while such polaron-exciton annihilation does not occur in PL since it does not form a polaron. The change in decay time upon changing the laser power or voltage was fit to our annihilation model, which yielded the annihilation rate for both EL and PL. We were able to distinguish the polaron-exciton annihilation process from the exciton-exciton annihilation process experimentally. Easy acquisition of the annihilation rate is expected to be of value in understanding the “efficiency roll-off” phenomenon and improving the OLED efficiency.

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In silico study of similarities between anionic gold and silver clusters

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Gold and silver have many different properties in the bulk phase although both of them belong to the noble metal family. However, as both elements have the same valance electron configuration ($d^{10}s^1$), small clusters of gold and silver having the same structure and similar size may exhibit similar properties. We carried out density functional theory calculations for anionic gold and silver clusters to investigate their similarities. We compared several properties of anionic metal clusters such as molecular orbital structure, energy levels, and charge distribution within the cluster, and found unexpected similarities between gold and silver clusters. With respect to a small molecular adsorbate, both gold and silver clusters showed nearly equal reactivity.

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Band gap states of cubic-$AgIn_5S_8$ nanoparticles

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경희대학교 화학과 [1]국민대학교 화학과 [2]국민대학교 생명나노화학과

The Ag-In-S system of ternary semiconductor nanoparticles had well-ordered phases with the general formular $AgInS_2$, $AgIn_5S_8$. The photoluminescence quantum yield of $AgIn_5S_8$ nanoparticles was much higher than $AgInS_2$ nanoparticles. Moreover, $AgIn_5S_8$ nanoparticles were easily synthesized at a molar ratio [Ag] : [In] = 1 : 5. $AgIn_5S_8$ nanoparticles had single phase of cubic spinel structure. We investigated the band gap energy of $AgIn_5S_8$ nanoparticles which are obtained from photoluminescence spectrum. In photoluminescence spectrum, the emission from band gap states showed that only cubic phase existed in $AgIn_5S_8$ nanoparticles. The band gap energy which was estimated from photoluminescence spectrum was similar to absorption band peak energy. We identified the lifetime of the emission from band gap states that much shorter than the emission from defect states. $AgIn_5S_8$ nanoparticles were synthesized in a variety of sizes at reaction temperature from 120 to 180℃. We observed the shift of emission from band gap states depending on the particle size. The variation of band gap energy indicated the quantum confinement effects.

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Optical properties of lead halide perovskites

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경희대학교 화학과

Recently, lead halide perovskites have emerged as promising materials in solar cells. The power conversion efficiency of perovskite-based solar cells have rapidly increased up to 20.1%. Such a high photovoltaic performance is attributed to optically high absorption coefficient and long diffusion lengths. Herein, we investigated the optical properties of methylammonium lead halide perovskites ($MAPbX_3$, where X= Cl, Br, and I or mixed halide) and cesium lead halide perovskites ($CsPbX_3$, where X= Cl, Br, and I or mixed halide) by spectroscopy. We observed photoluminescence and electron-hole recombination lifetimes of metal halide perovskites. The emission of band gap states of $MAPbX_3$ and $CsPbX_3$ nanocrystals can be tuned over the entire visible spectral region (1.6-3 eV) through change of composition ratio. Furthermore, we found a lasing phenomenon in $CsPbBr_3$ nanowire.

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Ultraviolet photodissociation spectroscopy of isolated adenine and 7-methyladenine complexes with alkali metal cations

백지영 김남준*

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We have obtained ultraviolet (UV) photodissociation (PD) spectra of adenine and 7-methyladenine complexes with alkali metal cations (M^+A and M^+7MA, M=Li, Na, K, Rb, and Cs) stored in a quadrupole ion trap (QIT) at ~10 K. The UV PD spectra exhibit well-resolved vibronic bands in the wavenumber region of 35900 ? 36700 cm^{-1}. The origin bands of M^+A and M^+7MA are red-shifted with increasing the size of the metal cation from Li^+ to Cs^+. Previously, it was determined that all of vibronic bands in the UV PD spectrum of K^+A are from a single conformational isomer, where K^+ is bound not to 9H-adenine (A9) but to 7H-adenine (A7). We suggest that all M^+A ions have the same structures as K^+A based on their similarities in the UV PD spectra. The most stable structures of M^+A and M^+7MA are predicted by theoretical calculations.

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Circular Dichroism Spectroscopy of Jet-cooled Ephedrine

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Circular dichroism (CD) spectroscopy has provided a powerful tool to elucidate absolute configurations and structures of chiral molecules. We obtained the resonant two-photon ionization (R2PI) CD spectra of jet-cooled ephedrine (ED) with circularly polarized laser pulses generated using a photoelastic modulator (PEM). The R2PI CD spectra of ED exhibit well-resolved vibronic bands, which have different CD signs depending on their vibrational modes. To determine whether or not the R2PI CD values represent the CD of the S_0-S_1 transition or the two-photon ionization process, we measured laser-induced fluorescence (LIF) CD spectra of ED. It is found that only the CD sign of a vibronic band at 38 082 cm^{-1} in the LIF spectrum is opposite to the CD in the R2PI spectrum. We suggest that these opposite CD signs between the LIF and R2PI spectra are due to mode-selective isomerization of ED occurring upon excitation to the vibronic band.

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Electronic Circular Dichroism Spectroscopy of 2-Amino-1-Phenylethanol and its Hydrated Clusters in a Supersonic Jet

정창섭 홍아람 장희선 허지영[1,*] 김남준[*]

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The circular dichroism (CD) values measured for molecules in solution represent only the averaged CD values of all conformational isomers present in solution. In contrast, the CD spectroscopy of gas-phase chiral molecules can provide conformation- and vibrational mode-specific CD values. We obtained the electronic CD spectra of (*R*)-(-)-2-amino-1-phenylethanol (*R*-APE) and (*S*)-(+)-2-amino-1-phenylethanol (*S*-APE) and their hydrated clusters in a supersonic jet using laser-induced fluorescence (LIF) and resonance-enhanced two-photon ionization (R2PI) spectroscopic techniques. Circularly polarized laser pulses alternating between left and right (LCP and RCP) were generated using a photoelastic modulator and were irradiated to jet-cooled APE and its hydrated clusters. We recorded the difference between the signals induced by LCP and RCP laser pulses as a function of the wavelength to obtain the CD spectra. In these spectra, we identified the origin bands of the S_0-S_1 transition for different conformers of APE, APE-$(H_2O)_1$ and APE-$(H_2O)_2$. IR-UV double resonance spectroscopy combined with theoretical calculations using DFT and TDDFT at the M06-2X/6-311++G(d,p) level were carried out to predict the most stable geometries of the conformers and their CD values. We will discuss the effect of hydration on the CD values of different APE conformers.

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Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism for Gas-Phase Molecules

장희선 홍아람 정창섭 김남준[*] 허지영[1,*]

충북대학교 화학과 [1]상명대학교 의생명공학과

Time-dependent density functional (TDDFT) theory becomes popular in calculations of the electronic excited state. The electronic circular dichroism (ECD) spectra of chiral molecules were computed by using TDDFT and compared with the experimental data. However, most ECD spectroscopy had been performed in solution phase; thus ECD values obtained were the averaged values of many conformers in solution, which made it difficult to interpret ECD spectra from the TDDFT calculations. Recently the ECD spectra of pseudoephedrine (pED) and ephedrine (ED) in gas phase have been reported and could be used for unambiguously evaluating the performance on TDDFT calculations of the CD values. Here we tested various types of functionals and levels of basis set in order to identify the best combination of the functional and basis set in predicting the accurate CD values. The basis set of 6-311++G(d,p) could provide the reliable calculation results, but we could not single out the best functional among seven different functionals. Further discussion of detailed results is presented in this poster.

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Linear Micro-rod Silver Cyanide Produced by Pulsed Laser Ablation in DMF

이슬기 최명룡*

경상대학교 화학과

A rapid and simple preparation of silver cyanide (AgCN) micro-rods (MRs) is presented in this study. AgCN micro-rods were prepared by a pulsed laser ablation method in N,N-dimethylformamide (DMF). A plausible mechanism for the formation of the AgCN micro-rods via a fast reaction between silver cations from silver nitrate and cyanide anions from DMF through a recombination process is proposed. The structural, morphological and optical properties of the AgCN micro-rods were characterized by various techniques, such as X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), transmission electron microscope (TEM), energy-dispersive X-ray spectroscopy (EDS), gas chromatography (GC), and Fourier transform infrared and Raman spectroscopy

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REMPI and UV-UV hole-burning spectroscopy of jet-cooled neutral p-phenetidine in the gas phase

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경상대학교 화학과

Jet-cooled neutral p-phenetidine (PPE) has been studied using the REMPI and UV-UV hole-burning spectroscopy in the gas phase. PPE as a precursor of phenacetine (PA) has an important intrinsic property for its enormous biological activities in biological systems. The mass-selective REMPI spectrum of the PPE monomer was obtained in the frequency range of 31000-34000 cm^{-1}. The most intense peak at 31587 cm^{-1} was found to be the origin transition of the PPE monomer. We investigated conformational information of the PPE monomer by fixing the pump laser at the origin band and scanning the probe laser (using the UV-UV hole-burning technique). We have also calculated the optimized structures of the PPE monomer by density functional theory (DFT) with a 6-311++G** basis set. Further discussion on the structures of the PPE monomer and its fluorescence lifetime will be presented in this poster

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Spectroscopic Study of Jet-cooled Indole-3-carbinol by Laser Desorption Technique: Franck-Condon Simulations and Anharmonic Calculations

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경상대학교 화학과

The conformational structure of indole-3-carbinol (I3C) has been investigated in the gas phase for the first time using a laser desorption technique. A UV-UV hole-burning technique revealed the presence of a single conformer of I3C in the mass-selected resonant two-photon ionization spectrum. The assignment of the observed IR spectrum of I3C is inconclusive due to almost identically predicted IR frequencies of the two lowest energy conformers from harmonic calculations. A conclusive assignment for the conformer of I3C has been reported with an aid of performing anharmonic calculations and Franck-Condon simulations on the two lowest-energy conformers.

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Enhanced visible-light photocatalytic activity of AgI nanocrystal with reduced graphene oxide

이승희 **devulapalliamaranathareddy** 최지하 박선화 마로리 양해식 김태규*

부산대학교 화학과

Novel reduced graphene oxide (RGO) enwrapped AgI nanocomposites were successfully fabricated by a facile template-free ultrasound-assisted method at room temperature. The structural, morphological, and optical studies demonstrate that the obtained nanostructures have good crystallinity and that the graphene nanosheets are decorated densely with AgI nanostructures. The photocatalytic activity of the composite was evaluated by the degradation of an organic dye, Rhodamine B (RhB), under visible-light irradiation. The results indicate that AgI with incorporated graphene exhibited much higher photocatalytic activity than the pure AgI due to the improved separation efficiency of the photogenerated carriers and that it prolonged the lifetime of the electron?hole pairs due to the chemical bonding between AgI and graphene. AgI (0.4 mg mL^{-1} of graphene oxide) nanocomposites displayed the highest photocatalytic degradation efficiency and the corresponding catalytic efficiencies within 70 minutes were around 96%. Moreover, with the assistance of H_2O_2 the photocatalytic ability of the as-obtained AgI-RGO nanocomposites was enhanced. The corresponding catalytic efficiencies within 30 minutes were about 96.8% (for 1 mL H_2O_2) under the same conditions. The excellent visible-light photocatalytic efficiency and luminescence properties make the AgI-RGO nanocomposites promising candidates for the removal of organic dyes for water purification.

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Spectroscopic studies of Jet-cooled methacetin and its water complexes in the gas phase

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경상대학교 화학과

Methacetin (MA) is one of the typical synthetic fever reducers as similar to acetaminophen (AAP), a major ingredient of Tylenol$^{?}$. MA and AAP are both derivatives of acetanilide (AA), substituted by methoxyl group and hydroxyl group in the para position of AA, respectively. In this work, we present the conformational investigations and photochemistry of jet-cooled MA 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 MA and its 1:1 hydrates by density functional theory (DFT). Here, we report the structural information of MA and its 1:1 hydrates with an aid of the experimental data and the ab initio calculations.

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Synthesis and Characterization of PbSe Nanoparticles by Pulsed Laser Ablation in Liquid (PLAL)

제민규 최명룡*

경상대학교 화학과

In many other studies, it takes a long time to synthesize PbSe nanoparticles and the processes are complicated. In this study, we present a facile synthesis method for the preparation of PbSe nanoparticles using a pulsed laser ablation in liquid (PLAL). PbSe nanoparticles were synthesized by a two-step method. Firstly, lead salt and selenium salt were used as the lead and selenium source, respectively. Each of the sources dissolves in distilled water with a reducing agent, $NaBH_4$. Then, PbSe nanoparticles were produced by a pulsed Nd:YAG laser (532nm, 10Hz, 7ns) ablation to the Pb and Se mixed solution. The morphological properties of PbSe nanoparticles via PLAL were characterized by X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and transmission electron microscopy.

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Ni-Pd alloy nanoparticles synthesized by pulsed laser ablation in liquid

정현진 최명룡*

경상대학교 화학과

Among various particle fabrication methods, pulsed laser ablation in liquid (PLAL) is currently attracting great interest due to its simplicity and versatility. In this study, a two-step process has been employed for the preparation of the Ni-Pd alloy nanoparticles. In the first step, laser pulses at 1064 nm (7 ns at 10 Hz) of a Nd:YAG system were focused to a 99.99% pure nickel plate placed at the bottom of a cell containing methanol. In the second step, laser irradiation using unfocused second harmonic Nd:YAG laser pulses (532 nm, 7 ns, 10 Hz) was applied to the as synthesized Pd-Ni alloy nanoparticles solutions. The Pd-Ni alloy nanoparticles prepared from PLAL were analyzed by X-ray diffraction measurement, field emission-scanning electron microscopy, transmission electron microscopy, and energy dispersive spectroscope.

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The Electronic Spectroscopic studies of Jet-cooled 5-cyanoindole and Its Water Clusters: IR-dip spectroscopy and Computational Calculation

민아름 문철주 안아름 성연국 최명룡*

경상대학교 화학과

5-cyanoindole (5-CI) as a derivative of indole has found some spectroscopic interest about excited state in the gas phase. In our previous study, we have reported 3-cyanoindole (3-CI) of another indole derivative via the REMPI and UV-UV hole-burning spectroscopic studies in the gas phase experiments. In this study, we have investigated 5-CI monomer and water clusters. For the 5-CI water clusters, their REMPI spectra having a red-shifted origin band compared to that of 5-CI monomer showed a clear identification of the single conformer of 5CI-(H2O)1. And then, we have also calculated the optimized structures of 5-CI monomer and water clusters by density functional theory (DFT). Here report the structural information of 5-CI water clusters by comparing the each IR-dip spectra and those from the theory. Further investigation on the structures of 5-CI and its water clusters will be investigated and discussed by IR dip spectroscopic studies in this poster.

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Green synthesis of Ag@AgI/ZnS microspheres with Enhanced Photocatalytic Activity and selective separation of methylene blue from aqueous solutions

devulapalliamaranathareddy 최지하 이승희 김유진 마로리 김태규*

부산대학교 화학과

A novel heterostructured Ag@AgI/ZnS microsphere have been fabricated through a soft chemical route with the assistance of polyvinylpyrrolidone (PVP). The formation of heterostructured Ag@AgI/ZnS nanocomposites was evident from the detailed morphological and structural analysis by SEM, TEM, XRD, XPS and FTIR analysis. Morphological and microstructural studies revealed that the Ag@AgI/ZnS nanocomposites are built up by tiny Ag, AgI and ZnS nanoparticles. Luminescence quenching in Ag@AgI/ZnS nanocomposites indicates that formation of a hetero-junction between Ag@AgI and ZnS, can effectively accelerate the charge separation and transferred electrons from the AgI to Ag and ZnS nanostructures. The photocatalytic activity was evaluated by the decomposition of dyes rhodamine B (RhB), under simulated sunlight light irradiation. All the Ag@AgI/ZnS heterostructures exhibited enhanced photocatalytic performance than the pure AgI and ZnS nanostructures. Ag@AgI-ZnS (10 wt.%) possesses the optimal photocatalytic degradation efficiency and the best photoelectrochemical performance. The enhanced photocatalytic activity is associated to the effective transfer and separation of photogenerated electron?hole pairs at the interface of Ag@AgI/ZnS nanocomposite due to their matching band positions. Further, the nanocomposites exhibit good photocatalytic stability, almost no loss of photocatalytic activity after five recycles. Moreover, these nanostructures show the best catalytic activity for the selective separation of methylene blue (MB) dye from the mixed dye-wastewater (RhB-MB, MO-MB). It is hoped that this work could promote further interest in fabrication of various heterostructured nanocomposites and their application to sunlight-driven photocatalysts for purifying polluted water resources.

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Spontaneous and Thermally Enhanced Charge Transfer at Graphene-Silica Interface

박광희 류순민*

포항공과대학교(POSTECH) 화학과

Low dimensional carbon materials undergo spontaneous hole doping in the ambient conditions. Thermal annealing enhances the degree of the charge transfer in silica-supported graphene exposed to oxygen and water vapor. In this work, we investigated the mechanisms responsible for the charge transfer using Raman spectroscopy and water contact angle measurements. Mechanically exfoliated graphene samples were annealed at various temperatures in a range of 100 ~ 1000 ^{o}C to induce the hole doping. While the annealing-induced charge density of graphene increased with increasing annealing temperature up to 700 ^{o}C, it decreased as increasing the temperature further higher. Graphene samples prepared in a low humidity condition lead to significantly decreased hole doping suggesting that water contained in the samples plays a key role. We will propose and discuss a charge transfer mechanism that involves thermal hydroxylation and rehydroxylation of silica surfaces.

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Spin-orbit Ab Initio Investigation of Photodissociation of Vinyl Iodide

문지원 김태규[1] 김중한*

가톨릭대학교 화학과 [1]부산대학교 화학과

Potential energy curves (PECs) of the low-lying excited states of vinyl iodide (VI) are calculated using the multiconfigurational spin-orbit ab initio method. The calculated splitting energy between $^2P_{1/2}$ and $^2P_{3/2}$ states at the dissociation limit is in good agreement with the experimental result. The location of the conical intersection where is crucial for the branching ratio is also estimated. On the basis of the calculated results, the correlation with the recent experimental results is briefly discussed.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Understanding the Mutation Effects on FAS1 Domain 4 Related to Protein Aggregation by Molecular Dynamics Simulation

조선희 함시현*

숙명여자대학교 화학과

Mutations of fasciclin 1 domain 4 (FAS1-4) are known to be the cause of phenotypically distinct corneal dystrophies initiated by protein aggregation. Extensive mutation studies have been carried out to identify the aggregation-prone mutations in FAS1-4. However, the structural information and mutation effects for the mutants of this protein at the atomic-level remain elusive. Here, we report structural and thermodynamics characteristics of the wild type FAS1-4 and its two mutants (R555Q and R555W) by using fully atomistic, explicit-water molecular dynamics simulations and the integral-equation theory of liquid. We find that the hydrophobic residues of α4-α5-α6 region are more solvent-exposed upon mutation. A significant decrease in stability in this region is also observed based on the free energy decomposition analysis. The increase in hydrophobic solvent accessible surface area and free energy in the α4-α5-α6 region will facilitate the association of FAS1-4 mutants, and our findings will contribute to understand the molecular mechanisms in FAS1-4 aggregation.

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Molecular Insights into the Fluorescent Probe for the Detection of the Aβ Oligomers: A Computational Study

조선희 함시현*

숙명여자대학교 화학과

Soluble oligomers of amyloid-beta (Aβ) have recently been demonstrated to be more neurotoxic than insoluble deposits related with Alzheimer's disease (AD). Since the chemical and topological characteristics of Aβ oligomers are unknown, the development of the Aβ oligomer-specific sensor has been a great challenge. Here, we represent computational results on the structural and thermodynamics properties of Aβ oligomer-specific fluorescent probe, BoDipy-Oligomer (BD-Oligo) as well as its complex with Aβ oligomer. We performed quantum mechanical calculations followed by a molecular docking and molecular dynamics simulations. The site-directed analysis of binding free energy was also carried out to understand why and how BD-Oligo is an Aβ oligomer-specific sensor. We find the critical role of hydrophobic residues (F19/V36) of Aβ oligomer on detecting BD-Oligo, which may provide insight into the development of AD drugs.

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Influence of D_2O on solubility and adsorption behaviour of surfactants at liquid/solid interface in aqueous solutions of H_2O/D_2O mixture

신태규

한국원자력 연구원 중성자과학연구부

Even though D_2O shows similar phase diagram as H_2O, D_2O has various peculiarities with respect to H_2O in many physico-chemical aspects: D_2O exhibits 4.95 mN/m smaller surface tension than H_2O and some salts are less soluble in D_2O, and the ionic mobility of D^+ and H^+ in D_2O exhibits 67.8% (K^+ and Cl^-, 84.9%) smaller value than in H_2O and so on. All these aspects can be reflected in the adsorption process of surfactants at liquid/solid interface. In this work, the adsorption behaviour of different cationic and nonionic surfactants in mesoporous silica SBA-15 with uniform pore size has been investigated by systematically varying H_2O/D_2O ratio. Results and analysis of Thermogravimetric Analysis and Small-Angle X-Ray/Neutron Scattering experiments will be presented.

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Cesium Exchange into Zeolite Y (Si/Al = 1.56) from High Salt Solution

김후식 문대준 이하영 임우택*

안동대학교 응용화학과

To study the tendency of Cs^+ exchange into zeolite Y (Si/Al = 1.56) dependence on Cs^+ concentration of aqueous solution during exchange, two single-crystals of fully dehydrated, Cs^+-and Na^+-exchanged zeolites Y were prepared by the flow method using a mixed ion-exchange solution whose $CsNO_3$:$NaNO_3$ mole ratios were 1:1 (crystal 1) and 1:100 (crystal 2), respectively, with a total concentration of 0.05 M, followed by vacuum dehydration at 723 K. Their crystals were determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group Fd3- m, respectively, and were refined to the final error indices R_1/wR_2 = 0.084/0.248 and 0.088/0.274 for crystals 1 and 2, respectively. In the structure of $|Sr_{40}Cs_{12}|[Si_{100}Al_{92}O_{384}]$-FAU (crystal 1), 40 Cs^+ ions per unit cell occupy five different equipoints; 3, 3, 14, 9, and 11 are at sites I, II', II, IIIa and IIIb, respectively, whereas, the remaining 35 Na^+ ions occupy three different sites: 9, 11, and 15 are at sites I, I', and II, respectively. In the structure of $|Sr_{29}Cs_{17}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 2), 21 Cs^+ ions per unit cell occupy three equipoints; 4, 6, 2, and 11 are at sites II, IIIa, and IIIb, respectively. The residual 54 Na^+ ions per unit cell are found at three different sites; 6, 20 and 28 are at sites I, I', and II, respectively. The degrees of ion exchange are 53 and 28% for crystals 1and 2, respectively. This result shows that the degree of Cs^+ exchange decreased sharply by decreasing the initial Cs^+ concentration and increasing the initial Na^+ concentration in given ion-exchange solution.

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Improved SERS Sensitivity by Using Hybrid Bilayer Membranes on SERS Substrates

<u>Weidong Ruan</u> 박연주 진실아 **Bing Zhao[1]** 정영미[*]

강원대학교 화학과 [1]State Key Laboratory of Supramolecular Structure and Materials, Jilin University

Surface-enhanced Raman scattering (SERS) has obtained huge attention in the fields of physics, chemistry, biology, and biomedicine. Till now, many metallic nanostructures, such as nanotriangles, nanorods, nanoshells, nanorings, nanocrescents, nanostars and nanoflowers, have proven to be SERS active due to the introduction of hot spots. Various SERS substrates have been fabricated by using e-beam lithography, colloidal lithography, nanoimprint lithography, and templated assembly of nanoparticles (NPs) [1,2].Herein we report a method for the fabrication of efficient SERS substrates by combination of hybrid bilayer membranes (HBMs) and NP films. The HBMs, composed of graphene oxide sheets and hexanethiol monolayers, are used as a novel nanoscale partition layer system on Ag NPs. Thus a new kind of compound SERS substrates is constructed successfully. These newly-designed SERS substrates have good adsorption performance on many probe molecules, such as p-aminothiophenol (PATP), rhodamine 6G (R6G), and 4-mercaptopyridine (4-MPy). Due to this special affinity, the analytical sensitivity of the target molecules is highly improved. Our preliminary work also shows that the biocompatibility of the SERS substrates after the HBM modification is better than the ones with bare modifications. This method might be useful for the future application in detection of biological probe molecules.

Keywords: SERS; substrate; hybrid bilayer membrane

Reference

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Characterization of Thermal Transition of Biodegradable Poly(butylenes adipate)/Poly(ethylene glycol) Blends

<u>Yujing Chen</u> 박연주 Isao Noda[1] 정영미[*]

강원대학교 화학과 [1]Department of Materials Science and Engineering, University of Delaware

Poly(butylene adipate) (PBA) is a biodegradable polymer, which exhibits two types of crystal forms, designated as thermodynamically most stable α- form and kinetically favorable β-form. It has been demonstrated that the α and β PBA crystal exhibit different physical properties and biodegradability. Thus, much attention has been paid to the formation mechanism and phase transition behavior of PBA from its β crystal to α structure[1]. In the present study, we investigated the thermal behavior and crystal transition of pure PBA and its blend with PEG upon heating process by FTIR spectroscopy and different scanning callorimentry (DSC) techniques. In addition, X-ray diffratcion was employed to examine the crystal structure of PBA/PEG blend. To gain further insight into the thermal behavior alteration and the phase transition of PBA with the addition of PEG, we performed 2D correlation analysis[2]. Detail information will be discussed in the presentation.

References

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Change in External Entropy upon Protein-Protein Binding

정성호 함시현*

숙명여자대학교 화학과

The non-covalent association involving biomolecules such as protein-protein, protein-DNA, and protein-ligand binding is of central importance in biology and pharmacology. Methods for computing the binding affinity of those biomolecular processes are therefore of great practical value. However, considerable uncertainty and controversy remains regarding the external entropy change, one of the principal terms constituting the binding constant, which is associated with the reduction in external (translational and rotational) degrees of freedom upon binding. Here, we present a statistical-thermodynamic method for computing the external entropy, which is an extension of the energetic approach we recently developed for unimolecular processes such as protein folding to association processes. The result of an application of this method to the external entropy change upon barnase-barstar complex formation will be presented.

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SERS biosensor using Au aggregates core-shell nanoparticles

진실아 박연주 **Weidong Ruan** 정영미*

강원대학교 화학과

Surface enhanced Raman scattering (SERS) based immunoassay has been extensively studied due to its high sensitivity and fingerprint information of molecules. In this study, SERS tag which is combining Raman reporter-labeled Au aggregates on a SERS-active immune substrate was prepared. Au aggregates-4-Mercaptobenzoic acid (4-MBA)@SiO_2 core-shell nanoparticles functionalized antibody were used for detecting thymine DNA glycosylase (TDG). Details of SERS spectra of TDG will be discussed.

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2D correlation analysis of thermal denaturation of HAMLET

김예슬 박연주 Bogusława Czarnik-Matusewicz1[1] 정영미[*]

강원대학교 화학과 [1]Faculty of Chemistry, University of Wroctaw, Poland

The intermediate state of α-lactalbumin (ALA) has an ability to form with oleic acid (OA) the complex, which is named, HAMLET (human α-lactalbumin made lethal to tumor cells). HAMLET possesses cytotoxic activity with respect to tumor. In this study, principal component analysis (PCA) and 2D correlation spectroscopy were applied to the temperature-induced FTIR spectra of ALA/OA complex to investigate the thermal denaturation of ALA/OA complex. Details of this results will be discussed in this presentation.

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The Stuctural and Electronic Properties of of CuO_n (n = 1 - 6) Clusters and their Water Reaction Effect using *Ab Initio* Monte Carlo Simulations

<u>배균택</u>

충북대학교 사범대학 화학교육과

Copper oxide nanoparticles are particularly effective catalysts for the formation of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) and other pollutants. *Ab initio* Monte Carlo simulations and density functional calculations are used to study the structural and electronic properties of copper oxide clusters, CuO_n (n = 1 ? 6) and their reactions with a single water molecule. All lowest energy structures of CuO_n and CuO_n-water clusters with n = 1 - 6 are optimized with the B3LYP functional and aug-cc-pVDZ basis set. We found that the lowest structures of CuO_n clusters with n = 1 - 6 are planar or near planar. Selected electronic properties including binding energies, ionization energies, electron affinities, second different energies, and Bader charges are calculated and examined of n.

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Hyperporphyrin Effects in the Spectroscopy of *Meso*-Bis(thiophenylethynyl)porphyrin Diacids

김준우 심상덕* 이석중[1]

순천대학교 화학과 [1]고려대학교 화학과

Porphyrins are of significant interest for a range of materials applications, including solar energy conversion, photodynamic therapy and light harvesting. However, the narrow absorption profiles of porphyrins limit their use in many photophysical applications; typical synthetic porphyrins such as *meso*-tetraphenylporphyrin (H_2TPP) constitutes an intense B band around 400 nm and less weaker Q bands in the region between 500 and 700 nm. Therefore, extension of the absorption spectra into the red and near-infrared region provides significant benefits for those application. Under appropriate conditions the UV-Vis spectrum of a porphyrin diacid bearing highly electron-donating substituents shows a split B band along with greatly enhanced, red-shifted absorption beyond where the Q bands usually end. These so-called "hyperporphyrin effects" are ascribed to charge transfer between the peripheral substituent and the porphyrin macrocycle. However, the nature of unusual spectra and the effect of structural change induced by protonation are still open question. To address these questions, we have carried out spectrophotometric titrations for several non-amino-substituted porphyrins with ethynyl spacers, *meso*-thiophenyethynyllporphyrins.

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Metal-enhanced fluorescence of rhodamine B on silver coated surfaces

송승민 조한국* 정병서*

인천대학교 화학과

We have studied metal-enhanced fluorescence (MEF) of rhodamine B to better understand metal-fluorophore interactions on metallic silver nanoparticles. The effects of different silver nanostructures on enhanced fluorescence properties were investigated using silver-island film or silver colloid coated surfaces. We employed rhodamine B molecules dispersed in poly(vinyl alcohol) or poly(methyl methacrylate) polymer matrices in order to control the distance between fluorophore and metal nanoparticles by varying the concentration of polymers. Variations of spectral properties as well as fluorescence enhancement were observed depending on the types of silver nanostructure and polymer film, and we discuss possible explanation of our findings.

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Femtosecond Rebinding Dynamics of Nitric Oxide to Iron Porphyrin Ring in Glycerol-Methanol Mixture

이태곤 이소현 박영상 김효준[1] 임만호[*]

부산대학교 화학과 [1]동아대학교 화학과

Iron porphyrin ring (FePPIX) and microperoxidase (MP) is a good model to investigate the reaction characteristics of the heme free from conformational change and protein structure. Femtosecond pump-probe spectroscopy was used to study the rebinding dynamics of carbon monoxide (CO) and nitric oxide (NO) to the heme model after photolysis of MpCO and MpNO with 0.1 mM to avoid aggregation in glycerol/water mixture. The geminate rebinding (GR) kinetics of photodeligated CO was different at various viscosity which was controlled by changing the glycerol volume ratio, but NO wasn't. Most of deligated NO rebinds to heme within 11 ps and almost similar in 18, 81, and 252 cP. Diffusion-controlled model or SRC model was used to explain the GR of CO, but two models are mixed in the GR of NO because of electron transfers from Mp to NO. We found that FePPIX doesn't aggregate even though its concentration is 8 mM when 1-methylimidazole (1-MeIm) is used as a proximal histidine and solvent. Moreover, 70% of photodeligated NO rebinds to Mp within 7 ps in 1-MeIm/methanol mixture and 30% doesn't rebind until 1 ns. To investigate solvent effect, we observed the GR of NO to (1-MeIm)FePPIX at various glycerol/methanol mixtures. Biexponential equation, $S(t)=A_1\cdot exp(-t/\tau_1)+A_2\cdot exp(-t/\tau_2)$ is used to calculated rebinding kinetics. The yield of fast rebinding component is increased and showed faster decays as viscosity increases.

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Elimination of Biofilm by Photo-induced Reactive Oxygen Species Generated from the Surface of Photofuctional Metal Alloy

허일 LIJING 송유진 심진회 신언필 왕강균 김용록*

연세대학교 화학과

The hospital strains may form the biofilm on the medical device which causes infection to the patient[1]. Therefore, the removal of the biofilm has actively been studied with physical and/or chemical treatments[2, 3]. In this study, reactive oxygen species (ROS) were utilized for the removal of the biofilm for the first time. The photofunctional metal alloy was fabricated for the generation of ROS. Photocatalytic effect of the photofunctional metal alloy was confirmed and the elimination of gram-negative and -positive biofilms was successfully demonstrated with the ROS generating metal alloy system. We believe that the photofunctional metal alloy has a great potential for the practical application in biomedical field.Reference1. Van der Borden, A.J., et al., Biomaterials, 2007. 28(12): p. 2122-2126.2. Denes, A.R., et al., Journal of Applied Polymer Science, 2001. 81(14): p. 3425-3438.3. Hequet, A., et al., Colloids and Surfaces B-Biointerfaces, 2011. 84(2): p. 301-309

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Design of Edge Terminated Ferromagnetic Graphene Nanoribbons: Doping Effect

남연식 조대흠 SHIHU 이진용*

성균관대학교 화학과

The intramolecular magnetic exchange coupling of doped zigzag graphene nanoribbon (ZGNR) edge terminated by diradical was studied with density functional theory calculations employing PBE functional. We investigated the effect of doping(B, N) on magnetic behaviors of pristine zigzag graphene nanoribbon with 8 zigzag chains (8ZGNR), 8ZGNRs terminated with trimethylenemethane (TMM) and 6-oxoverdazyl (OVER) radicals, i.e., TMM-ZGNR-TMM (TZT), OVER-ZGNR-OVER (OZO), and TMM-ZGNR-OVER (TZO) on its edges. As a result, TZT and OZO which have same radical on its edge respectively showed the same magnetic behavior: B or N doping at one edge showed ferromagnetic behavior while B and N doping at each edge shoed antiferromagnetic behavior. In case of TZO, however, which has different radical on its each edge showed opposite magnetic behavior: B or N doping on one edge showed antiferromagnetic behavior, while B and N doping at each edge showed ferromagnetic behavior.This magnetic behavoir depends on the number of unpaired p-electron on each edge. The same number of unpaired electron on each edge induces antiferromagetism while different number of unpaired electron induces ferromagetism. Also, doping on edge, terminated with TMM radical, increased magnetic coupling while edge with OVER radical decreased magnetic coupling. This changing magnitude of coupling was determined by resonance in radicals.

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Rebinding Dynamics of Oxymyoglobin and Oxyhemoglobin

박성철 박재홍[1] 신주향 임만호[*]

부산대학교 화학과 [1](주)코오롱 중앙기술원 분석평가센터

Time-resolved vibrational spectroscopy was used to investigate the photoexcitation dynamics of O_2-bound heme proteins in D_2O by probing the O-O stretch band in the time range from femtosecond to microsecond after excitation with a 575-nm pulse at 293K. Since the weak O-O stretch band is overlapped with the strong absorption bands in the 1200 ~ 1000 cm-1 region by water solvent, protein, and buffer molecule, difference time-resolved spectra (heme$^{16}O_2$ - heme$^{18}O_2$) were obtained to delineate O_2-related bands from the absorption changes due to conformational and thermal relaxation. In the early picosecond time scale, the fundamental bands of oxymyoglobin (MbO_2) and oxyhemoglobin (HbO_2) shift to lower frequency, showing a broadened absorption band, which decays on a 2.7 ps. After subtracting this contribution from the broadband absorption, the remaining bleaching bands decay with the same kinetics and were described by two (three) exponential functions plus an equation describing bimolecular reaction for MbO_2 (HbO_2). The recovered time constants for the exponential function were 6.7 ps (21%) and 36 ns (14%) for MbO_2 and were 2.1 ps (21%), 410 ps (13%), and 8 ns (6%) for HbO_2. The bimolecular rate constant of MbO_2 was $16 \times 10^6\ M^{-1}s^{-1}$ (12%) and HbO_2 was $90 \times 10^6\ M^{-1}s^{-1}$ (1%). The 2.7 ps decay of the broadened absorption band was attributed to thermal relaxation of six-coordinate heme subsequent to fast electronic relaxation without photodeligation. The cooling process for the six-coordinate heme group can be observed due to anharmonic coupling of low frequency modes with the observed O_2 stretching mode. We take the 6.7 ps (2.1 ps) decay of the MbO_2 (HbO_2) to be either partially or completely due to geminate recombination (GR) of O_2 after photodeligation. The 36 ns decay of the MbO_2 and 410 ps, 8 ns of the HbO_2 were attributed to GR of O_2 after photodeligation. When photoexcited in the Q-band, about 25~46% of MbO_2 undergoes photodeligation (quantum yield, QY = 0.25~0.46), about 25~46% of the deligated O_2 geminately rebinds in time constants of 6.7 ps and 36 ns, and the remaining O_2 escapes into solvent and bimolecularly rebinds with the rate constant of $16 \times 10^6\ M^{-1}s^{-1}$.

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 heme-O_2 suggest that the O_2 binding characteristics is independent of conformational substates of heme-O_2.

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Droplet Oscillation with Wide Range of Viscosities in DC Electrowetting

<u>채희도</u> 백승휘 권오선[1,*] 신관우[2,*]

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

With different concentrations of poly ethylene glycol(PEG), we made various viscosities and conditions of aqueous PEG solution. Herein we checked the viscosities and initial dimensions of droplet with the wide range as well as contact angles. As well known, applying the voltage to the droplet makes a very fast spreading and oscillation while the wetting phenomenon which is called electrowetting. We measured changes of dimensions, speeds of spreading, contact angle changes of droplets and it is plotted versus viscosities. We found the intimate relationship between viscosities and these parameters. This has a huge possibility for replacement of existing measurement methods of viscosity which has weak point for measuring a small scale and low viscous sample.

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Excited-state intramolecular proton transfer of dihydroxyanthraquinones studied by time-resolved absorption and emission measurements

이세복 장태형[1] 방윤수*

광주과학기술원(GIST) 물리화학부 [1]광주과학기술원(GIST) 화학과

Excited state intramolecular proton transfer (ESIPT) has been of great interest in chemistry and biology since it can be used in many applications including fluorescent molecular probes, chemosensors, molecular logic gates, and white-light emitting materials. Upon photoexcitation, the proton transfer can occur with a change of molecular geometry, and the dual emission from the locally excited and the proton-transferred states might be observed. The excited state dynamics related to the ESIPT might provide an important key in understanding the chemical reaction dynamics in many chemical and biological systems. In this work, dihydroxyanthraquinone (DHAQ) and its derivatives were used to study the ESIPT by transient absorption spectroscopy. The emission of DHAQ was strongly dependent on solvent polarities and excitation wavelengths. To further study the ESIPT of DHAQ depending on environmental properties, absorption and emission of DHAQ in AOT reverse micelles were also studied by steady-state and time-resolved absorption and emission measurements. Photophysical properties of DHAQ in AOT reverse micelles showed strong dependence on the size of reverse micelles, which might also be affected by the orientation dynamics of DHAQ molecules in the confined geometry.

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Oxidation of Alcohol Catalyzed by Dispersed Ruthenium Incorporated Titanium Oxides

김영용 권기영*

경상대학교 화학과

Ruthenium incorporated titanium oxides (Ru_x/TiO_2) are synthesized by one step hydrothermal method using $Ti(SO_4)_2$ and $RuCl_3$ as the sources of Titanium and Ruthenium, respectively. XRD, TEM, EDS mapping analyses confirm that ruthenium atoms are well dispersed in the anatase phase of TiO_2 and the size of crystallite of Ru_x/TiO_2 is smaller than that of pure TiO_2. The samples exhibit high reactivity and selectivity without formation of any byproduct for oxidation of benzyl alcohol into benzaldehyde using oxidant. Under N_2 condition not using any oxidant, benzaldehyde are produced with high selectivity for the oxidation of benzyl alcohol. The crystallites aggregate each other to change into crystal phase of rutile with the size of approximately bigger than 140 nm by after annealing $Ru_{0.07}/TiO_2$ at 700 oC for 6 hr. The annealed sample appears the formation of RuO_2 crystallites which are embedded in TiO_2 with phase segregation, and results in the decrease of catalytic activity for organic oxidation reactions.

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은 나노 구조체를 도입한 수산화인회석(HAP)의 촉매 활성 연구

표은지 권기영*

경상대학교 화학과

수산화인회석(Hydroxyapatite)는 칼슘과 인산염으로 구성된 무기물이다. 수산화인회석에 이온교환반응을 통하여 은 나노 입자를 도입한 뒤 다양한 농도의 $NaBH_4$ (0, 0.01, 0.1, 1, 10, 100 mM)로 은을 환원시켜 촉매를 합성한다. 합성한 촉매를 XRD(X-ray diffraction spectroscopy)와 TEM(Transmission Electron Microscope)을 통하여 촉매의 구조를 분석하였다. 합성한 촉매를 이용하여 다양한 종류의 알코올 류 (Benzyl alcohol, Cinnamyl alcohol, 1-Phenyl ethanol, 1-Octanol) 산화반응에 촉매 활성을 조사하였다. 두 가지의 전이금속이 도입 된 HAP 를 기반으로 하는 이동상 촉매를 또한 합성하였고, 이를 Methylene blue 분해반응에 응용하여 촉매활성을 조사였다.

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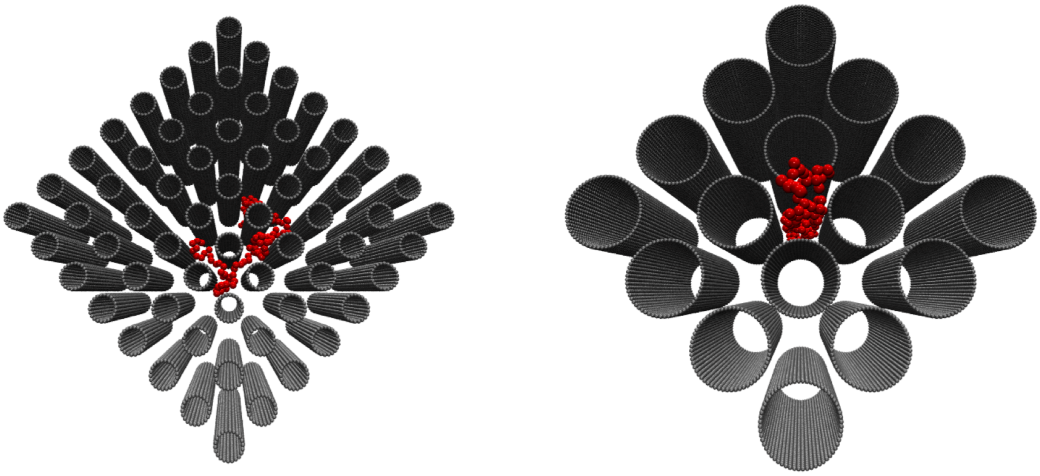
Conformation of a single polymer chain in a dense array of nanoposts

주희선 김준수*

이화여자대학교 화학나노과학과

Control of polymer conformations in heterogeneous confinement plays an important role in natural and engineering processes. We present a simulation study on the conformational structure and dynamics of a single, flexible polymer in a dense array of nanoposts with different sizes and separations. When a polymer is placed in the array of nanoposts, the size of polymer increases and polymer becomes elongated compared with that in the absence of nanoposts due to the confinement effect. As the interstitial volume between four nanoposts decreases either by increasing the nanopost diameter or by decreasing the separation between nanoposts, the chain elongation becomes more pronounced. On the contrary, the polymer size varies in a non-monotonic fashion, with an initial elongation followed by a chain contraction, as the interstitial volume decreases while keeping constant the width of the passageway between two nanoposts. The simulation analysis shows that the non-monotonic dependence of polymer size is determined by interplay between the chain alignment along the nanoposts in each interstitial volume and the chain spreading through passageways over several interstitial volume. This study suggests the possibility of utilizing a dense array of nanoposts as a template to control polymer conformations.



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은 나노 입자를 도입한 단결정 수산화인회석의 합성과 촉매 활성 연구

성홍규 권기영*

경상대학교 화학과

본 연구에서 지지체로 사용된 단결정 형태의 수산화인회석(Hydroxyapatite)은 칼슘과 인산염으로 구성된 무기물이다. 단결정 수산화인회석은 염기 조건 (10 M NaOH)에서 수열합성법 (Hydrothermal method)을 이용하여 합성하였다. 합성된 단결정 수산화인회석의 표면에 이온 교환 반응을 통하여 은 원자를 도입하였으며, 환원제 (0.01 M NaBH4)를 이용하여 은 원자를 은 나노 입자로 변화시켰다. 합성된 샘플은 XRD, TEM 분석을 통하여, 일정한 모양과 크기의 은 나노 입자가 형성된 것을 확인하였다. 합성된 샘플을 유기 반응 촉매로 사용하여 여러 가지 알코올 (1 차, 2 차 알코올)의 산화 반응에 응용하였다. 또한 UV-Visble light 영역에서의 오염물 분해 반응에 광촉매로서 적용하였다.

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Defocused differential interference contrast microscopy imaging of single plasmonic anisotropic nanoparticles

김연오 하지원*

울산대학교 화학과

We present the defocused differential interference contrast (DIC) imaging of gold nanorods. We found that the scattered light and the defocus aberration play an important role in the formation of orientation-dependent DIC image patterns of a gold nanorod (AuNR). Interestingly, the scattered light from a gold nanorod aligned closer to the polarization directions enables us to directly resolve its spatial orientation under a defocused DIC microscope.

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Synthesis, characterization, and photocatalytic applications of reduced graphene oxide supported copper oxides nanoparticles

오하나 박준범[1,*]

전북대학교 생리활성소재과학과 [1]전북대학교 화학교육과

Copper oxides have been widely used in various applications including photo-catalysts, antifouling paint, p-type semiconductor, and artificial coloring. Graphene is a well-known supporting material due to its large surface area, high chemical stability, and excellent thermal and electrical conductivity. In this study, we have synthesized reduced graphene oxide (RGO) supported metallic copper nanoparticles (NPs) (Cu/RGO) and copper oxide NPs (Cu_2O/RGO and CuO/RGO) by impregnation combined with thermal treatment method. The morphological and chemical structures of the as-prepared copper oxide nanocomposites were characterized using XRD, XPS, TEM, and XAFS, and their catalytic performance in photocatalytic degradation of dye molecules have been investigated. It has been found that CuO/RGO show a significant enhancement in the photo-catalytic activity compared with Cu/RGO and Cu_2O/RGO. Such excellent catalytic performance of CuO/RGO could be attributed to the synergistic effects of RGO, CuO, and H_2O_2. Further detailed decomposition mechanism will be discussed.

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ONIOM Investigation of Reaction Mechanism of Graphene Fluorination by XeF_2

백희현 문지원 김중한*

가톨릭대학교 화학과

Fluorographene is a fluorocarbon derivative of graphene which is unsaturated (sp^2 hybridized) two dimensional carbon sheet. With each carbon atom bound to one fluorine, all carbons are saturated and hybridization state is changed to sp^3. We clarify the reaction mechanism of graphene fluorination by XeF_2 using ONIOM(QM:QM) calculations. In addition, we found optimal theoretical level of low layer in ONIOM(QM:QM) calculations by comparing those results with the results of full density functional theory (DFT) calculations.

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Charge Transfer Mechanism Study of Polymer/PC$_{[70]}$BM Bulk heterojunction Films and Implications for Organic Photovoltaics

손지원 주태하*

포항공과대학교(POSTECH) 화학과

Organic photovoltaic (OPV) devices have advantages of low cost, light weight, flexibility and large area device applications by solution processing. In order to improve the PCE of OPV devices, understanding their mechanism is very important. However, there is still a need to explore the OPV materials in atomistic way and explain the underlying mechanism behind it. In this study, we investigated the effects of bridge central atoms of polymer molecule based on DT-fDTB polymers used as donor material, and PC[70]BM is used as acceptor material. The central chalcogen atom was changed in the polymer and femtosecond transient absorption experiment with 100 fs time resolution was tried in order to see the excited state population dynamics of blends. Chalcogen heteroatom blends of S and Se shows better PCE than O blend. We fitted the data kinetically with different rate constants, signifying various processes such as charge formation, separation and recombination occurring at different time scale and combined with time-resolved fluorescence data for measuring charge transfer states specifically. The measured kinetics shows intensity dependence in S and Se blends, while intensity independence in O blend. The results shows inefficient charge transfer in O blend compared to S and Se blend and is affected by geminate recombination which were started quite early. In case of other two blends, S is least affected by geminate recombination and has an efficient charge transfer therefore exhibits higher PCE. Also, Se blend shows better charge separation and least non-geminate recombination, but its larger size increases the charge densities in the blend due to its more interaction with PC[70]BM domains which later on were responsible for geminate recombination.

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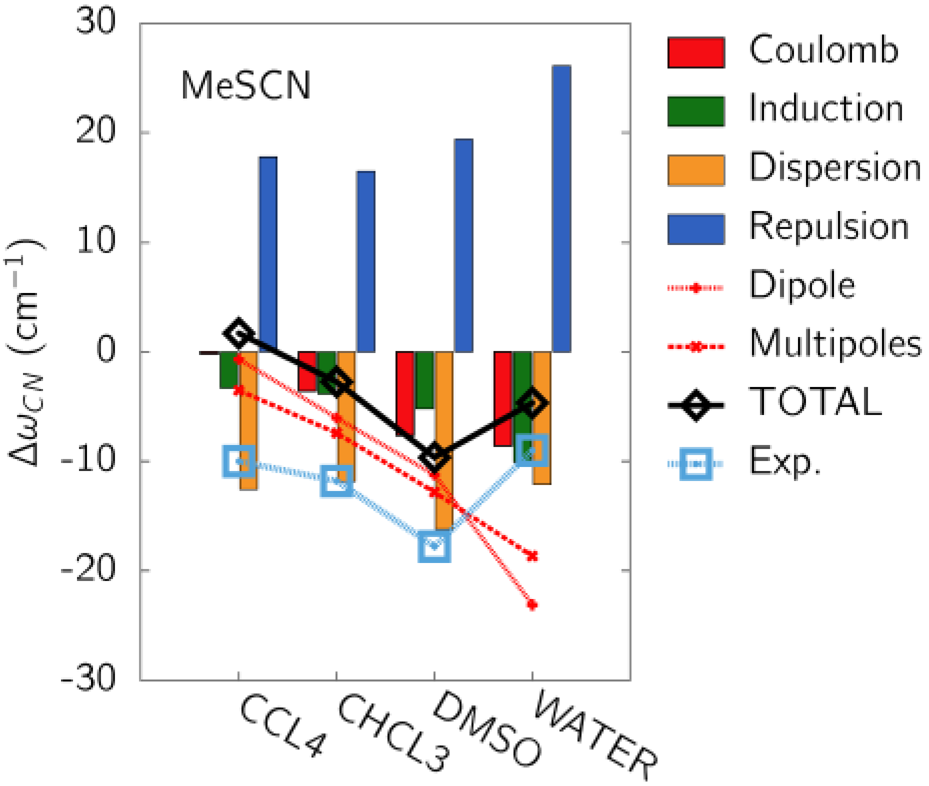
Vibrational solvatochromism from first principles - new insights

BLASIAK BARTOSZ 조민행*

고려대학교 화학과

Many simple semi-empirical models of vibrational solvatochromism reported so far were able to successfully describe, in some special cases, the vibrational response of small infrared probes due to external environment. However, modeling the effects of intermolecular interactions on the vibrational frequencies is challenging because they are quantum mechanical in nature. In fact, the existing models are generally not acceptable in some important cases because they are strictly electrostatic. Throughout the recent years, we have been developing the rigorous first-principles theory of vibrational solvatochromism of spatially localized infrared probes that are the reporters of the nearest molecular environments, and can provide crucial information about the structure and dynamics of biomolecules. In this presentation, we discuss the capability of our approach to reproduce experimental frequency shifts of model IR probes. In particular, we explain the observed breakdown of electrostatic models applied to nitrile stretch vibrational modes in H-bonding environments. We also provide the scope of further development and possible limitations of our method.


MeSCN
30
20
10
0
-10
-20
-30
Δω_CN (cm⁻¹)
CCL4
CHCL3
DMSO
WATER
Coulomb
Induction
Dispersion
Repulsion
Dipole
Multipoles
TOTAL
Exp.

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Synthesis and catalytic applications of graphene oxide supported manganese oxide (MnO, Mn_3O_4 and MnO_2), nanoparticles

이설희 박준범[1,*]

전북대학교 화학교육 [1]전북대학교 화학교육과

In this study, we have developed a straightforward synthetic route to prepare graphene (G) based manganese oxides (MnO/G, Mn_3O_4/G, and MnO_2/G) by controlling gas environment during thermal treatments. The preparation method involves (a) preparation of graphite oxide (GO) from graphite, (b) impregnation of Mn^{2+} precursor on GO, and (c) precise thermal treatment of Mn^{2+}/G in H_2, Ar, and air environment to produce specific MnO_x/G. The analyses of XRD, TEM, IR, and XPS data clearly demonstrate the formation of crystalline MnO, Mn_3O_4, and MnO_2 NPs on graphene. The prepared MnO_x NPs showed not only uniform size distribution but also fine dispersion on the graphene. Finally, the catalytic reactivity of the prepared MnO_x/G has been investigated in oxidation reaction of alkylaromatics to ketones and the final product ensures a new platform of MnO_x/G nanocomposites in the oxidation reaction.

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Molecular dynamics simulations of antimicrobial peptides in Gram-positive and Gram-negative bacterial membrane model

이아영 황현석*

강원대학교 화학과

Due to its potential antibiotic properties, antimicrobial peptides (AMPs) have drawn much attention. In this study, we have used molecular dynamics (MD) simulations to investigate the interaction of small AMPs with phospholipid bilayer membranes. For this purpose, DMPC/DMPG and POPE/POPG bilayers were prepared to mimic Gram-positive and Gram-negative bacterial membranes such as Staphylococcus aureus and Escherichia coli. A series of MD simulations for an AMP with or without proline, which was placed above the lipid bilayers, were performed. The insertion mechanism of the AMP through lipid bilayers was characterized by calculating the center-of-mass distribution of hydrophobic/hydrophilic part of the AMPs, secondary structure distribution, and lipid order parameter in the absence or presence of the AMPs.

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Conformational dynamics of D816 Mutations in c-KIT Receptor; Action mechanism of Inhibitors

김철희 김은애*

조선대학교 약학과

Various cancers are caused by a variety of specific amino acid mutated in the c-KIT tyrosine kinase. The c-KIT supervises many signal transduction pathways such as STAT3, MAPK, and PI3K and represents a typical allosterically regulated protein. In particular, D816(V/H/N/Y) mutations of the active binding site have drug resistance for Imatinib and then drug discovery for cancer has been a hot research area and a big challenge. In our mutation study, we modeled the D816 mutants based on X-ray structure of wild-type (PDB ID:1T45) and ran the molecular dynamics (MD) simulations at the physiological temperature. Also, we compared the binding mode of the mutants with inactive c-KIT/Imatinib complex (PDB ID:1T46) using the docking simulation. We will discuss the structural change of the mutants in the active site and the drug inhibition mechanism of imatinib and dasatinib.

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Adsorptions and Reaction Mechanisms of Amines on Ice Surface

Shoaib Mahbubul alam 최철호[1,*]

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Theoretical calculations have been carried out regarding the adsorption and reaction mechanism of ammonia (NH3), Methylamine (CH3NH2), Dimethylamine ((CH3)2NH) on ice surface with the help of B3LYP/6-31++G(d)//HF/6-31G(d) basis set using our QM/EFP scheme. The binding energies of amines are studied on different adsorption sites (H0, H1 and H2 site for neutral ice surface). It was found that H1 site yields the higher adsorption energies for amines compare to other adsorption site. Also adsorption of amines and proton transfer reaction from ice surface to amines was investigated on protonated H1 ice surface adsorption site. In the case of ammonia, low energy barrier (3.1 kcal/mol) was found for proton transfer reaction from ice surface to the adsorbate.

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Photoinduced Nonadiabatic Quantum Molecular Dynamics

<u>RashidMdAlMamunur</u> **최철호**[1,*]

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Dimethylnitramine, as one of the simplest compounds in the nitramine family, which attracted broad research interest in the energetic materials sector, has been used in the investigation of the unimolecular decomposition mechanism. To understand how chemical energy converts to the mechanical energy in the energetic materials, the photoinduced excited-state nonadiabatic processes and successive unimolecular dissociation of dimethylnitramine were investigated using ab initio calculation. Within 100 femtosecond, around 50% of the trajectories jumped from upper electronic state (S1) to ground electronic state (S0). Conical intersection was found to play an essential role for the ultrafast internal conversion from S1 state to S0 state in the initial steps of the decomposition of dimethylnitramine. Pyramidalization/bending motion of N-NO2 moiety are associated with the surface hopping followed by dissociation dynamics of dimethylnitramine. Some reaction channels may be accountable for decay features. Dimethylnitramine may either generate an NO2 product through an N-N bond fission mechanism or generate an NO product through a nitro-nitrile isomerization mechanism.

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Binding features of Δ-, Λ-[Ru(phen)2DPPZ]$^{2+}$ with G-quadruplex DNA

박진하 이영애 김석규*

영남대학교 화학과

Ruthenium complexes are widely used to investigate interactions with nucleic acids, but only weak selectivity between G-quadruplexes has been observed up to now. In this study, we used Δ-, Λ-$[Ru(phen)_2DPPZ]^2$+ in order to explore the interaction of that Ru-complex with human telomeric DNA, 5´-$G_2T_2G_2TGTG_2T_2G_2$-3´(15-mer). To compare the DNA binding of Δ-, Λ-$[Ru(phen)_2DPPZ]^{2+}$ for G-quadruplex and duplex DNA(Calf-Thymus DNA), Fluoresence emission, UV absorption, melting and CD measurements have been performed. The well-known enhancement of luminescence(the 'light-switch' effect) exhibited by when Δ-$[Ru(phen)_2DPPZ]^{2+}$ interaction with CT-DNA, approximately 8-times bigger than the Λ-isomer. In the presence of the G-quadruplexe, whereas, observed Λ-$[Ru(phen)_2DPPZ]^{2+}$ (K_b = 1.07 x 106 M^{-1}) binds approximately 3-fold higher than the Δ-isomer (K_b = 3.80 x 105 M^{-1}) case. From the job plot for G-quadruplex with Δ-, Λ-$[Ru(phen)_2DPPZ]^{2+}$, major inflection point for two isomers, at x = 0.65 was observed. These data are consistent with the binding mode at a [G-quadruplex]/[complex] ratio of 1:2. When bound to CT-DNA, meanwhile, x = 0.15 and 0.3 for Δ and Λ ? isomer were obtained, respectively. Corresponding to our results, The binding affinity and binding mode are seems to quite different between G-quadruplex and duplex DNA. One of isomer may binds at the lateral loop or under the diagonal loop or stacking on the external of G-quadruplex at the 5′-end or vice versa. The structural information and enantioselective binding mode for G-quadruplex are still unclear by this study.

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Spectroscopic Studies on the Interaction of DNA with Ru(II) Complexes

Hasi Rani

영남대학교 화학과

A series of mononuclear ruthenium(II) complexes have been prepared and their binding affinities toward double stranded native DNA was investigated by means of absorption spectroscopy, polarized light spectroscopy including circular and linear dichroism (CD and LD), fluorescence quenching and DNA thermal denaturation techniques. The complexes produce LD signal consisting of positive and negative signal in the absorption region upon binding to DNA although these complexes exhibited red-shift and hypochromism in the absorption spectrum. These contrasting observations indicated that the binding modes of the complexes are largely deviated from classical intercalative binding. These results suggest that the binding nature of the complexes to DNA is liable over an intercalative mode of binding to DNA. The small increase of DNA melting temperature in the presence of the complex indicates predominantly DNA groove binding propensity of the complexes. Absence of "molecular light switch effect" indeed further supports non-intercalative binding mode with DNA for the new complexes. This conclusion is also supported by the comparison of the resulting data with the $[Ru(phen)_3]^{2+}$. This study demonstrated the importance of the structure of bridging moiety in the intercalation of the Ru(II) complex.

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Behavior of guanine base into various DNA form

한지훈 이영애 황윤모 장윤정[1] 김석규[*]

영남대학교 화학과 [1]영남대학교 기초교육대학

Behavior of guanine base into single strand DNA and Quadruplex of G3, 5'$G_3T_2G_3TGTG_3T_2G_3$, was investigated by being replaced with 6-methylisoxanthopterin (6MI) as a conformational probe. The guanine (G) base at 10, 13 and 19th positions was replaced with 6MI. Under the same condition, relatively differences in the absorbance and fluorescence region of 6MI suggest that adjacent 6MI may have affect on the base to base interaction. Fluorescence decay curve was shown that all single strand DNAs have three components although 6MI nucleoside have an one components, which means that 6MI containing single strand DNA was reflected by adjacent 6MI bases. In contrast, various components were obtained in the case of quadruplex due to change of 6MI position when quadruplex is formed. It also can be aware of this fact that Anisotropy decay profiles are significantly different between single strand DNA and Quadruplex. The quenching and fast fluorescence decay study is under investigation.

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Binding properties of TMPyP with *calf thymus*-DNA induced by Molecular crowding

김영란 이영애 김석규*

영남대학교 화학과

Under the Molecular crowding, *meso*-tetrakis(*N*-methyl pyridinium-4-yl)porphyrin (TMPyP) with *calf thymus*-DNA(CT-DNA) complex produced different linear dichroism spectrum when forming the complex in aqueous buffer conditions. LD signal in the soret band region are much smaller than that of the CT-DNA LD value and shown different spectral change to our previous work. The angles calculated from LD were respectively 43.6° and 44.3° for B_x and B_y transitions of the porphyrin with respect to the local helix axis of the TMPyP-DNA complex in the presence of PEG. The range of angle 43.6° ~ 44.3°, may suggesting that the TMPyP molecular plane was tilted relative to the DNA helix axis under cell mimic conditions. Or it may suggest that the binding geometry of TMPyP to CT-DNA is not a canonical intercalative site. Under the PEG, hypochromism and red shift much less than aqueous buffer conditions. These may indicate that the interactions or binding characteristics of TMPyP with CT-DNA complex under different reaction buffer systems. Owing to be kept the experimental conditions of PEG were 37.5% (w/v) against to total reaction volume, we do not any longer focus on the conformational change of DNA helical structure induced by over amount of crowed media at this stage.

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Destabilization of RecA proteins by divalent cations

김래영 원아름 김석규*

영남대학교 화학과

RecA protein is widely known that DNA strand exchange reaction between single-stranded DNA (ss-DNA) and homologous double stranded DNA (ds-DNA). DNA strand exchange reaction required ATPase and higher concentration magnesium. In order to understand RecA protein structure by magnesium, we are investigated thermal profile using Circular Dichroism at 222nm. The addition of divalent ions did not affect the secondary structure of protein according to the CD measurement. Whereas, thermal profile of RecA protein was destabilized as increasing magnesium concentration. It was similar to thermal profile of RecA without the C-terminal tails. It may suggest that negative charged C-terminal tails interact with positive charge magnesium. The concentration of divalent ions required for destabilized protein was similar to that required to DNA strand exchange reaction. These results suggested that the divalent cation facilitate large conformational change in the protein, which may be required for the DNA strand exchange reaction.

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Length and sequence effect on the B-Z transition of $[d(A\text{-}T)]_n$ oligonucleotide induced by a cationic porphyrin

신종헌 황윤모 장윤정[1] 김석규[*]

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Trans-bis(*N*-methylpyrodinium-4-yl)diphenyl porphyrin induced the B-Z transition for alternated AT oligonucleotides as it was evident by inversed circular dichroism spectrum. Complete B-Z transition required at least 14 base-pairs long and [porphyrin]/[DNA base] ratio of 0.28. Insertion of one or two GC base pairs prevented the B-Z transition. No other polynucleotides including poly$[d(G\text{-}C)_2]$, poly(dA)·poly(dT), and poly(dG)·poly(dC), underwent the B-Z transition under similar conditions. The longer in oligonucleotide length resulted in slower the transition. This transition conceivably occurs from the end of oligonucleotide

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Study of ROS selective effects on Gram type bacteria with non-uptake condition of photosensitizer

심진희 왕강균 김봉진 황정욱 정승진 김용록*

연세대학교 화학과

Reactive oxygen species (ROS) have been extensive studied in chemical, environmental and medical fields due to their unique physicochemical properties and highly reactive nature. ROS induce both positive and negative effects by the involvement with metabolism of cells and organs due to the highly active reactivity and selectivity.1 In the bio medical science, there are many applications of ROS such as photodynamic cancer therapy, control of cell cycle, sterilization, and pest exterminations.2-5 The photophysical factors determining the efficiency of ROS generation has been investigated. In particular, the photo-induced ROS production initially consists of two different types (O2- and 1O2). The nature and functionality of the two critical species are distinctively examined. Based on the study results, the fabrication strategy of the photofunctional polymers which generate ROS is established for wide medical and environmental applications. The fabricated polymers are shown along with their excellent photo-induced functionalities for the photodynamic inactivation of various bacteria under non-uptake condition of photosensitizers.Reference(1) Ogilby, P. R. Chem. Soc. Rev. 2010, 39, 3181(2) Choudhary, S.; Nouri, K.; Elsaie, M. L. Lasers Med. Sci. 2009, 24, 971(3) Oh, H.-C.; Wo, J.-H. Kor. J. Pesti. Sci. 2011, 15, 87(4) Catherine, G.; Liam, D.; Plants Physiol. 2006, 141, 341(5) Floriane, L.; Angelique, B.-B.; Jean-Pierre, M.; PLoS Pathogens 2011, 7, 1

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Formation of Poly[d(A-T)$_2$] Specific Z-DNA by a Cationic Porphyrin

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Typical CD spectrum of the right-handed poly[d(A-T)$_2$] was reversed when *trans*-bis(N-methylpyrimidium-4-yl)diphenyl porphyrin (*trans*-BMPyP) was bound, suggesting that the helicity of the polynucleotide was reversed to the left-handed form. The formation of the left-handed Z-form poly[d(A-T)$_2$] was confirmed by ^{31}P-NMR, in which a single ^{31}P-peak of B-form poly[d(A-T)$_2$] was split into two peaks, which is similar to the conventional B-Z transition of poly[d(G-C) $_2$] induced by the high ionic strength. The observed B-Z transition is unique for poly[d(A-T)$_2$]. The other polynucleotides, including poly[d(G-C)$_2$], poly(dG)·poly(dC) and poly(dA)·poly(dT) remained as the right-handed form in the presence of the same porphyrin. This observation suggests that the porphyrin array that was formed along the poly[d(A-T)$_2$] provides a template to which left-handed poly[d(A-T)$_2$] is associated with an electrostatic interaction.

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Conformational isomers of isobutanal by vacuum ultraviolet mass-analyzed threshold ionization spectroscopy

이유란 김경은[1] 김명화[1] 김홍래 권찬호[*]

강원대학교 화학과 [1]이화여자대학교 화학 나노과학과

Conformational isomers, trans and gauche, of isobutanal were investigated by utilizing the high-resolution vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. The VUV-MATI spectra of isobutanal were measured by varying the supersonic expansion condition with He and Ar carrier gases to explore the conformational preference. Some peaks with different conformational cooling efficiency were displayed in the measured VUV-MATI spectra. All of vibrational peaks observed in the spectra could be nearly completely assigned by utilizing Franck-Condon analyses for each conformational isomer of isobutanal performed at the B3LYP/cc-pVTZ level. Consequently, it was found that trans and gauche isomers undergo their unique geometrical changes upon ionization and hence, have accurate adiabatic ionization energies of 78137 ± 6 cm^{-1} (9.6878 ± 0.0007 eV) and 78557 ± 6 cm^{-1} (9.7398 ± 0.0007 eV), respectively.References(1) J. H. Kim, J. H. Lee, H. Hwang, H. L. Kim, and C. H. Kwon, Phys. Chem. Chem. Phys. 16, 1590 (2014).(2) Y. R. Lee, D. W. Kang, H. L. Kim, and C. H. Kwon, J. Chem. Phys. 141, 174303 (2014).

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VUV generation in the 10.4 and 11.2 eV region by nonresonant four wave sum-frequency mixing in Kr and Xe

강도원 김홍래* 권찬호*

강원대학교 화학과

Generation of coherent and tunable vacuum ultraviolet (VUV) radiation has been mainly accomplished by utilizing resonant four wave sum and difference-frequency mixing (FWSM, FWDM) due to high conversion efficiency. FWSM and FWDM are commonly utilized in nonlinear medium such as rare gases rather than metal vapors because of easy handling. The most efficient gas is krypton or xenon, although it is difficult to generate the VUV in the 10.4 and 11.6 eV region. The VUV generation in this region was reported by R. Wallenstein et al. They generated the VUV radiation in that region by utilizing nonresonant sum-frequency mixing in xenon and krypton. This method has the advantage of use only a dye laser. Therefore, we adopted the FWSM in Kr and Xe cell to generate the VUV pulse in the range of 10.4 eV ~ 11.2 eV, with two dye lasers for the UV and VIS due to much higher conversion efficiency in the VUV generation.

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Reduction of 4,4’-dinitrobiphenyl on metal surface in acidic condition : SERS and DFT studies

이진철 엄소영 김홍래 권찬호*

강원대학교 화학과

We investigated the reduction of 4,4’-dinitrobiphenyl (DNBP) adsorbed on silver surface under various pH conditions using the surface-enhanced Raman scattering (SERS) spectroscopy. Silver surfaces such as high sensitive SERS substrate were systematically synthesized by using citrate as reduction agent. The observed SERS spectra could be definitely analyzed comparing with the density functional theory (DFT) calculations performed for the simple model. SERS spectrum of DNBP could be measured in only the acidic condition. It is found that the SERS spectrum of DNBP in the acidic condition well agreed with the SERS one of 4-amino-4’-nitrobiphenyl (ANBP) in the same condition. The spectral features displayed in the SERS spectra of DNBP according to the change from the acidic to the basic are same to the ones in the SERS spectra of ANBP and indicate that the DNBP on silver surface was reduced to ANBP under the acidic condition.

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Photodissociation dynamics of HN_3 at 205 nm : H + N_3 channel

박성만 윤상혁 권찬호* 김홍래*

강원대학교 화학과

Photodissociation dynamics of H atom formation channels from HN_3 (hydrogen azide or hydrazoic acid) at 205 nm has been investigated by laser-induced fluorescence spectrum of H. The measured Doppler broadened H atom spectrum was similar to the previously measured at 193 nm dissociation. At 248 nm, the fast dissociation takes place in the first excited singlet state of HN_3. However, the dissociation mechanism has not been exactly identified. We have performed quantum chemical calculations to construct potential energy surfaces to explain the detailed dissociation mechanism.

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Molecular Dynamics of Photo-induced Singlet Oxygen in Solid Phase

황정욱 왕강규 LIJING 심진희 신언필 송유진 김용록*

연세대학교 화학과

The photo-induced reactive oxygen species (ROS) initially consist of two types of oxygen molecules such as super oxide anion and singlet oxygen. Super oxide anion and singlet oxygen were generated through charge transfer process (Type I reaction) and energy transfer process (type II reaction) respectively.1 Among the two species, singlet oxygen has been studied for the purpose of bio-medical applications such as photodynamic therapy (PDT)2, sterilization3 . Although such investigations have widely been performed in many fields of researches, the quantitative and/or qualitative studies of singlet oxygen dynamics in solid phase have not been performed in details. In this study, we investigated the molecular dynamics of singlet oxygen in solid phase by using chemical reactions and near IR time-resolved spectroscopy. The results discuss various interesting and important aspects of singlet oxygen dynamics in solid phase.

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The constitution of nanostructures of Zinc oxide synthesized of microwave technique: Study of their antibacterial activity

이유로 김재욱 유정열 김종규*

단국대학교 화학과

ZnO-synthesized by microwave method was investigated. The products were prepared using zinc nitrate hexahydrate, ammonia solution and water. By adjusting the concentration of Zn2+ in the aqueous precursors, different morphologies of ZnO microstructures were obtained. The formation of oxide compound has been confirmed by X-ray powder diffraction (XRD), Field emission scanning electron microscope (FE-SEM), X-ray photoelectron spectrometer (XPS) and Infra-red spectrometer (IR). Antibacterial activity of ZnO was evaluated against Staphylococcus aureus (S.aureus) Gram-positive and Escherichia coli (E. coli) Gram-negative microorgnisms.

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Structural and Thermodynamic Study on the Binding Affinity of three Cyclic Naphthalene Diimides to G-quadruplex DNA

이진경 함시현*

숙명여자대학교 화학과

Specific guanine-rich regions in human genome called G-quadruplexes are of recent biological interest since they regulate a number of biological processes relevant to cellular functions. Developing small molecules that bind and stabilize the telomeric G-quadruplexes is an attractive strategy for specific anticancer agents. Cyclic naphthalene diimide (CND) is among such ligands, which exhibits greater affinity to G-quadruplex DNA than to a double stranded oligonucleotide. Here we investigate molecular origin on the binding affinity of cyclic naphthalene diimide toward G-quadruplex DNA by performing quantum mechanical calculations and molecular dynamics simulations. The effect of ions (Na+, K+) upon complexation in water is also quantified by the solvation free energy calculations based on the integral-equation theory. Thereby, we discuss the binding preference and the effect of solvent upon complexation between CND and G-quadruplex DNA.

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Theoretical Study on the Reduction Mechanism of CO_2 Catalyzed by $ZnCl_2$

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The reaction mechanism on the reduction of CO_2 in the presence of *N*-methylaniline and $PhSiH_3$ catalyzed by $ZnCl_2$ was studied by the density functional theory at the M05-2X[(SMD,CH_2Cl_2) 6-311++G(d,p)//M06-2X/6-31G(d) level. The calculations show that an initial catalytic formylation of the *N*-methylaniline using CO_2 followed by the 6 electron reduction of the carbamic acid intermediate is adopted for the formation of methylation product, which is energetically more favorable than the pathway involving the formation of the formoxysilane and methoxysilane species via the hydrosilylation of CO_2 with $PhSiH_3$. The rate determining step for the uncatalyzed reaction was the hydrosilation of CO_2 with $PhSiH_3$ but that for catalyzed reaction was the formylation of the *N*-methylaniline with CO_2. With respect to the uncatalyzed reaction, the energy barrier for the rate determining step is lowered from 41.7 to 34.6 kcal mol^{-1}, indicating that the simple zinc catalyst exhibits a good catalytic performance in the titled reaction.

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The nano/microstructures of ZnO synthesized by a simple way of microwave method and their photocatalyst activity

정상화 장연재 김재욱 유정열 이유로 김종규*

단국대학교 화학과

We report the nano/microstructures of ZnO powders were synthesised via microwave technique. The products were prepared using Zinc nitrate hexahydrate, sodium hydroxide in the aqueous. The variation of morphologies has been considered by influence of different concentration of sodium hydroxide solution and also it was changed by between zinc species and hydroxyl group. In this current study, the effects of reaction on the product morphology as well as crystallization mechanism were examined by using X-ray diffraction (XRD), scanning electron microscopy (SEM), Infra-red spectrometer (IR) and X-ray photoelectron spectrometer (XPS). The photocatalytic activity of both nanostructures has been examined by the degradation of Rhodamin B using UV light (253.7 nm).

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Preparation and Structural study of Fully Dehydrated Partially Zn^{2+}-exchanged Zeolite Y (FAU, Si/Al = 1.56)

문대준 김후식 이하영 임우택*

안동대학교 응용화학과

Four single crystals of fully dehydrated and partially Zn^{2+}-exchanged zeolites Y (Si/Al = 1.56) were prepared by the static ion-exchange method using a mixed ion-exchange solution in which $Zn(NO_3)_2$: NaCl mole ratios were 1 : 1 (crystal 1), 1 : 25 (crystal 2), 1 : 50 (crystal 3), and 1 : 100 (crystal 4), respectively, with a total concentration of 0.05 M, and followed by vacuum dehydration at 673 K. Their single-crystal structures were determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group Fd-3m and refined to the final error indices R_1/wR_2 = 0.0459/0.1454, 0.0449/0.1283, 0.0427/0.1284, and 0.0486/0.1680, respectively. Their unit-cell formulas are $|Zn_{25}Na_{25}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 1), $|Zn_{19.5}Na_{36}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 2), $|Zn_{19.5}Na_{36}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 3), and $|Zn_7Na_{61}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 4), respectively. The degree of Zn^{2+} exchange decreases from 62.9% to 18.9% as the initial concentration of Zn^{2+} decrease and the initial concentration of Na^+ increases in given ion-exchange solutions.

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Investigation of Dependence of Exchange of Cs+ and Na+ into Zeolite A (LTA) from Various Concentrations of Exchange Solution

이하영 김후식 문대준 임우택*

안동대학교 응용화학과

To study the tendency of $Cs^+$and Na^+ exchange into zeolite A, three single-crystals of fully dehydrated Cs^+ and Na^+ exchanged zeolite A were prepared by the static ion-exchange method using a mixed ion-exchange solution whose $CsNO_3$:$NaNO_3$ mole ratios were 1:11 (crystal 1), 1:2 (crystal 2) and 2:1 (crystal 3), respectively, with a total concentration of 0.1 M, followed by vacuum dehydration at 623 K and 1.33 × 10^{-4} Pa. Their structures were refined to the final error indices R_1/wR_2 = 0.0577/0.1555, 0.0575/0.1822 and 0.0496/0.1465 for crystals 1, 2, and 3, respectively. In the structure of $|Cs_2Na_{10}|[Si_{12}Al_{12}O_{48}]$-LTA (crystal 1), 2 Cs^+ ions per unit cell occupy large cavity, whereas, the remaining 10 Na^+ ions occupy sodalite unit. In the structure of $|Cs_{3.5}Na_{8.5}|[Si_{12}Al_{12}O_{48}]$-LTA (crystal 2), 3.5 Cs^+ ions per unit cell are located in the large cavity. 8.5 Na^+ ions are located in the sodalite unit and large cavity. In the structure of $|Cs_{4.5}Na_{7.5}|[Si_{12}Al_{12}O_{48}]$-LTA(crystal 3), 4.5 Cs^+ ions per unit cell occupy located in the large cavity and sodalite unit. 7.5 Na^+ ions per unit cell occupy are located in the sodalite unit. This result shows that the degree of Cs^+ exchange increased by increasing the initial Cs^+ concentration and decreasing the initial Na^+ concentration in given ion-exchange solution.

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Molecular Engineering of Metal-Free Dyes for Dye Sensitized Solar Cells

김동희* **<u>ESTRELLA LIEZEL</u>** **이상희** **Mannix Balanay[1]**

군산대학교 화학과 [1]Nazarbayev Univ. 화학과

To date, metal-free organic dyes are among the highly considered sensitizers for DSSC owing to their minimal environmental complications, low costs, ease of modification, and tunable optical properties compensating to high efficiency. In this study, a series of triarylamine-based dyes were designed after a known reference dye by systematically modifying the π-linker and donor moiety. The absorption spectra, electronic properties and energy gaps for these dyes were predicted using the density functional theory (DFT) and its Time-dependent counterpart (TD) methods. Also, key parameters of the dyes adsorbed on TiO2 surface related to short-circuit current (Jsc) and open circuit voltage (Voc) were evaluated. The simulated UV-vis absorption spectra shows the significant bathochromic shift as a result of planarization of the donor and π-linker moieties. Further improvement of the light-harvesting property of the dyes was observed upon incorporating auxiliary donor group. Moreover, the calculated ground-state and excited-state oxidation potentials signifies that efficient electron injection and dye-regeneration are energetically favored for all dyes. The results obtained in this study are expected to provide valuable insights for future molecular dye designs for DSSC applications.

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Formation mechanism of interfacial electronic structures between π-conjugated molecules and Au(111)

박선미 정재훈*

울산대학교 화학과

Understanding interfacial electronic and geometric structures at organic-metal contacts formed by the van der Waals (vdW) interactions is of great importance in organic electronic and photovoltaic devices [1]. The atomically-resolved scanning tunneling microscopy (STM) experiment combined to density functional theory (DFT) calculations recently revealed that a π-conjugated hydrocarbon (π-CHC) molecule, dehydrobenzo[12]annulene, can have a specific adsorption configuration, even on the noble Au surface [2]. The computational results proposed that the interfacial orbital interaction between a π-CHC molecule and the Au surface can play a decisive role in constraining adsorption orientation even in the typical weak vdW adsorption system. Herein, we perform periodic vdW density functional (vdW-DF) calculations in order to elucidate the more detailed formation mechanism of interfacial electronic and geometric structures between an isolated π-conjugated molecule and Au surface. We found that the interfacial electronic structures were formed in a way to maximize the interfacial orbital interaction through processes of interlocking-dragging-splitting induced by the local splitting of the Au d state due to electronic coupling with the molecular π-state. We believe that our results provide not only deeper insight into the formation mechanism of interfacial electronic and geometric structures in weak adsorption process but also new perspectives to organic electronics using π-CHC molecules on the Au electrodes.

1.H. Ishii, K. Sugiyama, E. Ito, and K. Seki, Adv. Mater. 11, 605 (1999); C.-a. Di, Y. Liu, G. Yu, and D. Zhu, Acc. Chem. Res. 42, 1573 (2009).
2.J.-H. Kim, J. Jung, K. Tahara, Y. Tobe, Y. Kim, and M. Kawai, J. Chem. Phys. 140, 074709 (2014).

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Charge transfer between an atomic gold and K-intercalated graphite

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울산대학교 화학과

The phenomenon of charge transfer is an essential process to reach the equilibrium of charge distribution at the interface, and thus considerable efforts have been devoted to understand it for controlling the chemical and physical properties of various potential materials, such as catalyst, sensors, molecular devices, and so forth. Charge transfer leading to ionized characters in a system, especially on a solid surface, is of great importance in tuning the chemical reactivity of heterogeneous catalyst. Negatively charged Au nanoparticle adsorbed on a defective MgO/Mo(100) or on an ultrathin MgO/Ag(100) through charge transfer was reported to result in the red shift of CO stretching mode, compared to on the neutral one adsorbed on bulk MgO [1]. K-intercalated graphite (K-Gr) can be a good candidate for studying the influence of charge transfer on the chemical reactivity of adsorbate because the higher charge carriers than the pure graphite (Gr) are induced at the surface due to the inserted potassium. Here, we investigate the effect of charge transfer on the adsorption properties of CO on both Au/K-Gr and Au/Gr using periodic density functional theory (DFT) calculations. We expect that our computational results provide deeper insights into the control of chemical reactivity through charge transfer in designing new catalytic system.

[1] X. Lin, B. Yang, H.-M. Benia, P. Myrach, M. Yulikov, A. Aumer, M. A. Brown, M. Sterrer, O. Bondarchuk, E. Kieseritzky, J. Rocker, T. Risse, H.-J. Gao, N. Nilius, and H.-J. Freund, J. Am. Chem. Soc. 132, 7745 (2010).

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STAP2: Refinement database of NMR structures with data expansion and new functionality

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과학기술연합대학원대학교(UST) 생명정보학과 [1]한국생명공학연구원 생명정보센터

STAP is a database of refined NMR structures obtained from the PDB. Since the first version release in 2011, STAP1 contains 2,405 NMR structures refined by statistical torsion angle potential and NOE distance restraint. Here, we present the new version of STAP (http://psb.kobic.re.kr/stap2). The STAP2 now includes more expanded data set (10,583 structures; most of NMR structures in PDB), a newly-developed refinement method, and various structural analyses. In STAP2, the flat-bottom distance potential is newly employed to refine the NMR structure with statistical torsion angle potential. This potential is useful when the NOE restraints are not available. It plays a role to prevent the structural dislocation during the refinement instead of NOE distance restraint. From the viewpoint of statistical analyses for STAP2, four quality scores (steric clash score, MolProbity and WHAT_CHECK Ramachandran plot appearances, and second packing generation packing quality) are significantly improved, and other seven protein-like scores become slightly improved in comparison with initial NMR structures. Furthermore, when we compared our results to well-known refinement databases (DRESS and RECOORD), the Ramachandran indicators and WHAT_CHECK structure z-score distribution are improved substantially. Moreover, the STAP2 provides more various information about the refined structures. The search table contains information of general properties and database information such as PubMed, CATH, SCOP, and experimental information. The main result page provides various analyses for refined structures: (i) the interactive structural visualization through 3D structure and secondary structure, (ii) the numerical/graphical protein-like scores as 'Structural Scores' table and intuitive radar charts in X-ray and NMR structural quality spaces, (iii) another molecular quality viewer by MolProbity, and (iv) functional domain information investigated by other related databases. Additionally, STAP2 provides mobile page to search refined information conveniently.

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Molecular Design of Tetraphenyl-Benzidine Derivatives as Hole Transport Material for Perovskite Solar Cells

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군산대학교 화학과 [1]Nazarbayev Univ. 화학과

Since its emergence in 2009, perovskite solar cell (PSC) has already achieved a confirmed PCE of 20.1%. The lower cost and high efficiency of PSC makes it a promising opponent of the commercially available silicon based solar cells. Spiro-OMeTAD, the widely used hole transport material (HTM), impedes the development of PSC due to its high cost and low performance in its pristine form. The search for an alternative inexpensive HTM with high hole mobility and proper HOMO levels is in urgent need to commercialize PSC. Recently, undoped carbazole substituted tetraphenyl-benzidine were used as HTM in perovskite solar cells and it shows comparable performance to spiro-OMeTAD. With the intention of designing potential HTM, we investigate the properties of the asymmetrically and symmetrically substituted tetraphenyl-benzidine derivatives. The HOMO level of the tetraphenyl-benzidine derivatives were accurately determined using density functional theory. Absorption spectra and electrochemical properties of the derivatives were also investigated.

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1차전이금속들의 메탈로센의 전자친화도의 밀도범함수 계산

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경북대학교 응용화학과

레독스 흐름전지는 에너지 저장장치로 많은 주목을 받고 있다. 전이금속 화합물은 레독스 흐름전지의 전기활물질로 사용하는 경우가 있다. 성능이 우수한 전기활물질의 선정하기 위하여, 전이금속 화합물의 산화환원쌍의 표준환원전위를 이용하기도 한다. 양이온 화학종의 환원전위의 계산에는 산화환원쌍의 이온화에너지와 용매화 에너지가 필요하고, 중성 및 음이온 화학종의 환원전위계산에는 전자친화도와 용매화 에너지의 차이가 필요하다. 이들 에너지들은 보통 밀도범함수 계산으로 얻을 수 있으며, 계산결과의 정확성은 계산에 이용하는 밀도범함수와 기본조함수에 따라 다르다. 본 연구에서는 다양한 밀도범함수를 이용하여 1 차전이금속들의 메탈로센들의 전자친화도를 계산하고, 계산값들을 실험값들과 비교하여, 전이금속화합물의 전자친화도 계산에서 밀도범함수의 성능을 평가하였다.

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Reaction Mechanisms of Proton Catalyzed Formaldehyde Hydration in Aqueous Solution

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Reaction mechanisms of proton catalyzed formaldehyde hydration in aqueous solution has been investigated by the quantum mechanical molecular dynamics simulation study. Both step-wise and concerted mechanisms were found for the proton catalyzed formaldehyde hydration in aqueous solution. However, the concerted path is more favorable contradicting the notion of forming a reactive intermediate by initial protonation. Although acid certainly has a catalytic effect on the free energy barrier, however, the trimolecular transition state of concerted path implies the importance of collision frequencies in a particular configuration. In this regard, the fast diffusion of hydronium into the reacting region with formaldehyde can be another important factor for its catalytic effect. Therefore, the increased reaction rate by acid can be better viewed as a combined effect of thermodynamic effect and the fast kinetic diffusion. In terms of transition state structure, a perpendicularly approaching direction between nucleophile and hydronium is found due to the reactant-like transition structure. It was also found that a dipole bound between formaldehyde and water nucleophile plays an important role.

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Computational Studies of Saccharide Absorption in Carbon Nanotube

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광운대학교 화학과

Saccharides as renewable energy sources have recently been a topic of active research because they are abundant, small, handy, and cost-effective. A typical example is the glucose fuel cell using catalytic enzymes. Although it shows high sensitivity and selectivity, the enzyme-catalyzed fuel cell requires sophisticated control over temperature, pH, and humidity because of its instability on the electrode. To solve this instability problem, noble metal porous electrodes have recently been introduced for the replacement of enzyme-based electrodes and tested for various saccharides such as glucose, sucrose, and cyclodextrins (cyclic oligo-saccharide). In one of experimental studies, it was observed that the current density which is normalized by the active area of electrode depends on both porosity and saccharide species. For example, while glucose and sucrose show weak dependence of current density on the porosity, cyclodextrin shows non-monotonic behavior as the porosity is increased. In order to understand this interesting phenomenon on a molecular level, we calculated the free energy profile during the process of saccharide adsorption in carbon nanotubes using atomistic molecular dynamic (MD) simulations of three different saccharides (glucose, sucrose, and gamma-cyclodextrin) and carbon nanotubes with various diameters. We observed that the adsorption free energy is mainly driven by dehydration penalty of saccharide as well as van der Waals attraction between saccharide and nanotube.

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SERS investigation of the first kinetic step in 4-nitrobenzenethiol photo-reduction

이강섭 최한규 신현항 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

By monitoring the spectral changes in surface-enhanced Raman scattering (SERS) spectra, we observe the initial photo-reduction step in the plasmon-assisted reduction of 4-nitrobenzenethiol (NBT). The Ag nanoparticle (AgNP)-NBTs-Au thin film (AuTF) junction is excited with laser at 632.8 nm wavelength, and we observe that the ν_{NO} SERS peak of NBT shows a red-shift (~10 cm^{-1}) prior to the appearance of the SERS peaks of product (DMAB). The peak could be decomposed into two components, which we assign as the peaks of NBT and NBT-. The electro-chemical SERS measurement and *ab initio* quantum chemical calculations are further carried out to support our assignment.

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SERS investigation of mode-specific vibrational excitation of organic molecules by plasmonic hot-electrons

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We investigate the vibrational excitation of molecules by plasmonic hot electrons using the surface-enhanced Raman scattering (SERS) spectroscopy. The individual 80 nm silver nanoparticle (AgNP) ? organic molecule ? gold thin film (AuTF, thickness : 10 nm) junction was illuminated by a laser (wavelength of 632.8 nm) to generate hot electrons and to monitor in real-time (20 ms) the Stokes and anti-Stokes SERS spectra of the 1,4-benzenedithiol (BDT), 4-methybenzenethiol (MBT), biphenyl-1,4-dithiol (BPDT), and biphenyl-4-thiol (BPT). By comparing the intensities of Stokes and anti-Stokes peaks of each vibrational mode, we discovered that the molecules that form covalent bridges to the metals (BDT and BPDT) show intermittent yet preferential excitation of a specific vibrational modes, whereas such selectivity is significantly reduced for MBT and BPT, strongly suggesting that the plasmonic hot electrons flow through the molecules and vibrationally excite specific vibrational modes via the vibronic coupling.

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Tip-Enhanced Near-field Spectroscopy with a nanostar particle probe

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To overcome the current limit of tip-enhanced spectroscopy that is based on metallic nano-probes, we have developed a new scanning probe with a metallic nanostar, the metallic nanoparticle with sharp spikes. We find that nearly all of the tips show the local field enhancement (up to 100 fold) for tip-enhanced Raman scattering (TERS) and tip-enhanced fluorescence (TEF) was confirmed. The current probe, however, exhibits large tip-to-tip variability, which may arise from the uncontrolled orientation of the apexes of the nanostar particle with respect to the sample surface, which calls for the further fabrication improvement. The result overall demonstrates a new probe fabrication that is effective for tip-enhanced spectroscopy.

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Infrared Nanoscopy Study on Bernal-stacked and twisted bilayer graphenes

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The bilayer graphene, generated by chemical vapor deposition method, show both Bernal (AB)-stcked domain and twisted bilayer structures. We employ the scattering-type scanning near-field optical microscopy (sSNOM) in visible and infrared wavelength to directly map out the distribution of the two domains. Through the wavelength-dependent sSNOM imaging and tip-sample near-field coupling model, we further obtain the information of band structures of each crystal structures.

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Evidence of Dissolution of Semi-conductor Nanocrystals in Organic Solvent: impacts on the formation mechanism of CdSe/ZnS Quantum Dot

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Through the optical spectroscopy, medium energy ion scattering (MEIS) spectroscopy, mass-spectrometry, and simulation, we have obtained evidences that strongly suggest that the CdSe/ZnS semiconductor nanocrystals (SNCs), which are synthesized CdSe/ZnS SNCs by seed-growth method, are dissolved to organic solvents. The dissolved SNCs appear to form small clusters, and such dissolution leads to the alloying at the interface between CdSe and ZnS, influencing their electronic band structures.

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Optimal active site model for quantum calculation of enzyme-substrate binding energy using counterpoise correction utility

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Estimation of enzyme-substrate binding energy is essential in drug design application of quantum chemistry. Within the static enzyme structure model, only the substrate molecule geometry is optimized docked in the active site which is relatively small region embedded in the whole enzyme molecule. To achieve computational efficiency, often limited number of peptide fragments are selected to model the active site surrounding the substrate molecule, and subsequently providing force field during optimizing substrate molecule geometry in quantum calculation. In this work, we use counterpoise correction utility in Gaussian calculation package and estimate the contribution of specific peptide fragment to the overall binding energy by comparing the calculation results obtained from bigger and smaller models of active sites. This method is tested to the previously studied Pim protein kinase-indole derivative complexes.

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Surface-enhanced Raman spectroscopy with spherical and triangular gold nanoparticles

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Surface-enhanced Raman spectroscopy (SERS) is an effective tool to study vibrational aspects of molecules adsorbed on noble metal surfaces. The strong Raman enhancement originates from the local electric field enlarged by the surface plasmons and the charge-transfer process between the metal and adsorbates. In this work, spherical gold nanoparticles for SERS were synthesized by using borohydride and citrate ions as reducing agents. Gold nanoparticles in triangular shaped were also synthesized by the lemongrass leaf extract. We found two consistent surface adsorption geometries of tryptophan and dipeptides containing tryptophan which adsorb on the spherical gold nanoparticle. With citrate-reduced gold colloids, tryptophan mainly adsorb via protonated amine group whereas the ? electrons of indole ring is preferred site for surface adsorption with borohydride-reduced gold colloids. pH dependent SERS spectra were also measured to understand the changes in adsorption geometry, which was confirmed by the DFT results.

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Water hydrogen-bonding network structure and dynamics at phospholipid multibilayer surface: Femtosecond mid-IR pump-probe spectroscopy

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고려대학교 화학과

One of the main components of the biological membrane is lipid. The lipid molecules spontaneously self-assemble into bilayers in aqueous environment. In fact, water molecules around the polar head groups of lipid molecules at the membrane surface strongly affect on a variety of membrane properties, both structural and functional activities of the membrane. For example, water-lipid interaction strengths are closely related to the membrane fluidity. The membrane fluidity of the gel phase is different from that of the liquid crystal phase, which suggest that the lipid-water interaction at the gel phase is different from that of the liquid crystal phase. Due to the underlying complexity of real biological membranes, we considered a phospholipid multilayer as a model biological membrane and studied water hydrogen bonding network structure and dynamics at different phases of the phospholipid multilayer by using femtosecond mid-IR pump-probe measurement method with HDO infrared probe.

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Langmuir-Blodgett Monolayers of Carborane-Poly(ethylene glycol) complexes

김선혜 유정주 이정욱 김효신 손대원*

한양대학교 화학과

Carboranes have a high content of ^{10}B atoms with the highest neutron capture cross section among all light elements. Such a unique property makes them a perfect potential candidate for boron neutron capture therapy (BNCT). Low water solubility is disadvantage when using carborane to BNCT. So solubility problem can be solved by connecting each carborane with Polyethylene glycol (PEG). This research used four different molecular weights of PEG (Mwt. 6000, 5010, 3800, 500). Carborane-PEG at the air-water interface and its Langmuir-Blodgett (LB) films were investigated by using surface pressure area isotherm and atomic force microscope (AFM). Surface pressure area isotherms show that Carborane-PEG has different limiting area according to the molecular weight of Carborane-PEG. AFM images also show the close-packed arrangement for the higher concentration of PEG. Carborane-PEGs make small domains, ~0.011μm^2 at the low pressure. As the surface pressure increases, the domains are aggregated and make large domains, ~0.18μm^2.

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Building a Multi-photon Fluorescence Microscope

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With few exceptions, biological samples strongly scatter light, prohibiting conventional microscopy from obtaining high spatial-resolution deep tissue images for them. Instead, multi-photon fluorescence microscopy is a useful tool for whole cell imaging and in-vivo tissue imaging, especially neuron because it uses light in near-infrared region that provides deep penetration depth.. Morover, its small excitation volume enables optical sectioning for 3D image reconstruction.In this poster we are reporting the recent progress in our lab of multi-photon microscope build-up. The home-build microscope is composed of a tunable high-power Ti:Sapphire oscillator, galvo scanning mirror, a motorized linear stage for z-axis scanning, and a PMT detector. The apparatus is controlled via custom software written in LabView. Signals are digitized and analyzed in Matlab. It shows lateral and axial resolution of xxx nm and xxx nm, respectively. It takes xx mintues to take an image of 512x512 pixels. Currently we investigate 3D the oxidative stress distribution in a live cell with the probe of ROS generation, CM-H2DCFDA. Three-photon fluorescence image can also be acquired on the same microscope setup. .

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REMD simulations to probe the melting temperature of the ice I_h

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경북대학교 화학과

An efficient parallel implementation of replica-exchange mol. dynamics (REMD) was suggested by employing the generalized distributed data interface (GDDI). A REMD simulation of water system has been performed in order to study the melting point of ice Ih. The results of REMD method are very robust ensemble which is able to sample both low and high energy configurations. We report the calculation of the liquid-gas phase transition of ice Ih at 1bar by using three different water models, i.e. TIP5P, EFP1, and EFP2. We set the 16 replica from 257K to 287K range of temperatures with interval of 2K. Each replica is simulated in the NPT ensemble. The melting temperatures at atmospheric pressure for the ice can be found 271K and 273K with TIP5P/MD and EFP1/MD, respectively.

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Developing a New Magneto-sensitive Fluorophore by Manipulating Chain Linker between Electron Donor and Acceptor

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In recent research Lee et al used intramolecular fluorescent exciplex of a magneto-sensitive fluorophore, Phen-(CH2)12-O-(CH2)2-DMA to visualize the magnetic field around nanostructures. [Nano Lett. 11 5367 (2011)] Its fluorescence intensity is increased by up to 80 % at 0.1 T of external magnetic field, which is call magnetic field effect (MFE). The sensitivity to the external magnetic field can be explained by the suppression of the intersystem crossing (ISC) of spin-correlated radical pair generated by photo-induced electron transfer (PET) from DMA to Phen* with UV absorption (355 nm). Such a high MFE is anticipated to long spin-correlation time kept by the chain that holds the proximity between the electron donor and acceptor. However, for better magnetic field images, biological application and simpler optical setup we need to develop new magneto-sensitive fluorophores having higher sensitivity to the magnetic field, higher water solubility and Vis excitation wavelength. In this poster we present our effort to synthesize Py-COO-(CH2)11-O-(CH2)2-DMA(Figure 1.)as a new magneto-sensitive fluorophore.The previous studies showed that unchained Py/DMA system showed ~10% MFE and a simple methylic carbon chained Py-(CH2)n-DMA showed up to 40% MFE. Substituting the Phen of Phen-(CH2)12-O-(CH2)2-DMA with Py showed ~60% fluorescence enhancement. We introduce -COO- group between Py and carborn chain as a electron withdrawing group to lower the HOMO energy level of Py. We expect a better electron transfer between the electron donor to acceptor and form stronger exciplex that is critical to the magneto-senstivity. Its response to the magnetic field is characterized by a programable bipolar electromagnet.

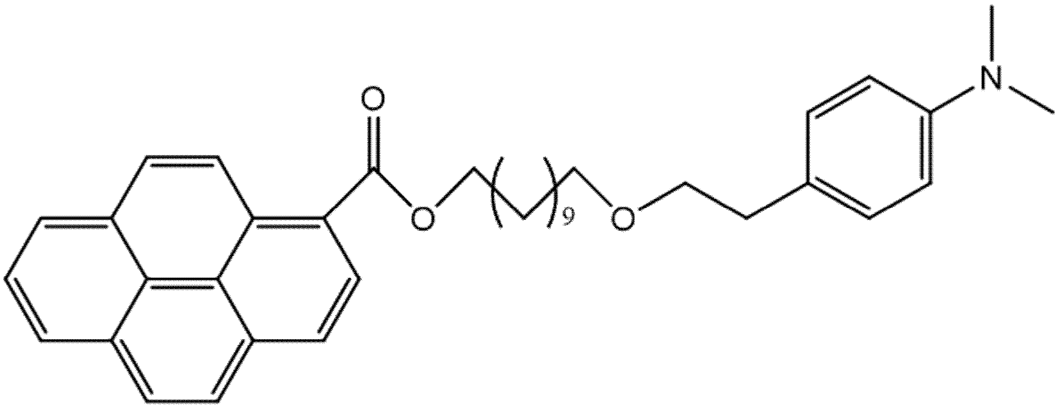

Figure 1. Molecular structure of Py-COO-$(CH_2)_{11}$-O-$(CH_2)_2$-DMA

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Molecular Interactions of Graphene Oxide with Aromatic Amino Acids

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대구대학교 화학과

Graphene oxide with functional groups of carboxylic acid, hydroxyl, and epoxide drew a great deal of attention as a promising nanomaterial for use in biosensors because of its ability of DNA adsorption as well as fluorescence quenching. Understanding the interaction between graphene oxide and the biomolecules is important for graphene oxide based bio-sensing applications. In this work, non-covalent interactions between graphene oxide and aromatic amino acids, tryptophan and tyrosine was studied by steady-state and time-resolved fluorescence measurements. Based on strong fluorescence quenching of Tyr and Trp by GO, the graphene was found to interact strongly with the amino acids. The fluorescence quenching mechanisms were investigated and the binding constants are estimated. The apparent Stern-Volmer quenching constants of GO-amino acid interactions were estimated to be similar for both Tyr and Trp ($1.88x10^4$ mL/g for Tyr and $1.93x10^4$ mL/g for Trp). From the ab initio MD simulations, different binding sites are suggested for tryptophan and tyrosine on graphene oxide and binding energies were estimated. It is suggested that fluorescence quenching of Tyr and Trp occurs through various non-covalent intermolecular interactions such as hydrogen bonding interactions and π-π interactions.

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액상 물 분자들의 진동 운동을 묘사하는 점전하 근사에서의 최적의 전하량 결정

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액체상의 물 분자의 OH 늘어남 진동에 대해, 진동하는 물 분자가 외부로부터 받는 상호작용과 이 때의 진동수의 관계를 이론적으로 묘사할 수 있다. 이 때, 물 분자가 받는 상호작용을 양자 역학적으로 계산해야 하지만 과도한 시간과 노동을 요한다. 그래서 이를 대체할 수 있는, 물 분자들의 원자들을 점전하로써 생각하는 점전하 근사를 도입할 수 있다. 하지만 물의 진동 시 발생하는 상호작용을 가장 잘 재현할 수 있는 점 전하들의 전하량이 결정되지 않았고, 우리는 이 전하량을 찾는 일을 하였다.

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Ionic liquid mediated relaxation of excited thymine

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부산대학교 화학과

Preservation of DNA is of paramount importance in biotechnology as well as medical sciences. Recently ionic liquids have been found as suitable media for preservation of DNA. Upon exposed to UV radiation, damage of DNA has been principally linked to dimerisation or photo-chemical changes of thymine, a constituent base of DNA. In the present work, time resolved vibrational spectroscopic study (Transient state IR) has been involved to study the excited state relaxation of thymine in ionic liquids having a variation in viscosity value. The relaxation mechanism in ionic liquids have been compared to that of organic molecular solvents to understand the interactions invoked by ionic liquids to stabilize thymine.

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Dynamic order from dynamic disorder

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중앙대학교 화학과

We investigated the reaction process where *l*-time intermediate reactions occurring sequentially yield one product molecule. It is known that a number of sequential steps result in a central limit process where the time interval between two consecutive reaction events is narrowly distributed around its mean time. However, each reaction rate involved in the process in concern fluctuates stochastically so that its stochastic properties have a significant effect on the convergence to the central limit. Because time intervals or waiting times are statistically correlated, depending on the magnitude of rate fluctuation and correlation time, it is shown that the long-lived memory effect significantly impedes *l*-driven narrowing of waiting time distribution. At intermediate values of *l* on the way to the central limit, the waiting time distribution shows even a remarkable bimodal feature. The randomness quantifying the dispersiveness of the waiting time distribution is shown to directly include the contribution from waiting time correlation function. In contrast, the resulting distribution of product copy number has a simple unimodal shape, which spreads more or less than a Poisson distribution. In the uncorrelated case, super(sub)-Poisson waiting time statistics must lead to super(sub)-Poisson counting statistics. It is clearly shown here that in the correlated case, sub-Poisson waiting time statistics can lead to super-Poisson counting statistics because of the slow convergence to the central limit.

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The Study of Context-Dependent Protein Hydrophobicity Based on Site-Directed Thermodynamic Analysis

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Hydrophobicity of a protein is one of the major factors controlling protein folding and protein-protein interaction. Conventionally, the protein hydrophobicity is estimated based on the summation of constituting amino acid hydrophobicity scales determined as an individual free amino acid, assuming that those scales are maintained in a protein-context. Here, we challenge this assumption by applying fluctuating thermodynamic framework for elucidating protein context-dependent hydrophobicity. We considered the following three globular protein systems with the distinct secondary structures, i.e. villin headpiece subdomain (HP35), WW domain, and B domain of protein A (BdpA). For those protein systems, the extensive atomistic MD simulations and the solvation free energy analysis were performed followed by the site-directed thermodynamic analysis to investigate the context-dependent hydrophobicity of constituting amino acids. We compared the hydrophobicity of a free amino acid, quantified by the free energy change upon hydration, with the residual hydrophobicity, quantified by the hydration free energy of a residue embedded in the protein context. We find that the residual hydrophobicity is significantly altered from the hydrophobicity of a free amino acid due to the protein structural effects such as secondary structure formation, salt-bridge formation and hydrophobic-core formation. Our results thus provide a new comprehension on the context-dependence of amino acid hydrophobicity, which will contribute to understanding how the hydrophobicity drives protein folding and protein-protein binding.

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the effect of the absorbance on the Raman scattering of chemical mixtures

고영진* 정영수[1]

국방과학연구소 5-3 [1]국방과학연구소 5본부 3부

The Raman spectroscopy is an attractive method for the identification of chemicals with similar structure. In this research, the effect of the absorbance on Raman scattering of chemical mixtures was studied. The Raman spectrum of mixtures show signature of only one chemical. the absorbance at the laser wavelength of chemicals was measured and the absorbance of chemiclas was related to the Raman spectrum of mixture, showing that the chemical with larger absorbance gives the Raman scattering signal.

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Introduction of Shimadzu spectrophotometer RF-6000 and IRTracer-100

이승장 김관수*

동일시마즈(주) 지원본부

DNA probes labeled with fluorescent dye are used extensively to detect and identify specific DNA when conducting life science studies. The mechanism involves the selective binding of the probe to specific DNA, thereby permitting the detection of that DNA. However, due to the wide variety of fluorescent dyes, it is important to know the exact wavelength at which the probe fluoresces to ensure DNA detection. Here, using the three-dimensional spectral measurement feature of the RF-6000 Spectrofluorophotometer, we introduce examples of fluorescence measurement of two types of fluorescent probes.Commercially available plastic products contain polymers, such as polyethylene (PE) and polypropylene (PP), as their main components, in addition to various trace component s that are added to enhance performance and maintain quality. Here we introduce an evaluation of additives used in plastic bags taking advantage of the high S/N ratio of the Shimadzu FTIR IRTracer-100 spectrophotometer.

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Photochemistry of DNA-intercalated Psoralen Derivatives

한기림 이종우[1] 황도익[1] 김성근[*] 연규진

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

Due to their conditional cytotoxicity under ultraviolet irradiation, psoralen and its derivatives have extensive history of being utilized for treating various skin diseases. In physiological environment they have several interesting photochemical properties, including their tendency to form various photoproducts after undergoing DNA intercalation. With the emergence of modern spectroscopic techniques, only recently researchers began to understand fundamental photochemistry of DNA-intercalated psoralen. In this research we attempted to elucidate excited-state dynamics of psoralen-DNA compounds by exploring different psoralen derivatives with various spectroscopic techniques including ultrafast transient absorption spectroscopy.

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DFT and Reactive Molecular Dynamics Simulation of CNT Container Loaded with Nitromathane

배세원* 조수경[1]

국방과학연구소 4본부 2부 [1]국방과학연구소 국방고등기술원

Molecular modeling of explosive nanocontainer was studied using various simulation methods, e.g. Grand Canonical Monte Carlo (GCMC), classical and Reactive Molecular Dynamics (MD), and Density Functional Theory (DFT). Encapsulation of energetic material, i.e. Nitromethane (NM) in this study, inside carbon based nanocontainer was used. Each of simulation method was employed to take into account the interpretation of controlled model systems; the amount of loading materials (GCMC), capping method of CNT and modeling (classical MD), energy release (DFT), and burst of nanocontainer (Reactive MD).

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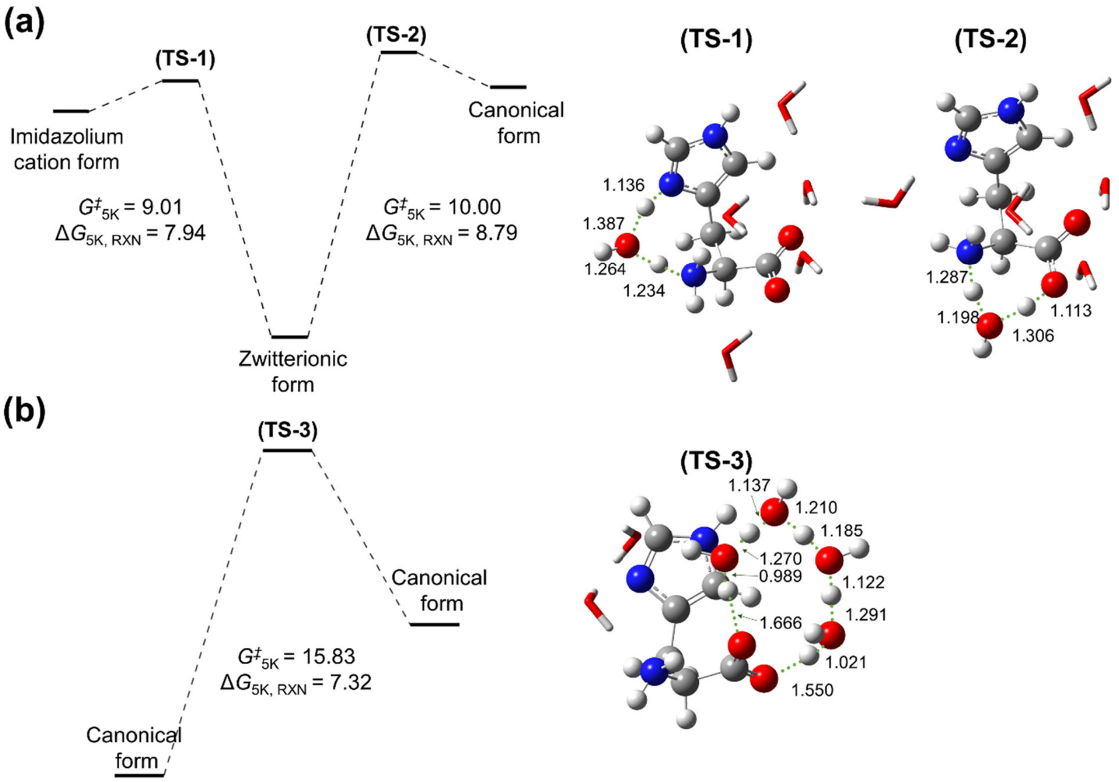
Thermodynamic and kinetic stability of zwitterionic histidine: Effectsof gas phase hydration

이성식 이성렬[1,*]

경희대학교 국제캠퍼스 화학과 [1]경희대학교 응용화학과

We present calculations for histidine?$(H_2O)_n$(n = 0?6) to examine the effects of micro-hydrating watermolecules on the relative stability of the zwitterionic vs. canonical forms of histidine. We calculate thestructures and Gibbs free energies of the conformers at wB97XD/6-311++G(d,p) level of theory. We findthat six water molecules are required to produce the thermodynamically stable histidine zwitterion. Bycalculating the barriers of canonical ↔ zwitterionic transformation, we predict that both the most stablecanonical and zwitterionic forms of histidine?$(H_2O)_6$may be observed in low temperature gas phaseenvironment.


(a)
(TS-1)
(TS-2)
Imidazolium cation form
Zwitterionic form
Canonical form
$G^{‡}_{5K}$ = 9.01
$\Delta G_{5K,\ RXN}$ = 7.94
$G^{‡}_{5K}$ = 10.00
$\Delta G_{5K,\ RXN}$ = 8.79
(TS-1)
1.136
1.387
1.264
1.234
(TS-2)
1.287
1.198
1.306
1.113
(b)
(TS-3)
Canonical form
Canonical form
$G^{‡}_{5K}$ = 15.83
$\Delta G_{5K,\ RXN}$ = 7.32
(TS-3)
1.137
1.210
1.185
1.270
0.989
1.122
1.666
1.291
1.021
1.550

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Theoretical study of the chemical reaction of benzoic acid with Ge(100)

김도환

전북대학교 화학교육과

We have performed density-functional calculations in order to investigate the chemical reaction of benzoic acid with Ge(100) surface. Benzoic acid undergoes O-H dissociation, forming benzoate. Resulting benzoate has two equivalent oxygen atoms, both of which may react with electron-deficient down-Ge atom. Mono-dentate product was found to compete with bidentate bridged structures. Bidentate structures may be end-bridged between adjacent dimers within the same dimmer row. The ontop bidentate structures have two σ bonds within the same dimers, similar to those in acetate on Ge(100). Another bidentate structure having inter-dimer row bridge was also calculated, but found to be energetically unfavorable. Aromatic phenyl ring remains unreacted and shows a bright spot in simulated STM images. All of the possible products from cycloaddition which have been suggested for benzene on Ge(100) resulted in unstable structures. Simulated STM images from the optimized adsorption structure explain experimental observations well. The location of phenyl ring affects the final image. The bright spot was from unreacted π-electrons from phenyl ring. The electronic density is very concentrated at phenyl ring.

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Improving AMBER Force field for RNA simulations

황태환 박영상*

부산대학교 화학과

In all-atom RNA molecular dynamics (MD) simulations, the standard AMBER99 parameters have some limitations, such as over-stabilization of base stacking and biased populations of the glycosidic syn-anti conformations. In an attempt to improve AMBER99 for RNA simulations, we proposed to modify van der Waals and glycosidic torsional parameters of the AMBER99 force field in conjunction with the TIP4p-FB explicit water model. For improving base stacking interactions, aqueous nucleosides clustering simulations were performed to compute association equilibrium constants (Ka), which were then directly compared to earlier experimental results measured by vapor pressure osmometry. For improving the glycosidic syn-anti ratio, we carried out mononucleoside simulations using the chiOL3 torsional potential by uniformly scaling the chiOL3 term for each base of rA, rG, rU, and rC. With all these new parameter sets, we found that UUCG and GCAA tetra loop hairpin RNAs remained stable within hundreds nanoseconds (ns). Further test has been undergoing to assess the feasibility of this force field for ab-initio folding of small RNA loops.

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Electrochemical CO_2 reduction by polymer modified electrode : Nafion/Polyvinylpyridine cathode

정호현 강영수*

서강대학교 화학과

Polyvinylpyridine polymer show catalytic property to reduce CO_2. In electrolyte containing PVP, cyclic voltammetry indicate similar tendency like pyridine molecule catalyst when CO_2 gas is purged to electrolyte. PVP coated FTO was used as a cathode for electrochemical cell to reduce CO_2 and 360 M of formic acid was produced during the reaction. To reduce CO_2 by pyridine groups, multi protons should be supplied to active sites. The Nafion polymer is well known for its water uptake and protons transport properties. Cast Nafion film on the PVP surface enhanced current of CO_2 reduction because pyridine groups of PVP is protonated more easily due to the Nafion film. This Nafion/PVP cathode enhanced formic acid production to 660 M at same condition. This polymer composite system provides new insight for CO_2 reduction as contrasted with previous researches which used metals as a catalyst for CO_2 reduction.

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Synthesis of Vis-to-UV Upconversion Phosphor Nanoparticles and its Application to Enhanced Smart Window

강하례 강영수[1,*]

서강대학교 화학 [1]서강대학교 화학과

Photochromism is the chemical transformation between two forms of molecules, which have different absorption peaks and are reversible. A smart window is one of its applications that controls the transmittance to minimize inefficient energy flows in buildings. Inorganic photochromic compounds have been attracted interests because of its better durability than organic ones, despite of their insufficient photochromic efficiency. To enhance the photochromic efficiency, an upconversion film which converts visible light into UV light could be attached on the top of the photochromic film as most photochromic films absorb UV light around 290 nm. Pr^{3+} has been chosen for an activator owing to its proper emission peak (280-400 nm). $Y_2SiO_5:Pr^{3+}$ nanoparticles were fabricated via hydrothermal method with size around 100 nm, and they were deposited on polyethylene terephthalate film using finger rubbing method.

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Synthesis of Highly Thin Reduced Graphene Oxide (rGO) by Electrochemical Method

정혜영 강영수*

서강대학교 화학과

Recently semiconductor/reduced graphene oxide (rGO) composites have been used for the reduction of carbon dioxide into hydrocarbon fuels like methanol, ethanol, etc. The intimate contact between semiconductor and rGO is proposed to accelerate the transfer of electrons from semiconductor to rGO. This leads to decrease charge recombination and enhance the carbon dioxide conversion efficiency. In this work, highly thin reduced graphene oxide sheet will be synthesized to prevent thick rGO sheet from concealing carbon dioxide reduction sites on the surface of semiconductor as well as maintain the high conductivity. After graphene oxide (GO) will be synthesized by modified Hummers method, GO spin-coated film will be reduced by electrochemical method of Rodney S. Ruoff’s group. According to their research, in PMMA/GO/metal composite cathode, electron transfer from metal to GO and proton ions of aqueous solution occurs and each of them are reduced to rGO and hydrogen gas. The hydrogen gas effectively delaminates rGO sheet producing thin rGO sheet. This would increase the charge separation and the conversion efficiency of carbon dioxide to hydrocarbon fuels.

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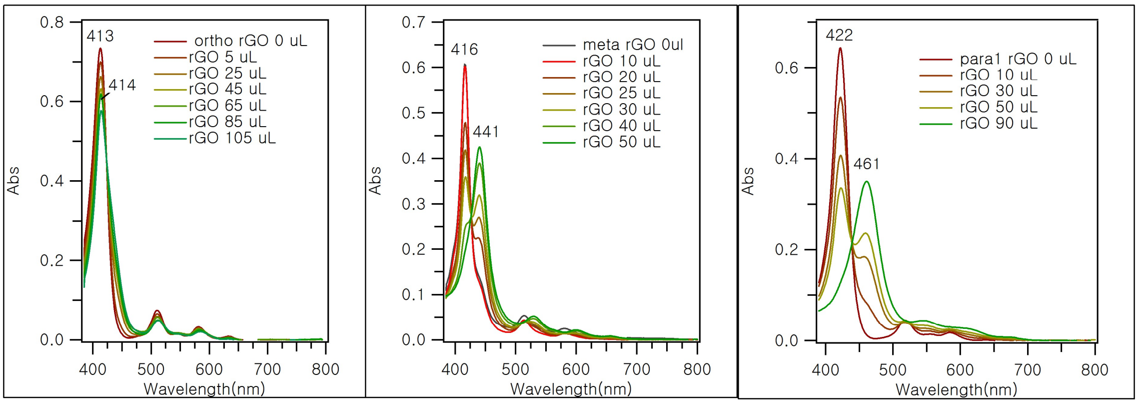
Comparative Study on Molecular Flattening of Porphyrin/rGO complexes and Their Applications to Optical Probes

이가현 심상덕[1,*]

순천대학교 기초의화학부 [1]순천대학교 화학과

Reduced graphene oxide (rGO) sheets exhibit physical and electronic properties similar to that of graphene. In addition to its solution-processability, they are being considered in electronic, sensor, and catalytic applications. Attempts to use blends of functionalized graphene has been made for a variety of applications including biological sensors, drug delivery, and tunneling electronic properties of graphene. As a kind of well-known functional dye, porphyrin derivatives also have been used for modifying graphene via covalent or noncovalent functionalization to achieve novel optoelectronic properties. Recently it has been reported the supramolecular complexation of negatively charged rGO and cationic porphyrin, 5, 10, 15, 20-tetrakis(1-methyl-4-pyridinio)porphyrin (*p*-TMPyP) induced a large bathochromic shift of the porphyrin Soret band in aqueous media, primarily due to the molecular flattening of TMPyP and resultant nonplanarity of the porphyrin macrocycle accelerated the coordination reaction with specific metal ions, Cd^{2+}. On the basis of this phenomenon the TMPyP/rGO complex could be used as a new optical probe for sensing a specific heavy metal ion with rapid sensitivity and improved selectivity toward specific ions. To study the correlation between the degree of macrocycle distortion and the selectivity, we investigate the *o*- and *m*-TMPyP/rGO as well as *p*-TMPyP/rGO. As expected, the *o*-, *m*-, and *p*-TMPyP/rGO complexes exhibit different bathchromic shifts of the Soret bands, indicating the different degree of molecular flattening. Based on this result, the selectivity control experiments of TMPyP/rGO complexes are now in progress.


0.8
0.6
0.4
0.2
0.0
Abs
413
414
ortho rGO 0 uL
rGO 5 uL
rGO 25 uL
rGO 45 uL
rGO 65 uL
rGO 85 uL
rGO 105 uL
400
500
600
700
800
Wavelength(nm)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Abs
416
441
meta rGO 0ul
rGO 10 uL
rGO 20 uL
rGO 25 uL
rGO 30 uL
rGO 40 uL
rGO 50 uL
400
500
600
700
800
Wavelength(nm)
0.6
0.4
0.2
0.0
Abs
422
461
para1 rGO 0 uL
rGO 10 uL
rGO 30 uL
rGO 50 uL
rGO 90 uL
400
500
600
700
800
Wavelength(nm)

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Photoreduction of CO2 to methanol by using CuInS2 cathode mixed with reduced graphene oxide

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서강대학교 화학 [1]서강대학교 화학과

Copper indium disulfide (CuInS2, CIS) is suitable for cathode cause it is a p-type semiconductor as visible light driven catalyst (band gap ~1.5 eV) and it has a high absorption coefficients (>105 cm-1) and appropriate band position for CO2 reduction to methanol. In general CIS electrode can be fabricated by electrochemical deposition followed by sulfurization but in our case CIS thin film was fabricated by simple annealing process using precursors dissolved in pyridine. Instead of water based solvent system, pyridine has a strong coordinating with solvent which can help the decomposition of the precursors catalytically. And also we incorporate reduced graphene oxide (r-GO) with CIS film. r-GO will be helpful to enhance photocurrent and also by varying the reduction level of graphene oxide we can control the reduction potential level for effective methanol production(~0.38 eV). r-GO-CIS film can be made simply by just mixing graphene oxide with precursors. This r-GO-CIS film can be applied well as cathode for methanol production which is our final purpose in artificial photosynthesis

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Effects of Polyhexamethylene Guanidine (PHMG) Adsorption on Cell Membranes

김원태 장락우*

광운대학교 화학과

In 2011, several children, pregnant women, and old men were dead of lung damage by a sterilizer of humidifier in Korea. The main chemical substances of sterilizer are Polyhexamethylene guanidine (PHMG) and Oligo(2-(2-ethoxy)ethoxyethylguanidium chloride (PHG). Since they have strong sterilizing power and showed a low toxicity by skin contact or intake, these molecules were used as a sterilizer for wet wipes, bleaching agent. However, it was recently found that they can cause pulmonary fibrosis when they are inhaled. In this study, we performed molecular dynamics simulations using atomistic models of the PHMG molecule and dipalmitoylphosphatidylcholine (DPPC) membrane systems. We studied the structural effects of PHMG adsorption on model cell membranes as well as lung surfaces by employing both bilayer and monolayer membranes consisting of DPPC lipids.

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Density functional theory study of *meso*-alkylidenyl carbaporphyrinoid compounds

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서울대학교 화학부 [1]강원대학교 화학과

The novel *meso*-alkylidenyl porphyrin systems are non-aromatic and conformationally flexible macrocycles that display unusual protonation selectivity and tautomeric equilibrium. We have performed density functional theory (DFT) calculations in order to investigate the optimized structures, energies, frontier molecular orbitals (MO), and molecular electrostatic potential (MEP) maps of *meso*-alkylidenyl carbaporphyrinoids. All calculations for the compounds were performed at the M06-2X/6-31G(d,p) level of theory. The obtained results from this study were compared with experimental data. Through the comparision, several issues are discussed.

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Hierarchically driven nanostructures of RuO2 nanorods on TiO2 nanofibers by a coaxial electrospinning process

정혜승 김명화[1,*] 오혜림[2] 함보영[3] 정유나[4]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과 [2]이화여자대학교 화학,나노과학과 [3]이화여자대학교 화학나노과학 [4]이화여자대학교 화학나노학과

We report a simple coaxial electrospinning process to directly prepare hierarchically driven RuO2 nanorods on TiO2 nanofibers followed by the thermal annealing. The single step fabrication of TiO2/RuO2 composite electrospun nanofibers can be readily achieved by the simultaneous injection of titanium precursor solution as core and ruthenium precursor solution as shell in the manner of the coaxial geometry. The careful control of various atomic ratios of Ti and Ru contents can give rise to well defined hybrid nanostructures of single crystalline RuO2 nanorods directly grown on polycrystalline TiO2 electrospun nanofibers. The morphology and crystal structure of the samples were carefully characterized with field emission scanning electron microscope (FE-SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). This rational crystal engineering is remarkably simple and versatile for the formation of hierarchical network architectures so that it can be readily applied for the design of other complex functional hetero-nanostructures that might find potential applications in broad range of the fields, such as electrode materials, sensors, catalysts, and energy related devices.

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TiO2/NiO composite electrospun nanofibers with the morphology of the hollow tube

이예정 김명화[1,*] 김성실 김세아

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

We present the fabrication of TiO2/NiO composite nanofibers by a simple electrospinning process by controlling various atomic ratios of Ti and Ni contents with mixed titanium precursor and nickel precursor solutions. The morphology and crystal structure of the samples were carefully characterized with field emission scanning electron microscope (FE-SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). Results show that the electrospun nanofibers consisting of titania and nickel(Ⅱ) oxide are uniformly formed with the shape of the hollow tube so that it is expect that composite nanofibers could be extended to apply for high efficient photocatalysts.

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Synthesis of Sintered $Sm_2Fe_{17}N_3$/*a*-Fe Nanocomposite Magnet for Exchange-Coupled Nanocompostie Magnet

안재우 강영수*

서강대학교 화학과

Nowadays, $Nd_2Fe_{17}B$ is the most popular permanent magnet. It has stronger magnetic energy product than any other hard magnet materials. But, this material has low curie temperature (585 K), so it is unstable in high temperature. On the other hand, $Sm_2Fe_{17}N_3$ has high curie temperature (749 K) and this can replace $Nd_2Fe_{17}B$ with higher stability at high temperature.Usually, $Sm_2Fe_{17}N_3$ can be synthesized by Ball-milling method (Top-down). But as-synthesized magnet shows phase separation at high temperature (>1473 K). But, in case of sintered $Sm_2Fe_{17}N_3$ magnet synthesized by wet chemistry (Bottom-up), purity of material is much higher and also size can be controlled. So the magnetic energy product of sintered $Sm_2Fe_{17}N_3$ magnet can be enhanced than that reported in the previous report. With this sintered $Sm_2Fe_{17}N_3$ magnet, final goal is the self-assembled hard/soft nanocomposite magnet for magnetic for higher maximum energy product than 55 MGOe by exchange-coupling effect.

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Co-solvent's Effect on Solute-Solvent Hydrogen-Bond Dynamics: Ultrafast 2D IR Investigations

백호용 이인성 김영삼*

울산과학기술대학교(UNIST) 자연과학부 화학과

Co-solvents strongly influence the solute-solvent interactions of biomolecules in aqueous environment and have profound effects on the stability and activity of several proteins and enzymes. Experimental studies have previously reported on the hydrogen-bond dynamics of water molecules in the presence of co-solvent, but understanding the effect from a solute's perspective could provide a greater insight towards protein stability. Our study uses 2D IR spectroscopy to investigate how DMSO as a co-solvent affects the dynamics of hydrogen-bonding interactions between the C=O group of ethyl acetate and water by quantitatively estimating the hydrogen-bond exchange rate with and without DMSO in aqueous solution. 2D IR results show spectral signatures of a chemical exchange process; the presence of the co-solvent is found to lower the hydrogen-bond exchange rate by a factor of 5. The measured exchange rates are 6.68×1011 s-1 and 1.48×1011 s-1 in neat water and 1:1 DMSO/water, respectively. The widely different hydrogen-bond lifetimes and exchange rates with and without DMSO indicate a significant change in the ultrafast hydrogen-bond dynamics in the presence of a co-solvent, which in turn might play an important role in the stability and activity of biomolecules.

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Electromagnetic simulations of noble-metal alloy nanoparticles' optical properties based on theoretical permittivities

류설[*] 김지은

조선대학교 화학과

We used discrete dipole approximations to calculate the optical properties of noble-metal alloy nanoparticles. The intrinsic permittivity properties of alloys were calculated using density functional theory methods with plane-wave basis sets. For ordered binary-component noble-metal alloys such as $CuAu_3$, CuAu, and Cu_3Au, the electronic band structures and electric permittivities in the linear response regime were calculated and the permittivities with alloy composition were compared. We performed electromagnetic simulations of the alloy nanoparticles' optical properties based on the theoretically obtained permittivity values. In this study, we show that by controlling the intrinsic property of nanoparticles it is possible to fine-tune the optical properties as red-shift or blue-shift with no changes in nanoparticle size and shape.

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발표분야: 물리화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

External Field Effects in Two and Three Dimensional Diffusion-Influenced Reactions

김태준 김효준*

동아대학교 화학과

The external field effects are ubiquitous in chemical reactions since they include gravitational, magnetic, and electric effects on diffusion-influenced reactions. Recently, we report the efficient lattice-based Monte Carlo simulation methods to treat the external field effects rigorously in one dimension. We were able to reproduce the exact analytical results in one dimension. In this presentation, we extend the simulation methods to higher dimensions, where no exact analytical solution has been known. We find that the external field against the escape of molecules actually increases the escape probability in two dimensions unlike one and three dimensions. This amusing result is caused by the correlation between diffusional movement and the field effect.

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Monte Carlo Simulation Studies on Anisotropic Diffusion Effects on the Diffusion-Influenced Reaction

황준필 김태준 김효준*

동아대학교 화학과

Many chemical and biochemical reactions are known to be influenced by anisotropic diffusion effects. However, the analytical solutions for anisotropic diffusion-reaction systems are very rare because of its complexity. In this presentation, we report the lattice-based Monte Carlo simulation methods to incorporate the anisotropic diffusion rigorously by simply introducing the stay probability. We test that simulations can reproduce the theoretical predictions and report the numerical results in anisotropic systems where theoretical predictions are absent.

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Synthesis, characterization and invivo application of gadolinium-dysprosium oxide nanoparticles as T1,T2 dual MRI contrasting agents

<u>SHANTI MARASINI</u> 이강호*

경북대학교 화학과

Several mechanisms have been proposed to synthesize water soluble T1,T2 based MRI contrasting agents. A new type of dual-mode T1 and T2 magnetic resonance imaging (MRI) contrast agent based on mixed lanthanide oxide nanoparticles was synthesized. We synthesized D-glucuronic acid coated GDO nanoparticles and measured their particle diameter, hydrodynamic diameter, r1 and r2 values, map images, and in vitro cellular toxicity. The water soluble and biocompatible D-Glucuronic acid coated GdDy mixed oxide nanoparticles have drawn tremendous attraction in the application of magnetic resonance imaging.

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Synthesis, Characterization and Surface Functionalization of Iron Oxide Nanoparticles

ADIBEHALSADAT GHAZANFARI SEYEDHOSSEIN 이강호*

경북대학교 화학과

Magnetic iron oxide nanoparticles have drawn tremendous attraction from both fundamental aspect as well as applications in biomedicine such as magnetic bio-separation, detection of biological entities, magnetic resonance imaging, magnetic fluid hyperthermia and targeted drug delivery due to their fascinating magnetic properties. These properties of iron oxide nanoparticles can be tuned by modifying their, size, shape and surface coating of the nanoparticles. This work deals with synthesis and characterization of iron oxide and iron nanoparticles with different surface coating. So we synthesized water soluble surface coated iron oxide and iron nanoparticles with Fluorescein-PEI, PAA-Folic acid, silica, and Fluorescent Brightener ? 28.

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Nocliniclal Dose Formulation : Method Validation of Mixture Dose Formulation

조원미* 김인희[1]

(주)바이오톡스텍 조제팀-조제물분석과 [1]바이오톡스텍 조제팀-조제물분석과

Nonclinical dose formulation analysis methods are used to confirm test article concentration and homogeneity in formulations and determine formulation stability in support of regulated nonclinical studies. There is currently no regulatory guidance for nonclinical dose formulation analysis method validation or sample analysis. Regulatory guidance for the validation of analytical procedures has been developed for drug roduct/formulation testing; however, verification of the formulation concentrations falls under the framework of GLP regulations (not GMP).

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Studies on Organic Light Emitting Diode (OLED) Emitters by Ultra Performance Liquid Chromatography and Supercritical Fluid Chromatography-Mass Spectrometry

조윤주 김성환*

경북대학교 화학과

Organic Light Emitting Diode (OLED) are widely used to digital display in devices such as television screens, computer monitors, portable systems such as mobile phones, handheld game consoles and personal digital assistances. Also, because of thin, light and flexible properties, OLED is drawing attention as the upcoming-generation material. For the applications, identification of side-materials in well-established OLED complexs is a very important for its purity and stability analysis. In this study, three iridium emitters and one material of photonic and optical device were identified by supercritical fluid chromatography (SFC) and reversed-phase ultra performance liquid chromatography (UPLC) coupled to electrospray ionization (ESI) Mass Spectrometry at the molecular level. SFC utilizes supercritical carbon dioxide, methanol as mobile phase and offers a faster runtime in comparison with UPLC and minimization of noise peaks in baseline for purity analysis in OLED samples. Overall, SFC- and UPLC-MS was successfully applied to OLED compounds for compositional and purity elucidation. Therfore, these results are examples of using powerful separation technique in the field of OLED and we expect that this developed technique will be involved in the actual OLED process.

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자동차용 폐리튬 이차전지의 효율적 분리와 희유금속 회수

유건상* 홍용표

안동대학교 응용화학과

자동차용 리튬이차전지 모듈은 전기자동차 또는 하이브리드 자동차의 배터리로서 충전과 방전을 거듭 시 사용 내구연수가 20 년 이내로 한정되어 있어 폐배터리로 버려지게 된다. 우리나라에서 자동차용 배터리 생산은 LG 화학, 삼성 SDI 에서 선도적인 이루어지고 있으며 이에 따른 폐배터리의 발생량도 앞으로 기하급수적으로 증가할 것으로 예상된다. 그러나 이러한 증가에도 불구하고 현재 전기자동차 배터리의 재활용 기술들은 매우 미흡한 상황이다. 자동차용 이차전지 폐모듈은 다양한 물리·화학적 성질을 갖는 정극, 부극, 격막, 전해질 등으로 이루어져 있어 핵심부품과 주변 기기들을 분리 정제하는 기술들의 확보가 우선적으로 필요하다. 따라서 본 연구는 자동차 리튬이차전지의 폐모듈을 안정적으로 해체하고 모듈을 구성하고 있는 Cu, Al, Li, Mn, Ni, Co 성분들을 효율적으로 분리하는 공정을 개발하여, Cu 와 Al 은 박막 형태로 분리해 내고 Li, Mn, Ni, Co 는 화합물 또는 혼합된 형태로 분리해 내는 것을 목표로 삼는다.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

역류산화반응을 이용한 변압기 절연유 중의 PCBs (polychlorinated biphenyls)의 파괴 및 제거

유건상* 홍용표

안동대학교 응용화학과

국내·외에서 변압기 절연유 중의 PCBs 의 화학적 탈염소화법은 나트륨금속과 절연유를 직접 고체-액체 반응시키는 방법과 PEG/KOH 의 glycoate 를 염소화 반응시키는 방법이 주로 이용되고 있다. 대체적으로, 나트륨금속을 사용하는 경우가 PEG/KOH 를 사용하는 경우보다 다소 높은 PCBs 처리효율을 나타낸다. 그러나 나트륨금속을 사용 할 때에는 절연유 중의 수분이 존재할 때 폭발의 위험성이 있어 반드시 수분을 미리 제거하는 전처리장치가 필요하다. 이외에도 화학적 탈염소화법은 절연유 중의 PCBs 처리 시 처리효율을 향상시키기 위해서는 PCBs 와 화학시약의 몰 비, 반응시간, 반응온도, 교반의 속도, 압력 등과 같은 많은 인자들의 정밀한 검토가 필요하다. 따라서 화학적 처리기술의 대안으로서, 변압기 절연유 중에 존재하는 PCBs 를 처리 (99.9999% 이상 혹은 2 ppm 이하)할 수 있으며 슬러지의 발생이 전혀 없고 비교적 처리비용이 저렴한 새로운 역류산화반응을 이용한 PCBs 처리기술 개발을 목표로 삼는다.

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Adsorptive removal of T-N and T-P in aqueous solution by yellow sand

유건상* 최종하

안동대학교 응용화학과

Nitrogen and phosphorous have aroused considerable public concern because of their increased discharge into water bodies including reservoirs, lakes, streams and rivers. They are essential elements necessary for all living cells as a component of cell membranes. However, their enrichment in water bodies leads to the algal blooms. The high growth of algae in aquatic system adversely affects the water quality. Among the various methods of wastewater treatment, adsorption is a quite popular method due to the simplicity and the absence of sludge, as well as the availability of a wide range of adsorbents. Activated carbon has become a favorite choice for removal of pollutants from wastewater because of its high surface area and pore volume, along with convenient regeneration of spent carbon. However, the high cost of activated carbon makes its use limited. Therefore, many studies have described the adsorption abilities of various low-cost adsorbents as the potential replacement. Of all low-cost adsorbents, yellow sand may be a good candidate as an adsorbent because it is environmentally friendly and can be easily obtained across the nation. The aim of the present study is to explore the possibility of utilizing yellow sand for the adsorptive removal of T-N and T-P from aqueous solution.

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Adsorptive removal of Pb and Cd in aqueous solution using fly ash

유건상* 최종하

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With the increase in industrial activities, a large amount of heavy metals have been continually brought into water bodies including reservoirs, lakes, streams, rivers and oceans. In the present, the presence of heavy metals in aqueous environments has been of great concern due to the disturbance of aquatic ecosystem. Pb and Cd is the non-essential elements for human health and well-known as the most toxic heavy metals. Therefore, it needs to be paid more attention to the solution of the contamination problem related with Pb and Cd. Fly ash, a combustion by-product generated from a thermal power plant, has been widely used in a range of applications and particularly as filler for cement in concrete. However, large amounts are not still used and this requires disposal. Therefore, it is necessary to broad the use of fly ash for favorable environmental benefits. The present study is to explore the possibility of fly ash for adsorptive removal of Pb and Cd in aqueous solution. Here, we investigated the effect of various factors such as temperature, contact time and concentration in details.

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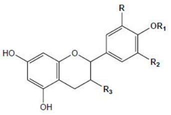
Basics of liquid chromatography-tandem mass spectrometry as a potential tool for profiling of polyphenolic compounds: Applied to flavonoid analysis from flowers of Rumex nervosus Vahl

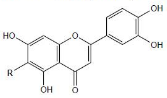
DestaKebedeTaye 신성철*

경상대학교 화학과

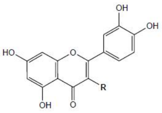
Liquid chromatography-tandem mass spectrometry (LC-MSn) is one of the most exploited hyphenated techniques used in many scientific researches including in clinical, medicinal, pharmacological, agricultural and nutritional analysis. It also attracted researchers' attention as a tool for profiling of the various polyphenolic compounds including flavonoids in plants. In tandem mass spectrometry, a mass analyzer is used to isolate a precursor ion, which then fragments to yield product ions that will be detected in the second mass analysis. By establishing relationship between precursor ions and their fragmentation products, MS/MS provides structural information. Characteristic fragmentation patters of aglycones, as well as O-, C-, and O-C-glycosylated flavonoids is the basis to use LC-MS/MS for characterization. Retro-Diels-Alder (RDA), quinone methine (QMF) and heterocyclic ring forming (HRF) are the most common fragmentation patterns used in tandem mass analysis of flavonoids. Using LC-ESI-MS/MS, characterization of 19 flavonoids from flowers of Rumex nervosus was achieved. The 19 flavonoids were quantified using external standards of the same aglycone chromophore and the performance of the method was validated. Majority of the detected flavonoids were reported in the most common edible fruits and vegetables.



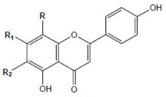
1. R = OH; R$_1$, R$_2$ = H; R$_3$ = *O*-gallate



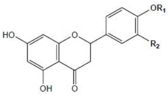
3. R = *C*-glucosyl
4. R = *C*-glucosyl



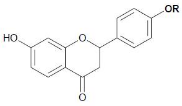
2. R = *O*-pentosyl
7. R = *O*-glucosyl
8. R = *O*-acetylhexoside
9. R = *O*-acetylhexoside
10. R = *O*-rhamanoside
11. R = *O*-acetylhexoside
12. R = *O*-rutinosyl
13. R = *O*-rutinosyl
14. R = *O*-acetylrhamanoside



5. R = H, R$_1$ = OH, R$_2$ = *C*-glucosyl
6. R = *C*-glucosyl, R$_1$ = OH, R$_2$ = H
17. R = H, R$_1$ = *O*-glucosyl, R$_2$ = *C*-glucosyl
18. R = H, R$_1$ = *O*-glucosyl, R$_2$ = *C*-glucosyl



15. R$_1$ = CH_3, R$_2$ = OH
16. R$_1$, R$_2$ = H



19. R = glucosyl

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Single bubble micro extraction for analysis of chlorophenols coupled with capillary electrophoresis

조성민 이인기 정두수*

서울대학교 화학부

In conventional headspace (HS) extraction, analytes evaporated from a sample donor phase in a sealed vessel can be enriched to an acceptor phase often in a liquid form or a sorbent coated on a fiber. The maximum enrichment factor is given by the ratio of the donor and acceptor volumes. Thus an acceptor of small volume is preferred and a single acceptor drop of small volume hanging to the capillary tip has been used in HS extraction for capillary electrophoresis (CE) [1]. To solve the stability problem of the hanging drop, we recently developed HS in-tube microextraction (ITME)/CE using a liquid plug inside a separation capillary as an acceptor in place of the drop [2]. Here, we present single bubble microextraction (SBME) technique coupled with CE, a simple but easy way of conducting HS extraction of a small volume sample for subsequent CE analysis. Instead of using a sealed vessel to prepare a HS, an bubble much smaller than 1 ?L was formed at the tip of a capillary by injecting a plug of air into the capillary containing an acceptor plug and ejecting the air plug after immersing the capillary into a sample donor. Then, SBME-CE was performed using the acceptor plug remained in the capillary. Due to the small volumes of the bubble and acceptor plug, it was possible even for a small volume donor to retain a high ratio of the donor and acceptor volumes for high enrichment factors. All steps of SBME-CE were carried out automatically using a commercial CE instrument without any modification. Therefore not only the sample volume could be dramatically reduced, but also the need for a special apparatus was eliminated.

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Measurement of lipid turnover rate in HeLa cell by heavy water labeling

고병숙 김태영[1,*]

광주과학기술원 화학과 [1]광주과학기술원(GIST) 기초교육학부

Heavy water (^2H_2O) labeling is a stable isotope labeling method that has been developed to quantify *in vivo* dynamics of biomolecules such as proteins, DNAs and lipids. Change in mass isotopomer distribution by deuterium labeling enable calculation of biomolecules' turnover rates. Here we describe an experimental strategy for measuring *in vivo* lipid turnover rate in HeLa cell by ^2H_2O labeling coupled with high resolution mass spectrometry. Lipids were extracted from HeLa cell grown in 5% (mol/mol) ^2H_2O enriched media at 6 time points between 0 and 48 hours of labeling. Lipid species of glycerophospholipids, glyceryl esters and sphingolipids were identified based on *in-silico Lipidblast* library. The turnover rate of lipids in HeLa cell was determined in a range of 0.02-0.1 hr^{-1}.

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Sequential Purge and Trap Technique for Sampling of Geosmin and 2-MIB in Aqueous Samples Using Needle Trap Device (NTD)

박선이 엄인용[1,*]

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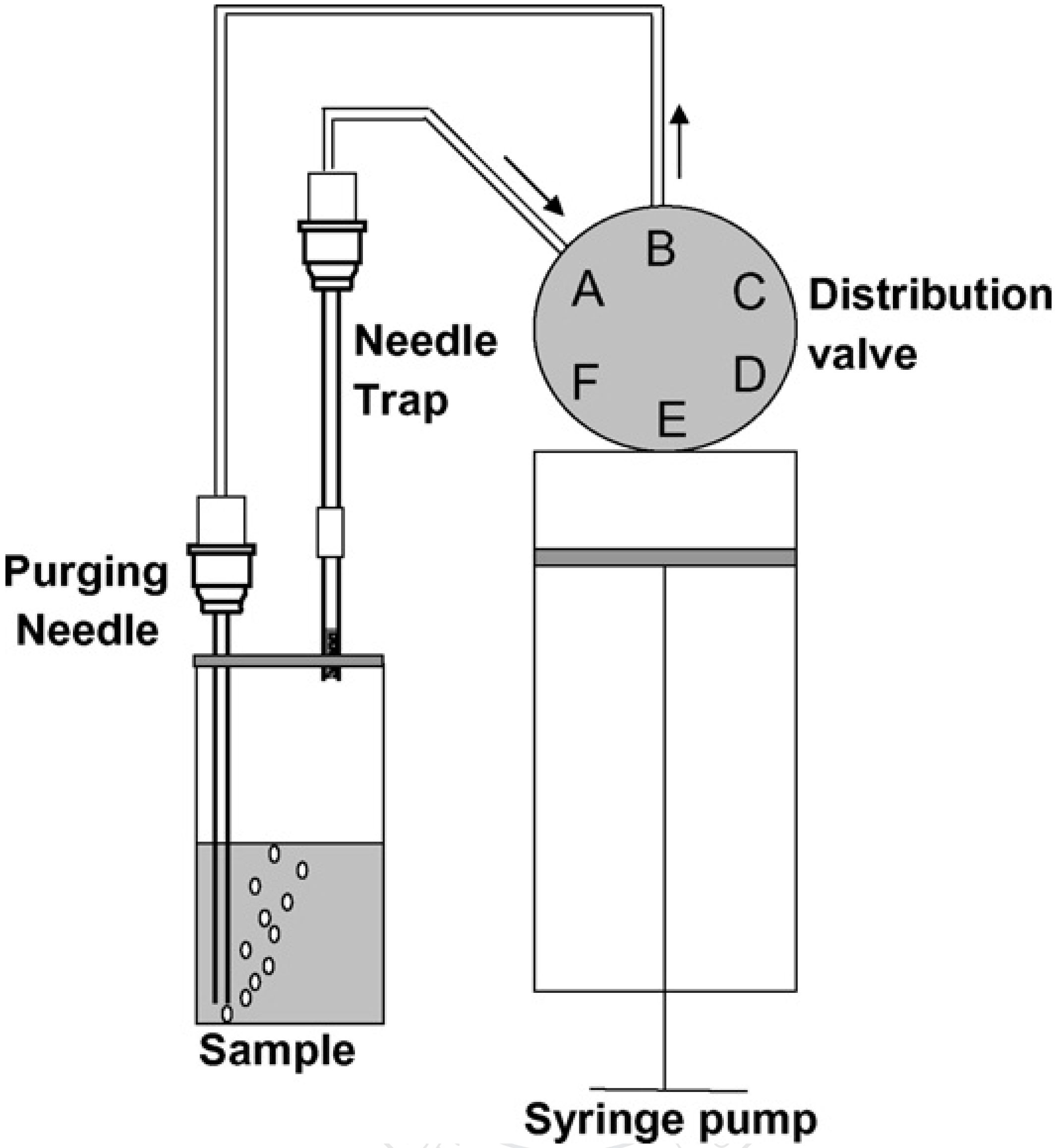
Recently, a needle trap device (NTD) was introduced to the scientific world of sample preparation. NTDs, like solid-phase microextraction (SPME) fibers, are another approach for one-step solventless sampling and sample preparation. The major advantages of NTDs as a sorbent trap technique are simplicity and convenience for sampling of VOCs from different matrixes and injection to the GC directly. Due to these reasons, they are widely used to analyze VOCs easily and efficiently in both gaseous and aqueous samples. However, fine sorbent particles packed in such a small tubing of the NTD do not make it suitable to use the conventional purge and trap technique which is one of the widely used active sampling techniques. To address this limitation, new approach called sequential purge and trap technique for NTD was reported few years ago. This technique adopted the purge and trap sampling mechanism but did not use an additional purge flow by recycling headspace air.1 We revisit this technique to sample and analyze geosmin and 2-MIB in aqueous samples. Geosmin and 2-MIB are naturally produced from blue-green algae and are known to cause earth-musty odor which are difficult to remove during tap water production process. Human noses are very sensitive to detect these compounds in ppt level (5 ng/L for 2-MIB and 30 ng/L for geosmin). In this report, we present concept of a syringe pump assisted headspace sampling technique (i.e. sequential purge and trap technique) for needle trap device again and several experimental factors to improve sampling efficiencies of geosmin and 2-MIB in aqueous samples.


B
A
C
Distribution valve
F
D
E
Needle Trap
Purging Needle
Sample
Syringe pump

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3-phase direct immersion in-tube microextraction coupled with capillary electrophoresis

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Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME, LPME requires more manual maneuvers. In order to overcome such shortcomings of LPME, We developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease. Since the acceptor phase is well protected inside the capillary, ITME can be carried out under severe extraction conditions. Moreover, given that the extraction and injection processes take place simultaneously, the extraction speed and efficiency are very high. Here, we present direct immersion ITME coupled with a commercial CE instrument (DI-ITME-CE) for three-phase configuration. In three-phase DI-ITME, acidic analytes in an acidic aqueous donor solution were enriched into a basic acceptor phase through athin organic layer by the driving force of pH difference.

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Constant current mode electromembrane extraction with capillary electrophoresis for sensitive arsenic speciation

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Arsenic is an element widely distributed in the crust of the earth, causing a worldwide problem of groundwater contamination. Four arsenic compounds dimethylarsinic acid (DMA), arsenites [As(III)], mono methylarsenic acid (MMA), and arsenates [As(V)] in a unbuffered water sample were enriched by constant current mode electromembrane extraction (CC-EME) and then analyzed by off-line coupled capillary electrophoresis (CE). Under an electrical potential, $CH_3(C_8H_{17})_3N^+ Cl^-$ (Aliquat 336) in the supported liquid membrane (SLM) acts as a carrier to mediate the transfer of anionic arsenic analytes such as DMA, MMA, and As(V) from the sample solution to an aqueous acceptor phase. Neutral As(III) was oxidized to As(V) by potassium permanganate and then enriched by CC-EME for indirect determination. Several parameters such as the electrode configuration, composition of SLM, pH of donor and acceptor phase, stirring rate, applied current, and extraction time were optimized. Under the optimal conditions, enrichment factors of 1200 to 3600 for the 4 arsenic species were obtained. The LODs for the 4 arsenic species in unbuffered water were 0.4 to 1.0 ppb As, each of which was below the WHO guideline of 10 ppb total arsenic. The established CC-EME was successfully applied for the arsenic species determination in unbuffered water with a high enrichment factor, high sensitivity, low cost and environmental friendly.

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Sensitive Arsenic Speciation with Capillary Electrophoresis

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서울대학교 화학부

Arsenic is naturally abundant in the crust of the earth and introduced into the aquatic system through dissolution and weathering of minerals. Chronic ingestion of arsenic in water may cause various diseases, including cancer and keratosis. The World Health Organization (WHO) has set a guideline for arsenic in drinking water at 10 ppb of total arsenic. However, arsenic toxicities vary significantly depending on the species; inorganic arsenics are known to be more toxic than organic ones. Hence the quantitation of specific arsenic species may be more meaningful than the total arsenic determination for the evaluation of the health risks from arsenic-contaminated drinking water. Capillary electrophoresis (CE) provides high performance separation suitable for the determination of arsenic species in real water samples but suffers from the low detection sensitivity. We used a counter-flow (CF) electrokinetic supercharging (EKS) technique to enhance the detection sensitivity. EKS is one of the most powerful sample stacking methods that combines field amplified sample injection (FASI) and transient isotachophoresis. For further improvements in sample enrichment and separation, CF-EKS uses a counter pressure to counterbalance the movement of the stacked sample zone during FASI, obtaining a pronounced increase in the amount of sample injected and the portion of the capillary available for electrophoresis. Four arsenic compounds were analyzed by CF-EKS to obtain 6,000 to 56,000-fold enrichments. The limits of detection (LODs) were in the range of 0.08-0.3 ppb As. For a tap water sample, LODs of 0.5-3.8 ppb As were obtained after 10-fold dilution with deionized water, significantly lower than the WHO guideline of 10 ppb total As.

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Detection of E. coli O157:H7 by ICP-MS immunoassay using metal-doped magnetic nanoparticles

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단국대학교 화학과

Enterohemorrhagic Escherichia coli O157:H7 (E. coli O157:H7) is a major food-borne pathogen causing severe disease in humans worldwide. E. coli O157:H7 is a pathogenic bacterium capable of contaminating food, causing food poisoning, bloody diarrhea, and occasionally kidney failure. For the detection, ICP-MS immunoassay employing magnetophoretic chromatography separation technique was to be used in this work. For target extraction and detection, amine-functionalized/Cs-doped multi-core magnetic nanoparticles (MNPs) were synthesized. The extraction is based on the highly bio-specific recognition interactions of antibody?antigen, i.e, antibody-conjugated MNPs captured E. coli O157:H7. The unbound excess MNPs were eliminated by magnetic separation in the presence of polyethylenglycol medium. The resultant immunoassay products were effectively extracted from sample solution by magnetic separation and then quantified by the determination of doped metal detection using Inductively Coupled Plasma Mass Spectrometer(ICP-MS). Since the proposed method reduced sample treatment time and amplify the signal, its application can be wide for various cell detection.

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Analysis of alpha-1 Antitrypsin in Serum Samples using Surface Plasmon Resonance compared to Enzyme Linked Immunoassay Sorbent Assay

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본 포스터에서는 세럼과 같은 실제 샘플에서 질병의 바이오마커로 이용되는 alpha-1 antirtypsin (AAT)를 surface plasmon resonance (SPR)로 분석하고자 하였다. 특히 알츠하이머질병과 연관있다고 알려져 있는 AAT 를 새로운 항체-압타머 어세이를 이용한 표면 샌드위치 플랫폼을 개발하여 SPR 로 정량분석하였고, 이 결과값을 enzyme linked immunoassay sorbent assay (ELISA) 실험결과값과 비교분석하였다.

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A Localized Surface Plasmon Resonance (LSPR)-based, simple, receptor-free and regeneratable Hg2+ detection system

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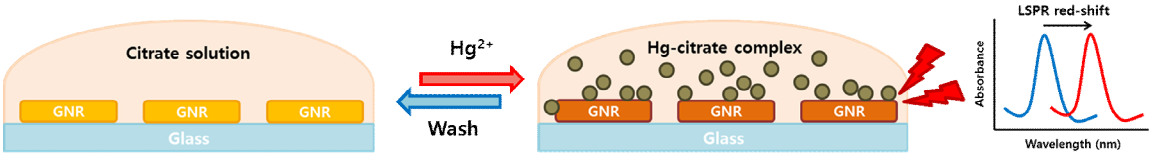
광주과학기술원(GIST) 화학과

A simple, receptor-free and regeneratable of Hg2+ sensor, which utilizes localized surface plasmon resonance (LSPR) shifts of a gold nanorod (GNR), has been developed. Precipitation induced by coordination of Hg2+ to citrate alters the local refractive index (RI) around the GNR surface on glass slide, promoting a red-shift in its LSPR absorption peak. This phenomenon is used to design a sensor that enables quantitative detection of Hg2+ in the 1 nM to 1 mM concentration range with good linearity (0.9507 correlation coefficient). A high selectivity of this sensor for Hg2+ is demonstrated by the specific LSPR red-shift of 27.67 nm promoted by this metal ion in comparison to those caused by other metal ions. In addition, the reusability of the new sensor chip is shown by its successful reuse eight-times following successive washing/precipitation steps. Lastly, the sensor displays excellent recoveries in spiking test with real water samples, such as tap water, lake and river. The simple combination of precipitation of Hg2+-citrate complex and the LSPR red-shift has led to the design of a novel sensing strategy for Hg2+ detection.



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A rapid and sensitive profiling of free fatty acids in biological samples by liquid chromatography coupled to tandem mass spectrometry with derivatization

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Free fatty acids (FFAs) that have roles in cellular energy and signaling are critical molecules in various biological states. Due to the poor ionization efficiency of FFAs under electrospray ionization mass spectrometry (ESI-MS), it is challenging to construct a robust platform to profile various FFAs in biological samples with LC-MS. In this study, we applied trimethylsilyldiazomethane (TMSD) derivatization to improve the sensitivity of FFA profiling by increasing ionization efficiencies. Multiple reaction monitoring (MRM) was used for the selective quantification of methylated FFAs. The performance of optimized TMSD methylation was validated for a reliable FFA profiling. By using liquid chromatography (LC)-ESI-MS, the high-throughput analysis of various FFAs were successfully carried out in 5 min. In order to prove the utility of our developed method, we performed the FFA profiling of mouse brain, liver, and plasma by using LC/MS/MS with/without methylation. As a result, comparing to nonmethylation, various FFAs were successfully analyzed by using methylation derivatization. Strikingly, we can successfully identify and quantify 14, 14 and 9 FFAs from mouse liver, brain and plasma among the 29 targeted FFAs.

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High Sensitive Analytical Platform for Glycolipids Characterization from Cells to Tissues using Negative Nano-LC/MS and LC/MS/MS

황재윤 안현주*

충남대학교 분석과학기술대학원

Gangliosides are glycosphingolipids containing one or more sialic acids. They participate in diverse biological processes including cell-cell recognition and the modulation of membrane protein function. In spite of the biological importance of cell surface gangliosides, the studies for gangliosides are being delayed due to the structural complexity, amphipathic nature, and lack of sensitive analytical method. Here, we introduces a robust analytical platform for the rapid profiling and quantitation of gangliosides on cell surface using membrane enrichment method and negative ion-mode nano-LC chip based mass spectrometry. The analysis of gangliosides using high resolution mass spectrometry with a membrane enrichment method provides not only comprehensive profile on cell surface gangliosides but also confident assignment of chain length and the degree of unsaturation of ceramide. We optimized the conditions such as solvents, gradients, and sample concentration to efficiently separate ganglioside standard in negative ion-mode. For profiling of cell surface gangliosides, cell membranes were isolated and enriched by ultracentrifugation. Membranes were further separated by Folch partitioning and then fractionated by C18 SPE to extract gangliosides. Gangliosides were comprehensively profiled by negative ion mode LC/MS and the structures were elucidated by tandem MS. We successfully explored cell surface gangliosides in MCF7 breast cancer cell and obtained over 70 compositions. GM3, GM2, GM1 and GD1 were commonly observed as major gangliosides showing various ceramide portions.

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Synthesis of Ruthenium oxide coated Silicon/Carbon Nanofibers composite as anode material for lithium secondary battery

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계명대학교 화학과 [1]계명대학교 화학시스템공학과

In this study, Silicon/Carbon nanofibers (CNFs) composite was synthesized and applied as anode materials of Li secondary batteries. Silicon/CNFs was grown via chemical vapor deposition (CVD) method. The source of silicon was a silane gas blended in a non-reactive carrier gas. Ethylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 600 ℃ and maintained for 10 min to synthesize Silicon/CNFs composite. After Silicon/CNFs composite was put into the 0.01 M $RuCl_3$ solution. The sample was dried in a dryer at 80 ℃. The morphologies, compositions and crystal quality of ruthenium oxide coated Silicon/CNFs composite were characterized by SEM, EDS, TEM, XRD, Raman spectroscopy and XPS. The electrochemical characteristics of ruthenium oxide coated Silicon/CNFs composite as an anode of Li secondary batteries were investigated using three-electrode cell. The as-deposited ruthenium oxide coated Silicon/CNFs composite on Ni foam were directly employed as a 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. 1M $LiClO_4$ was employed as electrolyte and 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. Acknowledgements : 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. 2015035858).

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Detection of Co2+ using automated drop-type chemiluminescence system for monitoring of nuclear reactor

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단국대학교 화학과

As well-known, the Fukushima nuclear disaster is the largest nuclear disaster since the Chernobyl disaster of 1986, releasing an estimated 10 to 30% of the radiation of the Chernobyl accident. It was an energy accident, initiated primarily by the Tohoku earthquake on 11 March, 2011, and the damage caused by the tsunami produced equipment failures in boiling water reactor systems, which induced a loss-of-coolant accident followed with nuclear meltdowns and releases of radioactive materials. In this work, a monitoring sensor of Co2+ ions as a clue of the leakage from a boiling water nuclear reactor was developed and its analytical performance was studied. The sensor system was based on a drop-type chemiluminescence which showed the merits of fast analysis with ultrahigh sensitivity. In addition, it has advantages of small sample consumption and less matrix interference or environmental influence in quantitative measurement. In this work, the limit of detection for Co2+ was 41.39 ppt, obtained from calibration curve. The interference by Cu and Fe ions were studied systematically, considering chemical and electrical behavior of interfering ions.

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Quantitative Analysis of 3 Major Nutrients in Milk Powder using Near Infrared Spectroscopy and Chemometrics

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경북대학교 화학과

A well-balanced diet is a very important factor to prevent various lifestyle diseases such as obesity, diabetes and hypertension. Meeting nutritional needs is essential for growing children, especially for infants. Therefore it is necessary to develop accurate as well as precise techniques to measure nutrient content.Even though previously established methods are relatively accurate, these are time consuming and cause environmental pollution by using organic solvents and strong acid. In these regards, spectroscopic methods would be great alternatives to official methods for the quantitative analysis.Mid infrared spectroscopy provides qualitative information regarding molecular functional group from fundamental vibrations. Near Infrared Spectroscopy(NIR) uses Overtone and Combination bands associated with the fundamental vibrations seen in the Mid-IR.A fast and eco-friendly method using FT-IR and NIR has been applied to qualitative and quantitative analysis in various fields.In this study, we applied Near Infrared Spectroscopy (NIR) combined with Chemometrics to quantitative analysis of fat, protein and carbohydrates in milk powder.

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Direct electrochemistry of Glucose Oxidase Based on Chitosan-Multi walled Carbon nanotubes composite for Glucose Sensor

오인돈 정지윤 김현욱 김정희 최영봉 김혁한*

단국대학교 화학과

We simply fabricated electrode of Chitosan-Multi walled Carbon nanotubes(Chi-MWCNTs) composite for enzymatic glucose biosensor without mediator. Chi-MWCNTs(1 mg/mL) of 20 μL was loaded on the cleaned Indium-Tin Oxide(ITO) electrode, and then dried Chi-MWCNTs suspension in the oven at 35℃. Glucose Oxidase(GOx) immobilized on the Chi-MWCNTs without cross-linker or binder. GOx of 20 μL was casted on the prepared Chi-MWCNTs working electrode, and then dried at room temperature. Lastly Chi-MWCNTs/GOx composite included working electrode was rinsed with distilled water after GOx completely dried for remove the unbinding substrate.For investigation of all electrode's morphologies, scanning electron microscope(SEM) was applied. And the electrical signal was measured by cyclic voltammetry(CV) and amperometry.We confirmed no effect of interference such as ascorbic acid(AA) and uric acid(UA) on the Chi-MWCNTs/GOx composite also.In this work, fabricated electrode for detection of glucose level was shown that has advantages such as simply process of electrode fabrication, high sensitivity, low-cost, fast electron transfer and wide detection range.

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판상화약의 자가발열 분해온도

이소정 김승희[1] 권국태 김진석[2,*]

국방과학연구소 4-2 [1]국방과학연구소 4본부2부 [2]국방과학연구소 4본부 2부

고에너지물질인 고폭화약은 사용기간 중 많은 외부 환경에 직간접적으로 노출되고 있다. 또한 화약과 같이 산화제와 연료가 공존하는 물질들은 특정온도 이상에서는 서서히 분해반응이 일어나고, 이들 열에너지가 내부에 축적되어 대규모 폭발반응이 진행되기도 한다. 따라서 화약의 열적특성을 정확하게 해석하여 사용 중에 원하지 않는 분해반응을 예방하여야 한다.일반적인 화약들은 원통형으로 시편을 제조하여 내부온도를 측정하여 열축적 측정이 가능하나 특수목적의 판상화약은 시편형태가 판상이기 때문에 열축적 측정을 직접 하는 것이 어렵다. 본 연구에서는 소량의 시료를 이용한 DSC 실험으로부터 얻은 데이터를 이용, 이를 AKTS kinetic 프로그램에 적용하여 자가 가속분해 온도(Self Accelerating Decomposition Temperature)를 계산하여 고에너지물질의 안전한 운용안정성을 예측하였다.

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Top-down Mass Spectrometry to Monitor Thrapeutic Protein with Glycan Heterogeneity

김현중 서영숙 안현주*

충남대학교 분석과학기술대학원

Biotherapeutic glycoproteins including recombinant monoclonal antibody(mAb) and Erythropoietin (EPO) are fast-growing sector in the current pharmaceutical market. They play a major role in the treatment of variety of conditions such as cancer, inflammation, auto-immune disease for mAb and anemia resulting from chronic kidney disease and inflammatory bowel disease for EPO. It is well known that glycosylation of therapeutic glycoprotein correlates with product safety, efficacy and quality. Thus it has become important to characterize its composition and molecular heterogeneity. In this study, we have developed a top-down approach using chip-based C8 nano-LC/Q-TOF MS. MS parameter was optimized such as gradient, flow rate, fragment voltage to get the best performance. The top-down approach should be preferable in the field of biopharmaceutical as it is relatively fast and more simplified sample preparation procedure. MAbs having neutral glycans and EPOs containing highly sialylated glycans are used to show the proof of concept for the method. We could directly monitor the multiple charge-state distribution and identified the presence and abundance of different glycoform with low nanogram levels of intact glycoprotein. The results can be applied to quality control evaluator and production of biotherapeutic glycoprotein. Especially method can satisfy the need for evaluating the similarity of the glycosylation profiles between biosimilar and innovator products.

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Application Research of Molecular Dynamics with Periodic Boundary Conditions for Long Alkyl Chain Aromatic Compounds by using CCS values and Ion Mobility

임동완 AHMED ARIF 이슬기다운 김성환*

경북대학교 화학과

Detailed structural characterization of compounds comprising crude oil is one of the important research topics in Petroleomics. Our previous study (Ahmed, A. et al., Anal.Chem. 86, 3300-3306, 2014) has shown the advantage of combining ion mobility mass spectrometry (IM-MS), ultrahigh-resolution mass spectrometry and theoretical collisional cross-section (CCS) calculations to increase the amount of information gained as well as to determine the molecular structures of aromatic compounds in crude oils. However, the result of previous study was limited to determine non-alkylated or short-chain alkyl aromatic compounds. In this research, we demonstrate that molecular dynamics (MD) simulation with Periodic Boundary Conditions (PBC) is a useful tool to investigate mutual relation between the theoretical CCS values from computational chemistry and experimental CCS values from ion mobility, especially for long-chain alkyl aromatic compounds in crude oil.

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Stability of Volatile organic compounds (VOCs) depending on storage temperature and duration of urine samples

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Volatile organic compounds (VOCs), ubiquitous environmental pollutants, are the organic compounds that have a high vapor pressure at room temperature. VOCs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA and cause cell mutations. Therefore, monitoring of VOCs in biological samples is very important to evaluate correlation between exposure of VOCs and human disease. However, the levels of VOCs in biological samples can vary depending on storage temperature and duration of samples because of low boiling points of VOCs. In this study, we investigated stability of 14 VOCs depending on storage temperature and duration of urine samples to establish optimal sample handling conditions. Aliquots of urine were stored at room temperature (25°C), refrigerator (4°C), or freezer (-20°C) conditions for either 1, 3, 7, 14, or 30 days. The levels of 14 VOCs in urine samples were detected by solid-phase microextraction-gas chromatograph-mass spectrometry (SPME-GC-MS). Alteration of urine samples is clearly storage temperature and duration dependent for almost all analyzed VOCs. This study provides detailed knowledge regarding stability of VOCs in urine samples and will help to ensure the reliability of laboratory test results.

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Structural identification of Nitrogen compound in Crude oils using high resolution MS/MS

조은지 김성환*

경북대학교 화학과

Oil is the energy source that become increasingly depleted. Therefore, it is important to find out the chemical composition of the oil and use it efficiently. There are many studies on analyzing the chemical compositions of crude oil. gas chromatography-Mass spectrophotometry (GC-MS) has been used to analyze light constituent of crude oil, but this is limited for the heavy constituents. This study shows the results of structural analysis of nitrogen compounds observed with different ionization methods, (+/-) ESI or APPI. The nitrogen composition mentioned either high molecular weight, polycondensed, or polar compounds that cannot be detected by using conventional techniques. Therefore, ultrahigh-resolution mass spectrometry (UHR-MS) is used to analyze heavy compounds. In addition, MS/MS spectra showed core structures of nitrogen compound of crude oil.

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The Analysis of TDI and TMP reactionproduct using MALDI-MS

이성엽 김혜진 강경민 전소라 김성호*

순천향대학교 화학과

TDI(toluene diisocyanate)와 TMP(trimethylolpropane)반응은 urethane 결합을 이루는 폴리머반응으로 진행된다. 따라서 반응 생성물은 13 종류 이상의 시리즈 형태로 생성된다. 모든 가능성 있는 분자량을 계산을 통하여 예측하고, MALDI-MS 를 이용하여 생성된 반응혼합물을 확인하였다. 이 방법을 통하여 MALDI-MS spectrum 의 대부분을 확인하였으며, 반응조건, 시간변화에 따른 생성물의 차이를 확인 및 검증 하는 방법으로 pre-polymer 형성에 대한 reaction monitoring 을 실시 하였다. 그리고 LC-MS, IR 등의 결과를 보조적으로 이용하여 pre-polymer 생성 반응을 체계적으로 설명하였다.

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Reliable DB for High-throughput Screening of Therapeutic Antibodies Glycosylation Using LC-MS and LC-MS/MS

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충남대학교 분석과학기술대학원

Biosimilar products of monoclonal antibodies (mAbs) are one of the most fast-growing segment of the biotherapeutic market. They commonly have advantages of specificity to targeted antigens and lower safety issues in clinical trials than many other type products. As patents on clinical mAb were beginning to expire, many pharmaceutical companies have been interested in developing for biosimilars. In producing recombinant mAb, glycosylation is considered as a crucial protein quality attribute. Because it is the key factor that can affect to biological activity, as protein stability and immunogenicity, of a therapeutic glycoprotein. Additionally, recombinant antibodies being expressed from non-human mammal cell lines could have the unexpected glycosylation that introduced by host cell's original glycosylation synthesis. Thus, glycosylation with micro heterogeneity should be screened for modulating protein quality. For identifying the desired/undesired glycosylation, accurate mass was used to compositionally annotate and profile N-glycans while tandem MS using CID was employed for structure elucidation. Here, we created glycoform database for rapid identification and structural elucidation of antibody N-glycosylation based on LC-MS and LC-MS/MS analysis. RT, accurate mass, and diagnostic fragment peak were summed up to identify each glycan. Up to now, glycans from five representative mAbs including adalimumab, bevacizumab, infliximab, rituximab and trastuzumab were analyzed and total 27 glycans were incorporated to database. The glycan DB could be applied with high-throughput glycan characterization method of therapeutic antibodies produced by various cell-based expression systems in pharmaceutical industry.

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Time-dependent ^{31}P NMR analysis of GTP hydrolysis in paclitaxel-stabilized microtubules

백윤기* **이효원[1]**

한국기초과학지원연구원 대구센터 [1]충북대학교 화학과

Microtubule dynamics is the chemotherapeutic target of several anticancer drug agents such as paclitaxe (Taxol, BMS), decetaxel (Taxotere, Aventis), and ixabepilone (Ixempra, BMS). The dynamics is regulated by rapid exchange and hydrolysis of the tubulin-bound guanine nucleotides [1]. However, the instability of microtubules and the small numbers (~2%) of the embedded nucleotides have made it difficult to directly observing the hydrolysis status of microtubule-bound GTPs. Recently, we have reported a protocol for NMR sampling of lyophilized microtubule in order to analyze quantitatively the biochemical effects of paclitaxel on the GTPase activity of tubulin [2]. Here, we report the ^{31}P NMR spectra of paclitaxel-bound microtubules acquired as a function of drug-loading time. The spectral analysis indicated that the fraction of unhydrolyzed guanine nucleotides in the polymerized tubulin increased as the duration of paclitaxel treatment time was increased from 1 to 20 hr. The NMR result is also consistent with general findings that paclitaxel lessens the GTPase activity of tubulin. References. [1] A. Dimitrove et al., Science 322, 1353 (2008). [2] G.H. Lee et al., Magn. Reson. Chem. 53, 330 (2015).

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Synthesis of silicon-coated carbon nanofibers on electroplated Co-Ni /C-fiber textiles for anode material of Li ion batteries

장건호 이상훈 이창섭*

계명대학교 화학과

In this study, carbon nanofibers(CNFs) were synthesized by thermal chemical vapor deposition(CVD) to Co-Ni electroplated on C-fiber textiles. The CNFs were coated with a SiO_2 layer by hydrolysis of Tetraethyl orthosilicate(TEOS) and Si@CNFs composite were synthesized by reduction of SiO_2@CNFs composite. SiO_2@CNFs and Si@CNFs were applied to the anode material of Li ion batteries. C-fiber textiles were oxidized with nitric acid before electroplating with Co-Ni catalysts. The oxidation process created the hydroxyl group on the C-fiber textiles, and the hydroxyl group was used as an active site for the electroplating of catalysts. After being electroplated, ethylene as a carbon source was flowed into a quartz tubular furnace heated to 700℃, and maintained for 1 h to synthesize CNFs. The CNFs were oxidized by nitric acid before being coated with silica via hydrolysis of TEOS. Coated silica layer on CNFs was reduced by inflow of H2 gas at 700℃. The characteristics of CNFs were analyzed by SEM, EDS, XPS and Raman. The SiO_2@CNFs and Si@CNFs were characterized using TEM, EDS and XPS. The as-synthesized CNFs, SiO_2@CNFs and Si@CNFs were directly employed as anode materials without any binder. The electrochemical characteristics of CNFs, SiO_2@CNFs and Si@CNFs as anodes of Li ion batteries were investigated using coin cell.

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Fabrication and Characterization of an Anode Materials for Li Secondary Batteries Based on four Carbon Materials - Si composites

김수진 박희구[1] 이창섭*

계명대학교 화학과 [1]계명대학교 화학시스템공학과

We have performed a study on the characteristics of Carbon materials -Si composites that used as an active anode materials for lithium secondary batteries. Samples employed for the battery test were commercial products of GNF, GNT, CNF and CNT. The test results of the samples were compared with the Si composites of each sample. The Si particles were ball-milled to a micron size and coated with pyrolytic carbon using by ethylene gas. Then it was finely mixed with respective two samples using ball mill. PTFE(Polytetrafluoroethylene) was used as the binder and glass fiber separator was used as the separator membrane for the composition of three electrode cell. As the electrolytes, 1M LiClO$_4$ was dissolved in a mixture of propylene carbonate(PC): ethylene carbonate(EC) in a 1:1 volume ratio. The four different Carbon materials-Si composites were evaluated as the anodic material in three electrode cells. The morphology and composition of the samples were analyzed by SEM and EDS measurements. Physicochemical properties of the samples were investigated using XRD, Raman spectroscopy and XPS. The electrochemical characteristics as an anodic material of Li secondary batteries were investigated using the galvanostatic charge?discharge and cyclic voltammetry measurements. Acknowledgements : 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. 2015035858).Acknowledgements : 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. 20151035858).

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Chemical behavior of non-visual on-line monitoring system in semiconductor manufacturing process

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단국대학교 화학과

Although semiconductor equipment industry is one of the high-profit fields integrated many state-of-art technologies, supporting material industry, its technical levels are not high as expected yet in our country. Since production efficiency and volume of chips have been improved by technical migration, the equipment control became very important for manufacturing process. So far, the efficiency control has been done by visual defect monitoring, However, it was revealed that the effect of non-visual defect on production loss is almost 30%. Therefore, a non-visual monitoring technique regarding on wafer contamination control and sample pre-treatment was developed in this work. Since the developed on-line monitoring system utilized various glassware, the chemical behavior of metal ions interested in the process was studied using ICP-MS, on the basis of lifetime of metal ions in acids.

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Combination of ring type separation and High resolution MS/MS for more information about constituents of Crude Oil compounds

하지현 조은지 김성환*

경북대학교 화학과

There are many studies on analyzing the chemical compositions of Crude Oil. Gas chromatography-Mass spectrophotometry (GC-MS) has been used to analyze light constituent of Crude Oil, but this is limited for the heavy constituents. The heavy constituents mentioned either high molecular weight, polycondensed, or polar compounds that cannot be detected by using conventional techniques. Latterly, Ultrahigh-resolution mass spectrometry (UHR-MS) is used to analyze heavy compounds. But UHR-MS technique has limitations. Ionization discrimination can limit the number of compounds observed by the technique. High-performance liquid chromatography (HPLC) ring-type separation is one of the methods to overcome limitations. The combined technique disclosed the aromaticity increased as the fraction number increased. The structures and distribution of heteroatom class compounds could be also explained using the combined technique. In addition, MS/MS spectra showed core structures of Crude Oil fractions.

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Identification of Lipsticks in the crime scene using analytical techniques

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경희대학교 화학과 [1]한국과학기술연구원(KIST) 특성분석센터 [2]국립과학수사연구원 화학분석과

In the crime scene, there remain many trace evidences and research that is related to trace evidence has been conducted actively to analyze the evidence more efficiently. Stain of lipstick, one of the many trace evidence, can be good evidence to find the suspect or anyone who is connected to the crime. It is necessary to make database because the components of the lipstick is slightly different depending on the kind of lipsticks. In this study, to make database for lipstick components, twenty one samples of three colors such as red, pink and orange were prepared. And we investigated the characterization of lipstick evidence using Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) and Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) and X-ray Fluorescence Analyzer (XRF). TOF-SIMS provides chemical information on surface of sample and their distribution without any treatment. ATR-FTIR is able to identify the molecular structure of lipsticks samples. And XRF is an instrument for analyzing component contained in the samples.

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Pepsin immunoassay for the diagnosis of laryngopharyngeal reflux disease

권지윤 현혜리 신재호*

광운대학교 화학과

A number of patients who complain of laryngopharyngeal reflux disease (LPR) is on the gradual increase due to changes in climate, environment, and eating habits. LPR causes hoarseness, frequent throat clearing, bitter taste in the mouth, referred ear pain, chronic cough and even larynx cancer. However, the effective treatment of LPR is difficult because the treatment yet stay in the inhibition of gastric acid secretion as well as the symptoms persist after treatment. Therefore, appropriate treatment through accurate and rapid diagnosis is necessary. Since pepsin is proteolytic enzyme produced only in the stomach, detection techniques of pepsin in saliva is useful as a sensitive and non-invasive method for the reflux of stomach contents. Therefore, pepsin is one of the most important biomarkers to diagnose LPR. Herein, we report on a new approach to design an immunoassay based on the enzyme-linked immunosorbent assay (ELISA). Binding of antigen-antibody converts a colorless substrate to a colored product by using enzyme. Furthermore, to confirm the presence of pepsin in saliva resulting from LPR, we checked the pH of saliva through the color changes of various kinds of indicator. The general pH of saliva is about 6.7, but in the case of saliva which contains pepsin, the pH decreases. We compared the color between different pH of phosphate buffer and artificial saliva in acidic and basic condition of indicators. In this ways, we investigate the utility of colorimetric immunoassay to determine pepsin in biological samples (i.e., saliva).

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Applications of LC-MS/MS and online H/D exchange experiments in metabolite identification and tissue distribution studies of an anticancer drug, cisplatin in rat kidney, liver and brain cancer tissues

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경희대학교 응용화학과

In vivo rat kidney, liver and brain tissue metabolites of an anticancer drug, cisplatin (CP), used for the treatment of mainly testicular and ovarian cancers, have been identified and characterized by using liquid chromatography positive ion electrospray ionization tandem mass spectrometry (LC/ESI-MS/MS) in combination with on line hydrogen/deuterium exchange (HDX) experiments. To identify in vivo metabolites, kidney, liver and brain tissues were collected after intravenous administration of CP to rats (n=3 per group). A total of thirty one, seventeen and four in vivo metabolites have been identified in kidney, liver and brain tissue homogenates, respectively. The structures of metabolites were elucidated based on fragmentation pattern using LC-MS/MS and accurate mass measurements combined with HDX experiments. These HDX experiments were used to further support the structural characterization of drug metabolites. The results showed that CP undergoes a series of ligand exchange biotransformation reactions with water and other nucleophiles like thio groups of methionine, cysteine, acetylcysteine, glutathione, thioether and thiol. Further, the developed LC/ESI-MS/MS method was successfully applied to investigate the distribution of CP in kidney, liver and brain tissues after intravenous administration of CP to rats. The results showed that the higher amount of CP was distributed in kidney followed by liver and brain which indicated that CP mainly accumulated in kidney tissues and renal excretion might be a primary and main elimination route. The identification of metabolites and distribution of CP in rats provide an essential information for further pharmacological and clinical studies of CP, and may also be useful to develop various effective new anticancer agents.

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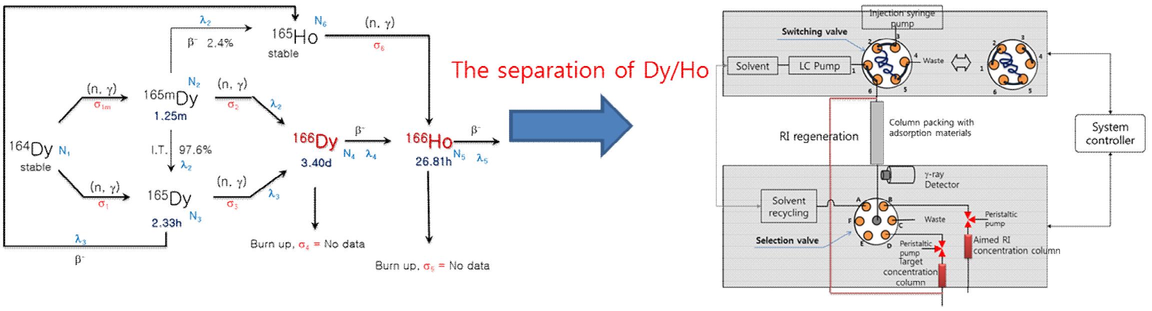
진단치료용 동위원소 생산을 위한 (n,γ)β핵종의 분리 (The separation of (n,γ)β reaction isotopes for production of theragnostic isotope)

최강혁

한국원자력연구원 동위원소이용연구부

방사성란탄족동위원소는 치료용 핵종으로 암환자의 암세포를 괴사시키는 능력이 있다. 특히, (n,γ)b 핵반응의 경우는 생성되는 모핵종과 딸핵종이 다르기 때문에 적당한 분리기술을 도입하면 비방사능(Specific Activity)이 높은 핵종을 얻을 수 있어 방사선면역체료제와 같은 방사선표적치료제 개발에 있어서 중요한 역할을 담당한다. 란탄족 동위원소의 특징은 용액상에서 +3 가이온을 가지며, 화학적인 성질이 유사하여 분리하는 방법이 쉽지 않다. 본 발표에서는 한국원자력 연구원에서 개발한 방사성동위원소의 차폐분리를 위한 분리 시스템과 방사성동위원소 취급에 있어서 작업자의 피폭을 최소화하며, 고순도, 고비방사능을 가진 동위원소의 분리 과정을 소개하고자 한다.



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Home-built solid-state NMR probes for the structural studies of biological samples like membrane proteins and the in-situ analysis of nano-materials

최성섭 정지호 김지선 김용애*

한국외국어대학교 화학과

The solid-state NMR spectroscopy has been widely used for various insoluble materials like industrial polymers and biological samples. Also, solid-state NMR analysis of membrane protein on a membrane-like environments, such as bicelle and bilayer, is especially valuable for their structure and function relationship. However, most of biological proteins on lipid bilayers have high dielectric property due to containing large amounts of lipids and salts. Therefore, specific probe with high efficiency and high capacity is required to study biological samples by using solid-state NMR. Also solid-state NMR methodologies for structural study of membrane protein in bicelle could be used for the in-situ analysis of liquid crystalline materials in LCD panels and lithium and fluorine in Li ion batteries. Here, we present the development of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil for structural study of membrane protein. We also present the development of a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a solenoidal coil for analysis of industrial materials. These probes provide short and strong RF pulses, high power capability, and good RF homogeneity.

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Expression, purification, and NMR Structural Studies of syndecan-4 as a transmembrane protein

김태형 김지선* 최성섭* 김용애*

한국외국어대학교 화학과

Syndecans as cell surface receptors participate in biologically important cell-cell and cell-matrix interactions and interact with numerous potential ligands including growth factors and extracellular matrix molecules. The syndecan protein family has four members. One of them, Syndecan-4 is a protein that in humans is encoded by the syndecan-4 gene. They may affect tissue development and repair and growth-factors as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4 is consisted of 25 hydrophobic amino acids and involved in formation of dimer, which is crucial for transduction of signals. Thus, we demonstrated an optimized methods for recombinant expression and purification of syndecan-4(Syd4), mutant Syd4-TM(mSyd4) and Syd4-eTC. The mSyd4 has a partially modified sequence of wtSyd4 and Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of syndecan-4.All peptides were purified by semi-preparative reversed-phase HPLC after cleaving the fusion partner with CNBr. Their biophysical properties of peptides were studied by circular dichroism (CD), mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy. CD spectra were presented that Syd4 analogues adopt a stable α-helical structure in micelle environments. Optimized structure of Syd4 analogues based on solution NMR spectroscopy and solid-state NMR spectroscopy based on 2D SAMPI4 were reinforced with Molecular Dynamics Simulation.

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Efficient analysis of arsenic contaminant in the ground water with capillary electrophoresis mass spectrometry

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서울대학교 화학부

In Korea, arsenic contaminants from trash yards and dead mines are becoming an issue. These contaminants dissolve in to the ground water and endanger water supplies for home, agriculture uses. We present using capillary electrophoresis and its applications to analyze arsenic compounds in the ground water with high efficiencies. Although capillary electrophoresis is suitable for aqueous sample analysis, In case of real samples, applications of capillary electrophoresis mass spectrometry with various enhancing methods still have some obstacles, such as excess amount of salt and other abundant residues. First we applied electrokinetic supercharging, consisting of transient isotachophoresis and field amplified sample injection, to overcome these obstacles. Then, we modified electrospray head unit to control flow in the capillary, which helps to conduct counter flow electrokinetic supercharging and online liquid microextraction. This poster presents the work of flow that approaches to analysis of arsenic contaminants.

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A Novel Non-enzymatic Glucose Sensor using Titanium dioxide(G)/Poly(3-aminophenylboronic acid)/Gold Nanocomposite Electrode

<u>Nallal Muthuchamy</u> 이광필[1,*] A.Gopalan[2]

경북대학교 과학교육학과 [1]경북대학교 화학교육과 [2]경북대학교 차세대에너지기술연구소

In this work, we have fabricated a non-enzymatic (enzyme-free) glucose sensing electrode using a new nanocomposite based electrode comprising of titanium dioxide (TiO_2), graphene (G), poly(3-aminophenylboronic acid) and gold nanoparticles (AuNPs) (designated as TiO_2(G)/PAPBA/Au-NCE) for electrochemical and photoelectrochemical glucose detection. The electroactivity and inter-facial characteristics of TiO_2(G)/PAPBA/Au-NCE were evaluated by cyclic voltammetry (CV), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS). The photo electrochemical behavior of TiO_2(G)/PAPBA/Au-NCE was evaluated in the presence of glucose by CV, CA and linear sweep voltammograms (LSV). The peak current for glucose oxidation showed a linear dependence with concentration of glucose in a wider range, 50 ?M to 18 mM. The TiO_2(G)/PAPBA/Au-NCE exhibits much higher and stable photocurrent intensities than that of the photoelectrochemical biosensors reported so far. Importantly, the peak current of glucose oxidation current was not influenced at TiO_2 /PAPBA/Au-NC in the presence of electrochemical interfering substances, such as L-ascorbic acid, acetaminophen and uric acid. The results from our studies clearly suggested that TiO_2(G)/PAPBA/Au-NCE would be ideally suitable for non-enzymatic glucose detection by electrochemical and photoelectrochemical methods.

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Preparation of various ground organic monolith particles as chromatographic separation media

김윤성 정원조*

인하대학교 화학과

We have recently reported a pioneering study on ground organic monolith particles as new chromatographic separation media in our laboratory. The reaction mixture was composed of methacrylic acid (MAA) as funtional monomer, Trimethylolpropane trimethacrylate (TPTM) as crosslinker, azobis-isobutyronitrile (AIBN) as initiator, polyethyleneglycol as special porogen, and toluene- Isooctane mixture as solvent. In this study, we have prepared different stationary phases by changing formulation of reaction mixture and reaction temperature in a variety of different ways. For example, xylene and n-octane were used as new solvent to increase the reaction temperature. The key idea of this approach is to make soft monoliths with large pore volumes for easy pulverizing. The variations of morphology and chromatographic separation performance of the resultant organic monolith particles will be comparatively discussed.

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Further study of PEEK encased monolith frits resulting upgraded separation performance in LC

박신영 정원조*

인하대학교 화학과

As a stream of studying for development of disposable HPLC column, our research group has been studying the technique of polymer encased monolith frits. It is very useful and novel technique owing to its reasonable price and potential of being further improved in a terms of theoretical number of plates. Thus, we have carried out some modification in the physical dimension of monolith frits encased in polymer tubing. To reduce the void volume of frit, the I.D. of poly ether ether ketone (PEEK) tubing was reduced from 500 um of the previous study to 250 um in this study. Catalyst assisted sulfornation of PEEK tubing and reaction with glycidyl methacrylate (GMA) were adopted again to improve the bonding strength between the monoltih core and the tubing inner surface. After sulfornation and anchoring of double bonds, the tubing was filled with a reaction mixture of lauryl methacryltate (LMA), ethylene glycol dimethacrylate (EDMA), initiator, and porogenic solvent. After in-situ polymerization, the tubing was thoroughly washed. Finally, it was ready to be used as frit element after cutting into thin slices. To check the frit performance comparatively, the packed columns installed with a PEEK encased frit of 250 um I.D., a PEEK encased frit of 500 um I.D., and a commercial stainless steel screen frit (1.6 mm I.D.), respectively, at the column outlet union, have been prepared. The separation efficiency with a monolith frit of 250 ㎛ I.D. showed the best results.

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A new C18 phase based on silica monolith particles showing enhanced separation efficiency in HPLC

AliAshraf 정원조*

인하대학교 화학과

Partially or fully sub-2?m porous silica particles have proved strong feasibility as column packing material due to enhanced separation efficiency and rapid separation in liquid chromatography. Partially sub-2 ?m porous silica monolith particles of relatively uniform size have been successfully prepared by sol gel process followed by grinding and calcinations at 550˚C. The production scale has been increased twenty times in comparison to our previous study. These particles were derivatized with C18 (chlorodimethyl octadecylsilane) ligand in anhydrous toluene under reflux followed by end capping with HMDS (hexamethyl disilazane) and TMCS (trimethyl chlorosilane). The C18 bound phase was washed thoroughly and packed in a glass-lined stainless steel micro-column (1.0 mm ID and 300 mm length) using a slurry packer at a high packing pressure (18000 psi). The separation efficiencies as high as 139,000 N/m were achieved for a test mixture containing benzene and its four derivatives in 60/40 acetonitrile/ water (v/v %) with 0.1% TFA at a flow rate of 25?L/min. The separation efficiency of current stationary phase is better than that of common commercial C-18 phase. This new phase also has shown the promising possibility for fast analysis when packed in a short column.

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Investigation on Raman spectral features of lactose/PE pellets prepared with different particle sizes

전슬아 정회일*

한양대학교 화학과

To investigate the variation of Raman spectral feature depends on particle size and its influence on accuracy of quantitative analysis, pellets composed of lactose (5-15wt%) and polyethylene (PE) were prepared, and the corresponding Raman spectra were acquired. For the preparation of pellets, the sizes of lactose were varied (below 50, 50-100, 100-200, 200-300, over 300um), while the size of polyethylene (PE) was unchanged. When the size of lactose particle was smallest, the band shape was dissimilar to those with different particle sizes. The origin for the difference is now under investigation in conjunction with the particle size as well as porosity using Monte-Carlo simulation. Finally, the lactose concentrations were determined using partial least squares (PLS) regression and the dependency of accuracy on the particle size was searched.

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Electrochemical detection of bisphenol A separated from molecularly imprinted polymer-solid extract phase tube

설다운 **PhamKhacDuy** 정회일*

한양대학교 화학과

Bisphenol A (BPA) is widely used for production of epoxy resin, polycarbonate and polyethylene. Since BPA is one of the endocrine-disruptors, its detection with simple and cost-effective scheme is greatly demanding. For this purpose, we developed a molecularly imprinted polymer (MIP) able to separate BPA in mixture samples and then a simple electrochemical detection utilizing a mechanical pencil lead as a working electrode was proposed. Since a mechanical pencil lead is cheap and easily obtainable, it could be potential for BPA detection. Initially, BPA-selective MIP was developed and its performances such as percent recovery were investigated. Then, the captured BPA was measured using a mechanical pencil lead electrode using stripping voltammetry and the resulting analytical merits such as limit of detection and response range were assessed. In addition, the same strategy was applied to detect capsaicin as a method for identify domestic and Chinese red peppers.

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Finding an optimal temperature able to improve accuracy for Raman spectroscopic identification of adulterated olive oils

류동현 정회일*

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Identification of adulterated olive oils is critically demanding for its fair product value evaluation. For fast and simple identification, Raman spectroscopy could be a proper candidate since it provides rich structural information of components and the spectral acquisition is non-destructive without requiring further sample pretreatments. Since molecular vibrations of components diversely vary according to temperature, an optimal temperature able to provide enhanced spectral difference between pure and adulterated olive oils would exist. For the study, adulterated extra virgin olive oil mixed with soybean oils was initially prepared. Then, a glass vial containing a sample was initially immersed in liquid nitrogen for sufficient cooling and the vial containing the sample was quickly taken out for continuous Raman spectral collection during natural temperature elevation up to near room temperature. During the temperature elevation, 50 snapshot spectra were collected. Using spectra collected at each snapshot, the identification of adulterated olive oils was attempted and a snapshot providing most discriminant spectral feature was found. The varied spectral feature at the optimal temperature was explained.

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Study on elution behavior of non-spherical gold nanoparticles in asymmetrical flow field-flow fractionation (AF4)

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Asymmetrical flow field-flow fractionation (AF4) is a diffusion-based separation technique that has been used widely for characterization of various types of colloidal particles and macromolecules. In AF4, the particles (or molecules) of different sizes migrate down the channel at different velocities due to the difference in their diffusion coefficients, yielding a size-based separation.Non-spherical particles have non-uniform diffusive (spreading) movement along the directions of the major and minor axis, while spherical particles have a uniform diffusive movement in all directions.In this study, a theory was developed on the elution behavior of non-spherical particles in AF4. In order to test the proposed theory, non-spherical gold nanoparticle (AuNR) of different aspect ratios were synthesized using the see-mediated growth method, which were coated with cetyl trimethyl ammonium bromide (CTAB) to prevent particle aggregation. The elution behavior of non-spherical particles in AF4 will be discussed based on the measured retention data of the AuNRs.

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C-terminal Modification with Putrescine for Relative Quantification by LC-MS

김상진 임재민*

창원대학교 화학과

Proteins are associated with many diseases such as cancer and diabetes. Recently protein quantitative analysis was diagnosed biomarker of many diseases by mass spectrometry. Protein quantification by mass spectrometry was generally used the isotope labeling. The use of typical isotope tags have developed in vivo or in vitro labeling techniques like the stable isotope labeling by amino acids in cell culture (SILAC), Isotope-coded affinity tag (ICAT) and H_2O^{18} protease technique.In this study, we have developed carboxyl modification of peptides as a method for quantitative analysis using normal putrescine (1,4-butanediamine) and heavy putrescine (1,4-butane-d8-diamine) by mass spectrometry. The carboxyl-reactive amidation reagent 1-[Bis(dimethylamino)methylene]-1H-1,2,3-triazolo[4,5-b]pyridinium 3-oxid hexafluorophosphate (HATU) is used to amidate the carboxylic acid group of the peptide angiotensin II and the tryptic digested albumin peptides to normal putrescine and heavy putrescine.As a result, amidation reaction using HATU with heavy putrescine as labeling shows 8 Da difference in comparison with original peptide which can overcome the isotope distribution overlapping. In addition, the carboxyl modified peptides increased the most abundant charge state compared to native peptides to enhanced fragmentation for electron-transfer dissociation (ETD).

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Quantitative Analysis of Perfluorinated Compounds (PFCs) in Stream of Changwon by LC-ESI-MS

서현경 임재민*

창원대학교 화학과

Recently, as a new environmental pollutant is increasing interest in perfluorinated compounds (PFCs). PFCs is a materials which is substituted by fluorine on the hydrogen position of the hydrocarbon chain. The high stability of the molecule because of strong covalent bonding between carbon and fluorine. Therefore, it does not react with other materials hydrolysis, photolysis, biodegradable, has a resistance to metabolic degradation. Because of these properties water-resistant, oil-resistant, surface treatment agent, surfactant was used in many industries for over 50 years. It is detected in almost all the environmental media. The purpose of this study is a quantitative analysis of PFCs in stream of Changwon using LC-ESI-MS. To obtain a calibration curve, the PFCs standards were used for quantitative analysis. The concentration distribution of the PFCs was mapped at the sixteen sampling site in stream of Changwon.

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Analysis of fluorescence-labelled starch using asymmetrical flow field-flow fractionation (AsFlFFF) with multiple detectors

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한남대학교 화학과 [1]Hebei University, China [2]Lund University, Sweden

Starch is a mixture of amylose (AMY) and amylopectin (AMP). AMY molecules are essentially linear, while AMP molecules have branches with 5-6% alpha-(1,6) linkages. Usually AMY and AMP are different in physical properties such as molar mass, radius of gyration (R_g) and hydrodynamic radius (R_h). The rheological and functional properties of starch are influenced by various factors including the molecular size, molar mass distribution and the concentration ratio of AMY to AMP. It is also important to analyze proteinaceous material in starch for characterization of starch.In this study, asymmetrical flow field-flow fractionation (AsFlFFF) was employed for separation and quantitation of AMY and AMP. AsFlFFF was coupled with multiple detectors such as multi-angle light scattering (MALS) and refractive index (RI) detectors for determination of absolute molar mass, molar mass distribution, and molecular structure without the need for system calibration. And then, for analysis of proteinaceous matter in starch, starches were fluorescence-labelled, and then analyzed by AsFlFFF coupled with a fluorescence detector.

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Collection and characterization of airborne using an electrical charge-based particle collector and field-flow fractionation (FFF)

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Airborne is a particulate matter (usually having the particle size ranging 0.1~200 μm) that floats or flies in air. They are formed by either natural or artificial occurrence such as sand dust or the use of fossil fuels in power plants. They react with chemical substances, and produce compounds such as sulfate or nitrate. Frequently they contain heavy metals or toxic organic compounds. Depending on the particle size, they show different behaviors, and sometimes, affect the human health and the environment. It is thus necessary to be able to identify the cause of occurrence and to analyze the particle size and chemical composition of the airborne. For accurate analysis of airborne particles, efficient and representative sampling is required. In this study, a new airborne collector was implemented and tested. This new airborne collector employs an electrical force, and does not need a filter, allowing to avoid adsorption or modification of the particles by the filter. Also it does not require the sample concentration such as drying, washing, vortexing and centrifuging. Split flow thin cell fractionation (SF) is a continuous separation method, allowing a large-scale separation of particles into two populations of different size ranges. SF was employed to separate the collected airborne particles into two populations (one in nanometer and another in micrometer ranges). Field-flow fractionation (FFF) is a size-based separation technique that is useful for analysis of colloidal particles. Collected airborne particles were analyzed by FFF for determination of the particle size and its distribution. An inductively coupled plasma mass spectrometry (ICP-MS) was also employed for compositional analysis of the collected airborne particles.

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Preparation and characterization of lipid vesicles using dynamic light scattering and asymmetrical flow field-flow fractionation

한수정 최재영 Lars Nilsson[1] Haiyang Dou[2] 이승호[*]

한남대학교 화학과 [1]Department of Food Technology, Lund University [2]Hebei University

Vesicles are spherical shells composed of lipid bilayers that encapsulate an aqueous space. They have been used frequently as model membranes, and as nanoscale containers for drugs and other substance in the pharmaceutical and cosmetic industries. When vesicles are used for drug delivery, the stability (and the life-time) of the vesicles is directly related with their medicinal effect. Generally the stability of vesicles is related with the size and size distribution of the vesicle. Thus size characterization of vesicles is necessary for understanding of the vesicle stability. The dynamic light scattering (DLS), optical microscopy (OM), electron microscopy (EM), nuclear magnetic resonance (NMR) and nanoparticle tracking analysis (NTA) have been used for size analysis of particulate materials. Among them, DLS is simple to use, and has been widely used for measuring the particle size and its distribution. Sometimes, however, application of DLS is limited, especially when dealing with samples of complex mixtures or those of broad size distributions. Field-flow fractionation (FFF) is useful for separation and size characterization of particles having broad size distributions from a few nm up to about 100 μm. Asymmetrical flow field-flow fractionation (AsFlFFF), a member of FFF, is useful particularly for characterization of aqueous colloidal particles. In this study, nano-sized vesicles were prepared by extrusion, and then were analyzed by AsFlFFF for determination of the particle size distribution and for the stability test. Results from DLS and AsFlFFF were then compared.

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Optimization of fractionation efficiency (*FE*) and throughput (*TP*) in a large scale splitter less full-feed depletion SPLITT fractionation (FFD-SF)

유영석 최재영 김운중 음철헌[1] 이승호*

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Split-flow thin cell fractionation (SPLITT fractionation, SF) is a particle separation technique that allows continuous (and thus a preparative scale) separation into two subpopulations based on the particle size and the density. In a conventional mode (conventional SF), there are two inlets and two outlets in the SF channel, which is equipped with a flow stream splitter at the inlet and the outlet of the channel, respectively. On the other hand, in the full-feed depletion mode (FFD-SF), there are only one inlet for the sample feed, and the channel is equipped with a flow stream splitter only at the outlet. In SF, there are two basic performance parameters. One is the throughput (*TP*), which was defined as the amount of sample that can be processed in a unit time period. Another is the fractionation efficiency (*FE*), which was defined as the number % of particles that have the size predicted by theory. In this study, a FFD-SF channel was developed for a large-scale fraction, which has no flow stream splitters ('splitter less FFD-SF'), and then was tested for optimum TP and FE by varying the sample concentration and the flow rates at the inlet and outlet of the channel. Polyurethane (PU) latex beads having two different size distribution (about 3 ~ 7 μm, and about 2 ~ 30 μm) were used for the test. The sample concentration was varied from 0.2 to 8 %wt/vol. The channel flow rates were varied from 70 to 160 mL/min. The fractionated particles are monitored by optical microscopy (OM). The sample recovery was determined by collecting the particles on a 0.1 μm membrane filter.

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Quantitative Analysis of Calcite in Desulfurization Gypsum Using Raman Spectroscopy

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한양대학교 화학과

According to the recent study some of gypsum board release Radon. Because a few gypsum board made by only phosphate gypsum. Phosphate gypsum has radioactive elements like U, Th. And Radon is formed as one intermediate step in the normal radioactive decay chains through which thorium and uranium slowly decay into lead. So many gypsum board manufacturer reduce amount of phosphate gypsum and increase amount of desulfurization gypsum. FGD Gypsum is a unique synthetic product derived from flue gas desulfurization (FGD) systems at electric power plantsTherefore increase demand of desulfurization gypsum analysis.In this study, It purpose that Existing analysis method of desulfurization gypsum replace new analysis method using Raman spectroscopy. Raman spectroscopy have many advantage like quick analysis, On-line analysis, nondestructive analysis. And it is possible that real time analysis.

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Chromo/fluorogenic detection of metal ion in sancho (zanthoxylum schinifolium) by the simple Schiff base sensor

정연기* 이기환* 최남규 강충호 **Muhammad Saleem** 최창식[1]

공주대학교 화학과 [1]극동대학교 한약발효학과

Recently, the hazard may appear due to the use of synthetic preservatives that have been used widely in the existing industry revealed by several studies. Therefore, the development and discovery of natural preservatives is a necessary condition. The natural substance derived from an organic material including lower fatty acid, lysozyme, lactoferrin, bacteriocins, and a polylysine can be frequently employed as a preservative in various foodstuffs. In particular, the utility of preservatives in the cosmetics products is of immense interest. One of herbal oriental medicines, sancho (zanthoxylum schinifolium) has revealed medicinal activities including anti-platelet aggregation, anti-oxidant, anti-inflammatory, and anti-tumour effects. Also, sancho has the potential to nutraceutical and cosmetic resources having biological activities. Therefore, we attempted to detect hazardous pollutants such as metal ion to use the sancho extracts for the cosmetics preservatives.

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Displacement phenomena in Serial Affinity Column Set (SACS)

<u>윤민규</u> 조원련*

원광대학교 바이오나노화학부

The work described here examines displacement phenomena that play a role in lectin affinity chromatography and their potential to impact reproducibility. This was achieved using Lycopersicon esculentum lectin (LEL), a lectin widely used in monitoring cancer. Four small LEL columns were coupled in series to form a single affinity chromatography system. The serial affinity column set (SACS) was then loaded with human plasma proteins. At the completion of loading, the column set was disassembled, the four columns eluted individually, the captured proteins trypsin digested, the peptides deglycosylated with PNGase F, and the parent proteins identified through mass spectral analyses. Significantly different sets of glycoproteins were selected by each column, some proteins appearing to be exclusively bound to the first column while others were bound further along in the series. Clearly sample displacement chromatography (SDC) occurs. Glycoproteins were bound at different places in the column train; identifying the presence of glycoforms of different affinity on a single glycoprotein.

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Highly sensitive SERS-based immunoassay as an early diagnostic tool in rheumatoid arthritis

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Rheumatoid arthritis is both common and chronic, with significant consequences for multiple organ systems. The key to therapeutic success lies in identifying individuals who will have severe destructive disease as early as possible, so that effective treatment can be initiated before irreversible damage occurs. Anti-cyclic citrullinated peptide (anti-CCP) antibody is well known biomarker as a particularly useful biomarker in the diagnosis of RA, with high specificity, presence early in the disease process, and ability to identify patients who are likely to have severe disease and irreversible damage.In this study, we assessed the clinical feasibility of conducting immunoassay based on surface-enhanced Raman scattering (SERS). An anti-CCP was used as a biomarker, magnetic beads conjugated with CCP were used as substrates, and the SERS nano-tags were comprised of anti-human IgG-conjugated hollow gold nanospheres (HGNs). We were able to determine the anti-CCP serum levels successfully by observing the distinctive Raman intensities corresponding to the SERS nano-tags. At high concentrations of anti-CCP (>25 U/mL), the results obtained from the SERS assay confirmed to those obtained via an ELISA-based assay. Nevertheless, quantitation via our SERS-based assay is significantly more accurate at low concentrations (

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Development of SERS imaging-based lateral flow immunosensor for rapid and sensitive detection of food toxin

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Lateral flow immunoassay (LFIA) is uncomplicated and intended assay method to detect the presence of an antigen in sample without the need for specialized or costly equipment. However, some of the problems associated with low sensitivity and limitations in quantitative analysis have made this technique less attractive. Here, we developed a surface-enhanced Raman scattering (SERS) imaging-based lateral flow immunosensor to overcome the limitation of conventional LFIA kit. In SERS imaging-based LFIA strip sensor, all the measurement principle is same with conventional LFIA strips except detection nanoprobes. The Raman-reporter labelled hollow gold nanosphere (HGN) was used as a SERS nanoprobe instead of gold nanospheres used in conventional LFIA strips. To verify the feasibility of the devised SERS imaging-based LFA strip platform, an immunoassay of staphylococcal enterotoxin B (SEB) was performed as a model reaction. The presence of SEB can be identified through the color change of the test zone. In addition, a highly precise quantitative evaluation of SEB is possible by averaging the SERS mapping signals. The sensitivity of proposed LFIA sensor was compared with contrast imaging analysis of test zone and conventional ELISA method. The LOD of the proposed LFIA sensor was estimated to be 1 pg/mL, and this low LOD value demonstrates that our SERS imaging-based LFIA immunosensor is approximately three orders of magnitude more sensitive than corresponding control methods. Accordingly, our SERS-based LFIA strip sensor shows significant potential for the rapid and sensitive detection of target markers in a simple manner.

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Wash-free immunoassay of prostate specific antigen using SERS-based microdroplet sensor

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We report a conceptually new immunoassay technique using SERS-based microdroplet sensor. Our proposed method offers a fast and sensitive assay applicable to PSA cancer marker in serum. The sensor used in this study is composed of four different compartments; the generation of microdroplets for fast PSA immunoreactions, the separation between immunocomplexes and supernant solution, the isolation of magnetic immunocomplex droplets, and the collection of SERS nano tag droplets for Raman detection. This technique allows a convenient immunoassay of PSA marker without any washing process since the magnetic immunocomplexes can be easily isolated by the droplet splitting into two smaller parts after the application of magnetic bar. Raman signals of the remaining SERS nano tags in the large droplet (supernatant solution) were measured for the quantitative evaluation of PSA marker. SERS signals for 240 droplets (8 Hz) were measured and averaged for the quantitative evaluation of PSA. The LOD, determined by our SERS-based microdroplet sensor, was estimated to be below 0.1 ng/mL for PSA cancer marker, and this value is much lower than the clinical cut-off value for the diagnosis of prostate cancer. In addition, rapid analysis with a tiny volume of sample is possible since all the process can be automatically carried out in the specially designed microdroplet channel. As a result, this SERS-based assay technique is expected to be a potential clinical tool for early diagnosis of prostate cancer.

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Highly sensitive detection of HIV-1 DNA using SERS-based lateral flow immunosensor

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We report a surface-enhanced Raman scattering (SERS)-based lateral flow assay method for the highly sensitive detection of target nucleic acids. Human immunodeficiency virus type 1 (HIV-1) DNA was used as a model analyte in this work. Here, Raman reporter (Malachite green isothiocyanate (MGITC)) and detection-DNA co-functionalized gold nanoparticles (AuNPs) were employed as SERS nano tags for targeting specific nucleic acids. In the presence of HIV-1 DNA, the sandwich type “detection DNA-conjugated SERS tag - target DNA - capture DNA” hybridization reactions occurred and the SERS tags induced strong Raman intensities on the test line. On the contrary, without HIV-1 DNA, the SERS tags could not be captured on the surface of test line, resulting in very low or no SERS intensities. With the increase of HIV-1 DNA concentration, the SERS intensities on the test line were gradually increased. The characteristic Raman scattering peak intensity of MGITC was measured for the quantitative detection of HIV-1 DNA. Under optimized conditions, the minimum detectable concentration for our SERS-based lateral flow assay was 0.5 pM, which was improved about 200-fold compared with the colorimetric detection approach or fluorescent method. This result demonstrate the potential feasibility of SERS-based lateral flow assay to detect a broad range of genetic marker for in-field or POC diagnostics.

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Protein stability in the presence of ions

박순호

강릉원주대학교 치의학과

Acid-denatured variant ubiquitin (named as HubWA) was observed to refold in the presence of ions, such as chloride, bromide, and sulfate ions. Thus it is thought that the effect of these ions to the stability of highly positively charged protein can be studied by using HubWA as a model protein. At pH 5, the stability of HubWA was increased as increasing concentrations of chloride, bromide, and sulfate anions. The stabilizing effect of sulfate was observed to be bigger than that of chloride and bromide anions. This observation indicated that the stability of protein is strongly influenced by the Hofmeister series effect at neutral pH. At pH 2, the stability of HubWA was also increased linearly in the increasing concentrations of chloride, bromide, and sulfate anions. Interestingly, the degree of stability increase at pH 2 was same in all three anions. It is considered that the effect of charge screening effect override the Hofmeister series effect for highly positively charged proteins. The effect of ions to the stability of proteins appears to be highly influenced by the charged state of a protein.

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Ultrasensitive Quantitative Analysis of Proteins Using Atomic Force Microscopy

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The detection of proteins at ultra-low level is quiet challenging, because biochemical processes are present at very low levels during the early stages of the cell development. In particular, neuronal protein plays an important role in the regulation of development and synaptic plasticity. So it is important to analyze of the protein distribution and quantification of the neurons.Conventional methods to analyze proteins are western blotting, ELISA, and immunofluorescence. However, these tools have limitation of detect spatial localization of proteins in high resolution. Therefore, a new approach for protein detection tool is atomic force microscopy (AFM). Using the mapping capability and imaging mode of AFM, it is possible to obtain an image of a single neuron and performing a quantitative analysis of the protein distribution in nanometer order resolution. In this research, quantitative analysis of a specific protein is performed by AFM using model system and it is applicable in neuron analysis.

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Analysis of Non-coding Cellular RNA Using Atomic Force Microscopy

박익범 김영규[1] 박준원[2,*]

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MicroRNA (miRNA) is a class of short (19-25 nt) noncoding single-stranded RNA molecules that regulates in post-transcriptional gene expression. MiRNA controls the expression level of target proteins, and plays key roles in multiple biological functions such as cell differentiation, proliferation and apoptosis. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Detection of miRNAs has become an important emerging topic in biomedical fields. Therefore, accurate quantification of miRNAs from biological samples will lead us to better understanding of the role of miRNAs. 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 sensitive detection of miRNAs. Therefore, a new approach for miRNA detection tool is atomic force microscopy (AFM). AFM has been extensively used to observe interaction of molecules and manipulate biomolecules in the physiological conditions at the single-molecule level. Because AFM has high lateral resolution of sub-nanometer, the nanoscale distribution of individual molecules on the sample surface could be imaged. Here, we established an AFM-based miRNA quantification and distribution method with no requisite of labeling for modification of miRNAs. In this research, the detection of a specific miRNAs in biological samples is measured by force-based AFM and help to understand functions of miRNA in depth.

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Optimized overexpression and purification of human transmembrane proteins for NMR structural studies

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한국외국어대학교 화학과

Structural and functional studies of membrane proteins which have biologically crucial roles have been a difficult and time-consuming task, primarily because of technical difficulties in the purification and handling of membrane proteins. We tried to produce large amounts of human amyloid-β (hAβ) that is related to the dementia and human melanocortin-4 receptor (hMC4R) that is related to the severe early onset of obesity. The hAβ transmembrane protein shows that the nonfibrillar hAβs form the calcium-permeable ion channel in the cell membrane and these channels would enable disrupt the normal cellular calcium homeostasis. It plays a central role in pathogenesis of dementia and Alzheimer disease. The hMC4R is critical regulator of energy homeostasis and key switch in the leptin-regulating pathway like the energy intake and expenditure. Heterozygous mutation located in second transmembrane domain of hMC4R results in human obesity, hyperphagia. In this research, we succeed to produce the transmembrane domain of the hAβ and second transmembrane domain of hMC4R. To directly assess the role of these proteins, it is important to clarify the three-dimensional structure of them. Therefore, we obtained enough quantities of proteins by using recombinant DNA technologies. And highly purified proteins were applied to various biophysical techniques. Structural characterizations of these proteins in the membrane-like environments were obtained by solution and solid-state NMR spectroscopy. Also, we present the optimized design, construction, and efficiency of a home-built 1H-15N solid-state NMR probe. 1H-15N 2D SAMPI4 spectra from membrane proteins in oriented bicelles was successfully obtained by using these solid-state NMR probe.

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Radiation Damages Analysis by Single DNA Molecule

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서강대학교 화학과

We present single DNA molecule imaging approach to analyze the DNA breaking damages. Traditional ways for DNA damage analysis such as comet assay or smearing assay in electrophoresis are not sensitive for single strand break and difficult to quantitative analysis. However, our novel single molecule approach allows the visualization of single strand break and double strand break of DNA damages using fluorescent labeled d-NTP. By analyzing DNA single strand break and DNA double strand break, we can find the location and frequency analysis of the single strand break. Moreover, we can distinguish damage sources caused by UV and ROS using nicking enzymes. By using E. coli K-12 (MG1655) strain, we analyzed the amount of DNA damages induced by UV irradiation, ethanol, and alcoholic beverage.

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Measuring Telomere Length of Chromosome Using Atomic Force Microscopy

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포항공과대학교(POSTECH) 화학과

The length of the telomere in the chromosome is known to be related to longevity, health status, and also the presence of the disease. Telomere is a fragment of DNA that has the role of cell clock. Telomere is the end of the chromosome as a buffer area to prevent loss of the cell information. That is lost when cell division and is supplemented by telomerase. Human telomeres contain hundreds and thousands of repeats of the six specific nucleotide sequence (5`-TTAGGG-3`) and the total length of telomere is about 5 ~ 25kb. Every time a cell divides once telomere loses 50 to 200 nucleotides. In other words, the telomere length is reduced it means that the cell is old. We will be able to open up new services to predict the life, if able to accurately know the telomere length. Currently, methods such as Quantitative Fluorescent in situ hybridization (Q-FISH) are used to predict the lifetime by measuring the approximate length of telomeres, but those methods are not accurate because standard deviation of the measurement is greater. However, if we use atomic force microscopy (AFM) it is expected to be able to measure the telomere length of a particular chromosome with an accuracy of several tens of nm. The method using of AFM will be more useful in the field of medical diagnostics

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Synthesis of Cyclic and Linear Peptoids for Their Cellular Uptake Evaluation

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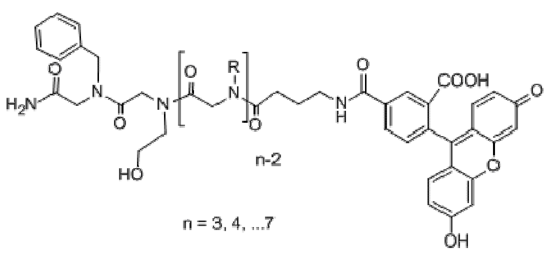
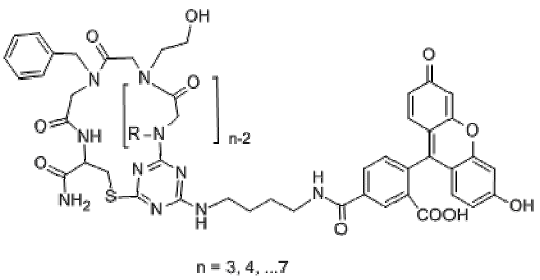
포항공과대학교(POSTECH) 화학과

Peptoids, oligomers of N-substituted glycines, have great potential in therapeutic applications and chemical biology. In particular, cyclic peptoids have received attention by many researchers because of their conformational rigidity and pre-organized structure. However, very little is known about cell permeability of cyclic peptoids. The cell permeability of cyclic peptoids, corresponding linear peptoids, linear peptides will be compared in the near future. The synthesized cyclic/linear peptoids/peptides have phenylalanine and homoserine residues with different sizes (3mer ~ 7mer), and they were labeled with fluorescein to analyze cell permeability. Confocal microscopy was carried out on HeLa cells treated with the 3mer compounds and controls. Other compounds will be treated on the cells, and the cell permeability of the compounds will be imaged by confocal microscopy. FACS analysis will further determine cellular uptake, identifying whether the cyclic peptoids are more cell permeable than the linear peptoids or not.





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DNA nanomaterials for drug delivery

이소연 안대로[1,*] 김학중

고려대학교 화학과 [1]한국과학기술연구원(KIST) 테라그노시스연구단

RCA is a useful tool for preparing DNA based nanomaterial. In this presentation, we can control the size of nanomaterials formed by RCA reaction using modified DNA. DNA nanomaterials are attractive candidate in delivery system since it can be intercalate some molecules. For this reason, we also study utilities of DNA nanomaterials based on RCA as a carrier in drug delivery.

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Traceless and site-directed fluorescent labeling of transmembrane proteins in live cells

이의연 권영은*

동국대학교 의생명공학과

Proteomics has become one of the fastest growing fields in life science research, and the demand for tools to analyze proteins has increased significantly. Engineering and modifying proteins *in vivo* or *in vitro* can aid the understanding of the protein-protein interactions and cellular dynamics. For this purpose, live cell imaging using fluorescent proteins (FPs) has been widely utilized to visualize target proteins under a microscopy by constructing fusion proteins. However, methods of FP-based imaging have a few limitations, such as slow maturation kinetics or issues with photo-stability under laser illumination. In order to address these drawbacks, we employed a pair of engineered *Npu* DnaE split-intein for labeling of recombinant target membrane proteins. By utilizing short 14 amino-acids synthetic C-intein instead of 36 amino-acids native sequence, this method offered novel opportunity to build more practical and sufficiently efficient labeling system. The labeling reaction occurred in two different modes, namely either via specific binding of two split-intein fragments or via covalent bond formation through split-intein mediated protein trans-splicing reaction. No external energy was required for the labeling reaction. Labeling reaction was carried out efficiently on HeLa cell-line at the concentration of reagent as low as 4 μM within 1~30 min with minimal background staining. This approach will lead to new methodologies for investigating protein localization, transportation, and cell signaling.

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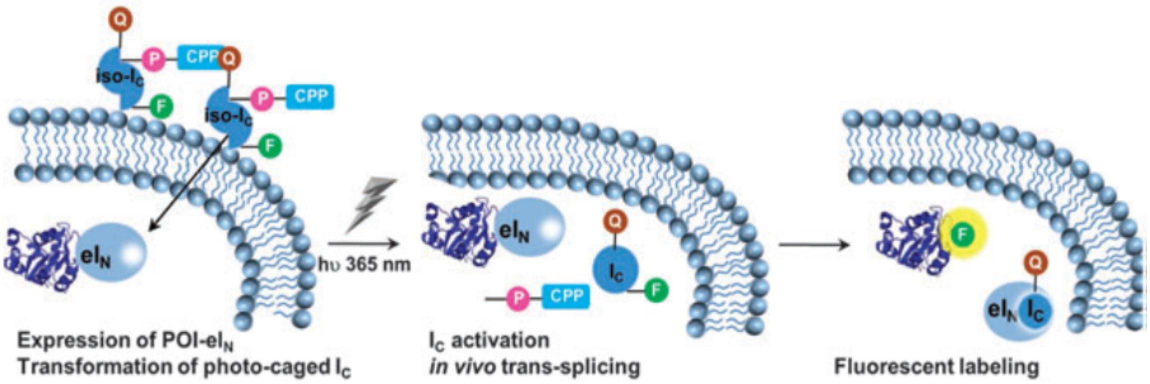
Photo-triggered fluorescent labelling of recombinant proteins in live cells

전현진 김다희 권영은*

동국대학교 의생명공학과

A method to photo-chemically trigger fluorescent labelling of proteins in live cells is developed. The approach is based on photo-caged split-intein mediated conditional protein trans-splicing reaction and enabled background-free fluorescent labelling of target proteins with the necessary spatiotemporal control.



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Discovery of a small compound named as Neurodazine which promotes neural differentiation from Skeletal muscle to specific neuron

이창희 신인재*

연세대학교 화학과

Neurogenerative diseases such as stroke, Parkinson’s, and Alzheimer’s diseases result from the loss of neurons and are prevalent throughout the world. Recent advances in stem cell biology offer the prospect of a new therapeutic approach for the treatment of these diseases. However, this approach requires a sufficient source of stem cells a precise control over differentiation, a suppression of tumor formation by undifferentiated cells. These technical problems as well as ethical issues concerning the use of discarded embryos restrict stem-cell-based therapies. Adult stem cells have the potential to differentiate into several cell types and thus could be also used for cell therapies. However, the adult stem cells have reduced efficiency to grow and differentiate into various types of cells compared to embryonic stem cells.

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Sensitive detection of Helicobacter pylori which expresses BabA and SabA by implementing fluorescent glyco-conjugated nanoparticle

박상현 신인재*

연세대학교 화학과

Helicobacter pylori is a Gram-negative, microaerophilic bacterium found in the stomach which causes chronic gastritis and gastric ulcers. Furthermore, it is also associated with the development of duodenal ulcers and stomach cancer. Therefore, sensitive detection of H. pylori is critical for early diagnosis and effective treatment of H. pylori associated diseases. Recently, it has been studied that H. pylori constantly expresses sialic acid binding ahdesin which is also known as SabA, and a Leb-binding adhesion, BabA that adhere to the human gastric mucosa by interacting glycan-adhesin to cause infection. In order to spot BabA expressing H. pyroli, fluorescent magnetic glyconanoparticles had been implemented by utilizing conjugated aminoethylated Lea, Leb and H1 oligosaccharides to carboxy-containing fluorescent magnetic nanoparticles. Zeta potential and transmission electron microscopy (TEM) was employed to check whether glyconanoparticles were made accurately. In a case which J99 strain of H. pyroli expresses BabA was incubated with three kinds of glyconanoparticles, fluorescence microscopy analysis showed that Leb and H1 conjugated but not Lea conjugated nanoparticles bound to this strain. However, these glyconanoparticles did not recognize H. pyroli strains lacking BabA. Finally, they were employed to enrich BabA expressing H. pyroli by using a magnet. It is expected that fluorescent magnetic glyconanoparticles will be powerful tools to sensitively detect pathogens including H. pylori.

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A Simple, rapid detection for drug-resistant Mycobacterium tuberculosis using allele specific primer

최지영 김진호 문명진[1] 김민선 전승훈 이유로 이환이 정상화 장연재 장원철*

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Tuberculosis remains a global problem due to high infection and human transmission, mortality and morbidity. Generally, high mortality rates due to inefficient treatment of multidrug-resistant (MDR) Mycobacterium tuberculosis strain. MDR is defined as resistance both fist-line anti-tuberculosis drugs including isoniazid (INH) and rifampin (RIF). Recently, several studies reported that 315 codon mutation in katG and 516, 526 and 531 codons mutation in rpoB were associated about 50-95% INH-resistance and 95% RIF-resistance, respectively. Conventional tests like culture based method for Mycobacterium tuberculosis strain takes 6-8 weeks. For these reason, rapid and accurate diagnosis is needed for efficient treatment of TB patients. In this study, we established to detect mutation that related to drug-resistant gene by combined multiplex allele-specific PCR (MAS-PCR) and real-time PCR. Allele specific-primer designed to MDR related mutation. Real-time PCR data is confirmed by DNA sequencing. Our results showed that using allele-specific primer is inexpensive and efficient method for rapid detection of multidrug-resistant tuberculosis.

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A genetic association between small ubiquitin-related modifier 2 gene polymorphisms and risk of Alzheimer's disease in Korean population

김민선 김진호 문명진[1] 최지영 전승훈 이유로 이환이 장연재 정상화 장원철*

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Alzheimer's disease (AD) is a neurological disorder affecting the elderly such as cognitive decline and loss of autonomy. To produce excessive amounts of β-amyloid (Aβ) protein is the widely accepted theory as to the cause of AD. Aβ is produced by amyloid precursor protein (APP) that is cleaved by β-secretase and γ-secretase. Small ubiquitin-related modifier (SUMO) proteins are consisted of 97 amino acids and similar in tertiary structure of ubiquitin. SUMO proteins are a type of post-translational modification to target proteins that are involved in the regulation of gene transcription, cell cycle, DNA repair, and protein localization. Previously studies reported that two SUMOylation sites (K595, 587) are adjacent to the β-secretase cleavage site (M595-D597) of APP. In addition, APP SUMOylation by SUMO2 is associated with decrease of Aβ aggregations. In this study, we hypothesized that SUMO2 gene polymorphisms may be related with risk of AD. We aimed to investigate the association between two polymorphisms (rs35271045 and rs9913676) of SUMO2 gene and risk of AD. These SNPs were selected in linkage disequilibrium (LD) information from HapMap database. The genotype analysis was performed by PCR-Sequencing. All statistical analysis was used a fisher's exact test for comparing genotype frequencies between AD patients and healthy control subject.

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Solid-Phase Synthesis and Sequence Analysis of α-Helix Mimetic Oligobenzamides

문희조 임현석*

포항공과대학교(POSTECH) 화학과

Protein-protein interactions (PPIs) play a central role in various cellular events including cell development, differentiation, and proliferation. However, misregulation of such interactions often leads to diseases. Accordingly, modulation of PPIs is along highly attractive therapeutics for chemists. Nonetheless, targeting PPIs with small molecules has been considered undruggable due to the flat, large, and even featureless interfaces of proteins, which make PPIs intractable.α-Helices, accounting for approximately 40% of total protein secondary structures, often occur at the protein interfaces. It has been reported that the short segment of α-helix functions as a mediator of PPIs by projecting the side chains of three residues, i, i+3 or 4, and i+7 along one side of helices that contact significantly with interacting proteins. Taking advantage of such features, the development of small molecules that can mimic the role of these three side chains has been advanced. Oligobenzamides have been shown to successfully replace the function of natural helices in α-helix mediated PPIs. By maximizing structural diversity with aids of split-and-mix methods, we expected to enhance the possibility to develop a hit compound with high binding affinity towards disease-related target proteins. Generally, construction of small molecule chemical library on polymer beads requires encoding tags for the characterization of hit compounds. In this work, we constructed a benzamide-based α-helix mimetic library without encoding parts that facilitates the characterization of hit compounds using tandem mass spectrometry.

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A Simple Method to Sequence Bicyclic Peptoids via One-Pot Ring-Opening and Cleavage Reaction

서창덕 임현석*

포항공과대학교(POSTECH) 화학과

Cyclic peptide and peptidomimetics are important in drug discovery and chemical biology. It is well known that macrocyclic structures provide structural rigidity and improved cell permeability, so the cyclic molecule libraries have been used widely. Bicyclic peptide and peptidomimetics have much more structural rigidity and prevail in natural compounds, so it is more interesting structure than linear or monocyclic form. However, bicyclic peptide and peptidomimetics can’t be sequenced by Edman degradation or tandem mass spectroscopy (MS/MS). To solve this problem, I used CNBr cleavage method for bicyclic peptoid. Bicyclic peptoid containing two homocysteine residues was synthesized by solid phase synthesis and cleaved by CNBr cleavage solution. Cleaved fragments were sequenced using MALDI-TOF MS/MS. This strategy can provide a new and improved tool for chemical biology.

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Encapsulation and stabilization of all-trans-retinol by new fatty acylated-cyclic glucan derivatives

김환희 호예라 임지은[1] 조은애[2] 정선호[3,*]

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Encapsulation of bioactive ingredients into cyclic glucans can be one of effective means to protect them against chemical degradation. In this study, the new fatty acylated-cyclic glucans for all-trans retinol (vitamin A) were formulated to improve the stability of vitamin A, whose chemical instability has been a limiting factor in its clinical use. Various novel conjugates of fatty acylated cyclic glucan such as mono [6-deoxy-6-(octadecanoic amidomethyl)]-cyclosophoraoses, mono [6-deoxy-6-(octadecenoic amidomethyl)]-cyclosophoraoses, mono [6-deoxy-6-(octadecanoic amidomethyl)]-β-cyclodextrin, mono [6-deoxy-6-(octadecenoic amidomethyl)]-β-cyclodextrin, mono[3-deoxy-3-(octadecanamido)]-β-cyclodextrin and, mono [3-deoxy-3-(octadecenamido)]-β-cyclodextrin were prepared from the isolated bacterial cyclooligosaccharides. Synthetic fatty acylated-cyclosophoraoses and -cyclodextrins were characterized using ^{1}H nuclear magnetic resonance (^{1}H NMR), Fourier-transform infrared spectroscopy (FT-IR), matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS), differential scanning calorimetry (DSC) and X-ray diffraction (XRD). Based on the structure of novel fatty acylated-cyclic glucans, the encapsulation capacities and stability towards retinol were investigated by fluorescence spectroscopy, dynamic light scattering (DLS) and scanning electron microscopy (SEM). These amphiphilic cyclic glucans capable of effectively incorporating vitamin A will be potential for the drug delivery and other nanotechnology applications.

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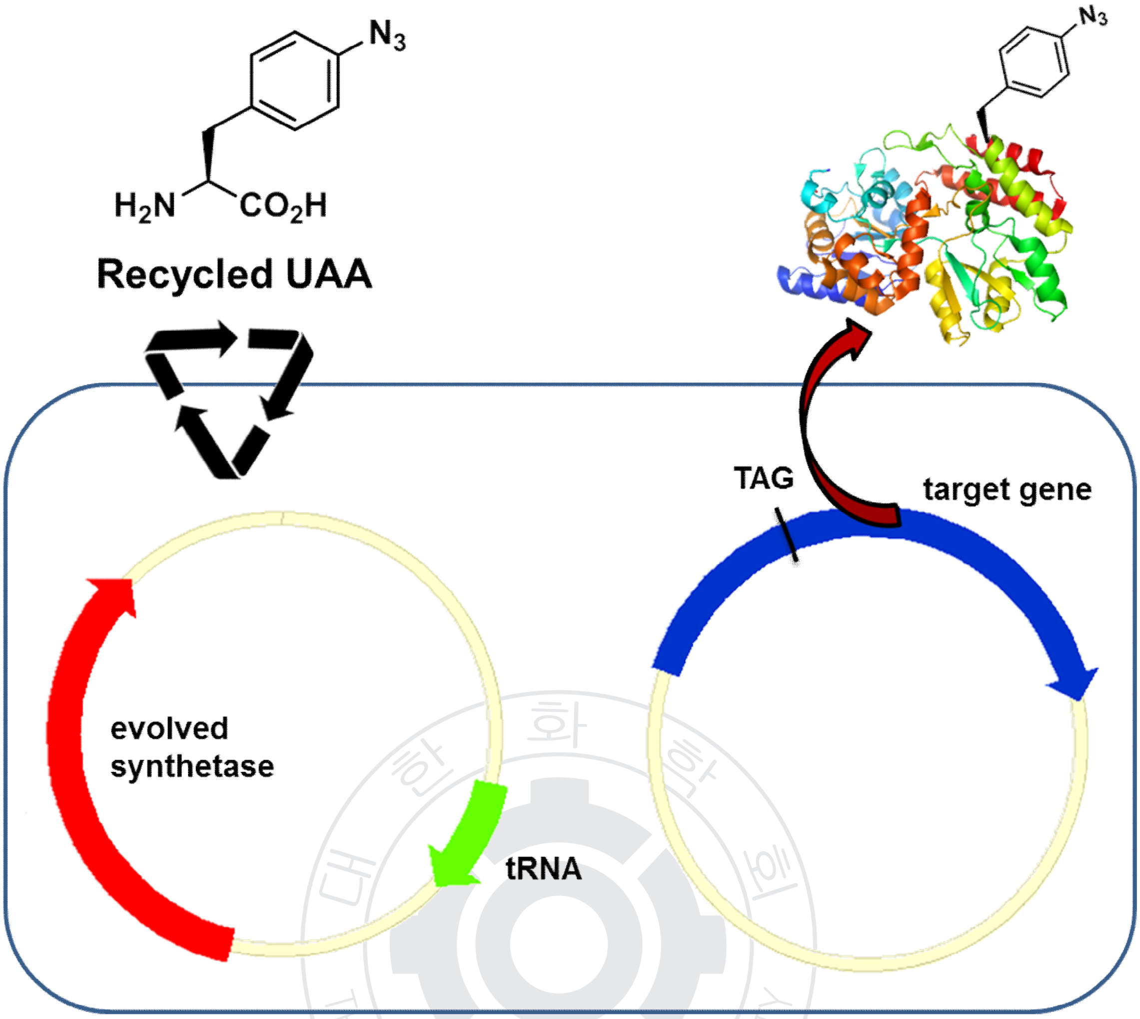
Genetic incorporation of recycled unnatural amino acids

김상길 이현수*

서강대학교 화학과

The genetic incorporation of unnatural amino acids into proteins has been a useful tool for protein engineering. However, most of unnatural amino acids are expensive, and the method requires high concentration of unnatural amino acids, which has been a drawback of the technology especially for large-scale applications. In order to address this problem, a method to recycle cultured UAAs was developed. The method is based on recycling a cultured medium containing an unnatural amino acid, in which some of essential nutrients were re-supplemented after each culture cycle, and induction of protein expression was controlled by using glucose. In an optimal condition, five UAAs were recycled for up to seven expressions without decrease in expression level, cell density, and incorporation fidelity. Because this method can be generally applicable to other UAAs, it would be useful to reduce the cost of UAAs for the genetic incorporation and helpful to expand the technology to industrial applications.


N3
H2N
CO2H
Recycled UAA
N3
TAG
target gene
evolved synthetase
tRNA

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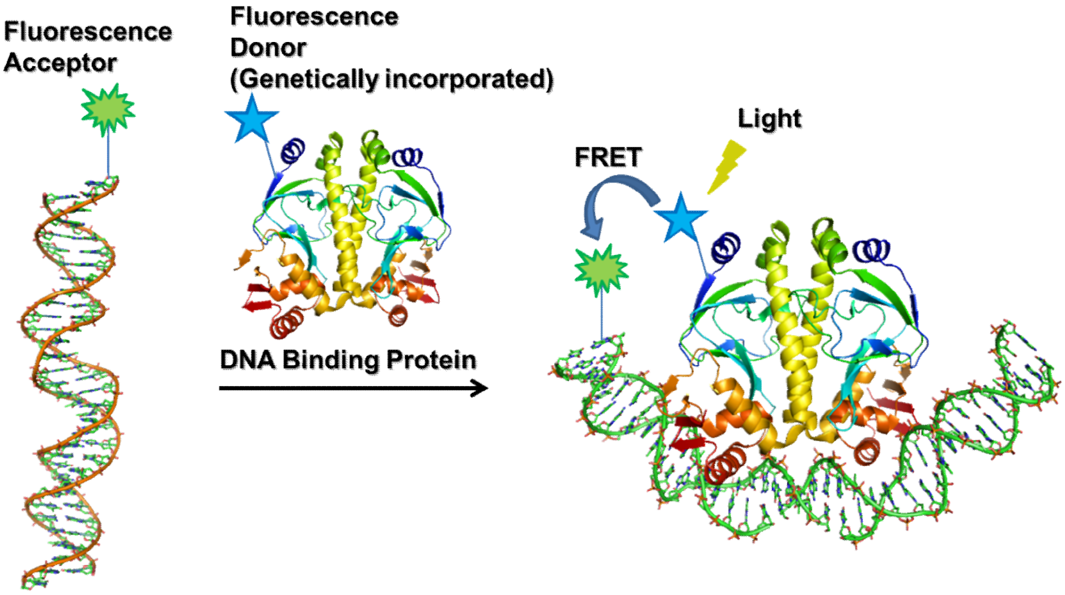
FRET-based analysis of protein-nucleic acid interactions by genetically incorporating a fluorescent amino acid

고우석 이현수*

서강대학교 화학과

Protein-nucleic acid interaction is an important process in many biological phenomena. In this study, a fluorescence resonance energy transfer (FRET)-based protein-DNA binding assay has been developed in which a fluorescent amino acid is genetically incorporated into a DNA binding protein. A coumarin-containing amino acid was incorporated into a DNA binding protein, and the mutant protein specifically produced a FRET signal upon binding to its cognate DNA labeled with a fluorophore. The protein-DNA interactions were then measured under equilibrium conditions. This method is advantageous for studying protein-nucleic acid interactions because it is technically easy and applicable to any nucleic acid binding protein.



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Design a novel imaging agent using peptide coated gold nanoparticle towards CD133 as Biomarker for brain glioma

조준행 이상춘 윤문영*

한양대학교 화학과

CD133 was first identified as a marker for cancer initiating cell in brain tumor and contributor to cancer stem cell (CSC) which possess tumorigenesis and resistance of conventional therapeutics. Also, CD133 was known as marker for CSC on Glioblastoma (GBM), most common type of brain tumor in adults, and key factor as maintenance the tumorigenic potential GBM. So, CD133 was a potential target to accurate diagnosis of GBM and target therapy to enhance the prognosis of patient. Herein, we designed the peptide coated gold nanoparticle (GNP) to form an imaging agent with cellular stimuli dependent cleavage activity. GNP was prepared as a quencher for fluorescein isothiocyanate (FITC) labeled on a peptide specific to CD133. The high amount of glutathione (GSH, 10~20 mM), presence in cancer cell, was a key role as stimuli agent on our probe complex. The peptide-GNP shown target specific fluorescence signal when the bonding of peptide-GNP was dissociated by GSH. Also, the peptide-GNP have no cellular cytotoxicity when it binds to target. This result given that the peptide coated GNP can be utilized as imaging agent for accurate diagnosis of GBM and further drug carrier for therapeutic effect.

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Mechanistic analysis of ecumicin from Mycobacterium tuberculosis Caseinolytic protease C1 (ClpC1)

정인필 윤문영*

한양대학교 화학과

Caseinolytic protease C1 (ClpC1) in Mycobacterium tuberculosis (MTB) is a general stress protein which belongs to the heat shock protein 100 (hsp100) family of molecular chaperones. ClpC1 is a promising target for the development of new anti-tuberculosis agent, since ClpC1 have been identified as having a role in protein homeostasis in MTB strains. Ecumicin targeting to ClpC1 is one of the potent inhibitor in growth of MTB strains. In this study, we characterized the interaction between MTB ClpC1 and Ecumicin via both In-silico analysis and site-directed mutagenesis study. In molecular docking analysis, the Ecumicin was analyzed that it binds at the N-terminal domain (NTD) of ClpC1 and matched with previously report, in which the MTB strain with a mutated ClpC1 at NTD was exhibited Ecumicin resistance. Specifically, R83 and E89 residues of ClpC1 interacted with Ecumicin through hydrogen bond. Therefore, we selected the both residues for site-directed mutagenesis in order to analyze an interaction of between Ecumicin and ClpC1. Most mutant ClpC1s similarly exhibited the enzyme activities and kinetic parameters with wild-type ClpC1 except for one of R83 mutant ClpC1s. Especially, R83A mutant ClpC1 did not change the activity as increasing the Ecumicin concentration. Furthermore, a result of molecular docking for mutant ClpC1 also indicated that the R83 mutants (R83A: -3.9 Kcal mol-1, R83K: -4.9 Kcal mol-1, respectively) interact with much lower binding energy than wild-type (-5.7 Kcal mol-1). In this result, we concluded that the R83 might be a key residue in interaction of MTB ClpC1 and Ecumicin. This research might provide an impetus for identification of inhibitory mechanism of Ecumicin and development of potent anti-tuberculosis agent.

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Effect of Pachymic Acid on Autophagic apoptosis

이수경 김문무*

동의대학교 화학과

Pachymic acid is a main chemical constituents in Poria cocos which has been used as a medicinal herb for treatment of chronic gastritis, acute gastroenteric catarrh, gastric atony, oedema, nephrosis, dizziness, nausea and emesis in East Asia. However, the effect of pachymic acid on induction of autophagy remains unclear. Autophagy is the main lysosomal degradative machinery and plays a major role in maintaining cellular homeostasis. Therefore, in this study, it was investigated whether pachymic acid has an effect on cellular senescence by induction of autophagy in human lung fibroblast, WI38 cells. First of all, pachymic acid showed cytotoxic effect in a dose dependent manner. In addition, it was observed that pachymic acid induced autophagy activity. Moreover, pachymic acid increased the expression levels of LC3, Bcl-2 Atg3 and p-mTor associated with autophagy. Furthermore, pachymic acid increased the expression levels of p53, p-p53, Ac-p53, p-p21 and IGFBP3 in IGF-1/p53 signaling pathway. In particular, treatment of pachymic acid increased the expression levels of p-FoxO1, glutation reductase, catalase and SOD-3 which are involved in oxidative stress defense mechanism

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β-Caryophyllene Oxide Inhibits Invasion of HT1080 Cells

홍수경 김문무*

동의대학교 화학과

In recent years, β-caryophyllene oxide (CPO) has been reported to have not only bioactivity of anti-inflammatory activity and immune activity, but also inhibition of growth and induction of apoptosis in tumor cells. CPO is a sesquiterpene isolated from essential oils of medicinal herbs with aroma such as guava leaves, oregano, cinnamon and black pepper. The purpose of this study is to investgate an inhibitory effect of CPO on matrix metalloproteinases (MMPs) that play an important role in tumor cell invasion using human fibrosarcoma cells (HT1080). First of all, the effect of CPO on cell viability in HT1080 cells was observed using MTT assay. Its cytotoxicity was increased in a dose dependent manner. In addition, the inhibitory effect of CPO on the activities of MMP-2 and MMP-9 related to cancer metastasis was examined using gelatin zymography. In our study, it was found that CPO above 2 μM significantly inhibited on MMP-9 activity as well as MMP-2 activity. futhermore, CPO declined expression of MMP-2 compared with phorbol-12-myristate-13-acetate (PMA) group. The available data let us to suggest that CPO could contribute a potential chemoprevention on metastasis as an inhibitor.

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Preparation and Characterization of Pullulan Microspheres Conjugated with Microbial β-(1,2)-D-glucans

최재민 이벤엘 박경희 정선호[1,*]

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Polysaccharide pullulan, originated from yeast like fungus Aureobasidum pullulans, was crosslinked with various cyclic glucans such as Rhizobium leguminosarum biovar viciae VF-39 originated cyclic β-(1,2)-D-glucans, and chemically modified hydroxypropyl cyclic β-(1,2)-D-glucans by epichlorohydrin for creating microspheres. The morphological differences of these pullulan- β-(1,2)-D-glucans microspheres were obtained by scanning electron microscopy (SEM). Pullulan- β-(1,2)-D-glucans microspheres were investigated for encapsulating target molecules. The loading ability of each microsphere was monitored and the microspheres were compared with pure agents about the loading capacity for each target molecules by UV-vis spectrometry. According to the results, pullulan-cyclic glucan microspheres were able to capture drugs, and it is suggested as the potential biomaterial for encapsulating agent.

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Development of the novel protein cage platform for the easy and controlled protein conjugation

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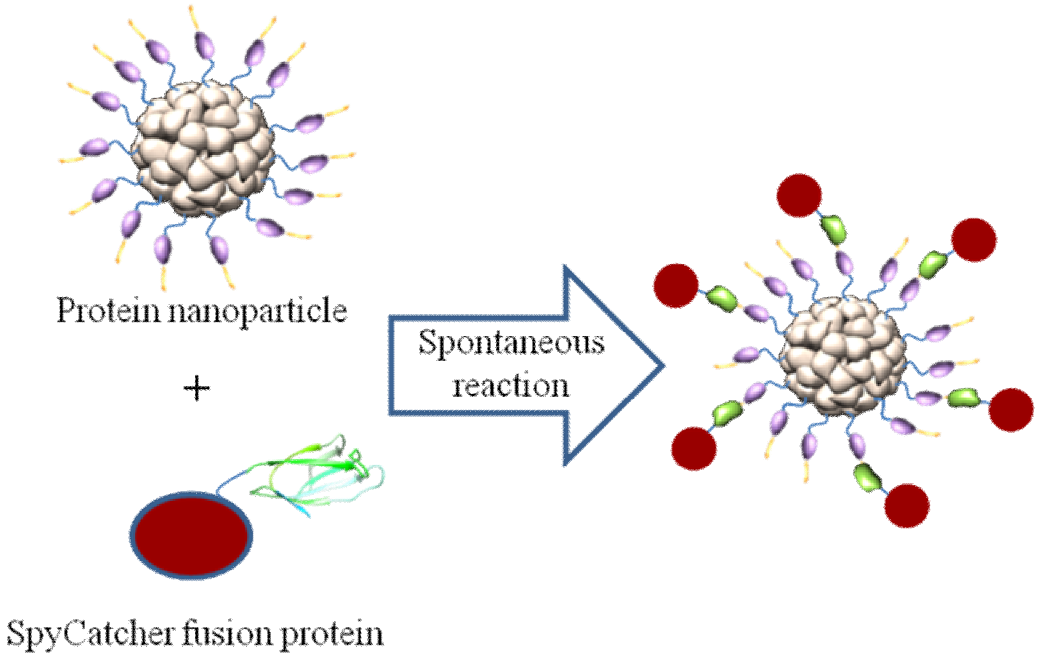
Ten is better than one. In the case of the biochemical world, this also makes sense. The more the enzyme exists, the faster the substrate is consumed. And many biological interactions occur in the multivalent manner. Here, we suggest the evolved protein based nanoparticle that can be conjugated with other proteins. We used protein cage named Lumazine Synthase which forms the uniform cage structure by self assembly of the 60 subunits. And to make this protein nanoparticle as a specific biosensor, we also genetically fused the antibody binding domain to the protein cage. To achieve the protein-protein conjugation, we used SpyTag and SpyCatcher. SpyTag and SpyCatcher are the peptide and protein that form irreversible isopeptide bond each other specifically and spontaneously. By making Genetic fusion of the SpyTag to the protein cage and SpyCatcher to the target protein, we can induce protein ligation which cannot be achieved by the genetic fusion. Finally, we found that protein conjugation really occurs and it does not interrupt the function of each functional protein.The biggest advantage of this method is the extreme conjugation efficiency that we can generate number controlled uniform cage structure by charging all of the ligation site or multifunctional cage by using more than 2 kinds of SpyCatcher fusion proteins. We expect this newly developed novel bio-nanoparticle can be potentially used as the various protein based biosensors.


Protein nanoparticle
+
SpyCatcher fusion protein
Spontaneous reaction

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NMR dynamics study of defective isoforms of the type III antifreeze proteins from *Zoarces elongates Kner*

최서리 이준화*

경상대학교 화학과

Antifreeze proteins (AFPs) are found in a variety of cold-adapted (psychrophilic) organisms to promote survival at subzero temperatures by binding to ice crystals and decreasing the freezing temperature of body fluids. One of most widely studied classes of AFPs is the type III from arctic fish such as the ocean pout and Japanese notched-fin eel pout. The type III AFPs are small globular proteins that consist of one α-helix, three 310-helices, and two β-strands. The type III AFPs have been categorized into two subgroups, quaternary-amino-ethyl (QAE) and sulfopropyl-Sephadex-binding (SP), based on differences in their isoelectric points. The QAE proteins can be further divided into two subgroups, QAE1 and QAE2. QAE2 isoforms can slow, but not stop, the growth of ice crystals by binding to pyramidal ice planes. The other group (QAE1) binds both pyramidal and primary prism planes and is able to halt the growth of ice.In this study, we have investigated backbone dynamics analyses of four kinds of type III AFPs from Japanese notched-fin eel pout (Zoarces elongates Kner), nfeAFP6 (SP), nfeAFP8 (QAE1), nfeAFP11 (QAE2), nfeAFP6_tri (P19L/A20V/G42S), nfeAFP8_tri (Q9V, L19V, V20G) and nfeAFP11_tri (V9Q, V19L, G20V) at various temperatures. We also characterized the structural/dynamic properties of the ice-binding surfaces by analyzing the temperature gradient of the amide proton chemical shift and its correlation with chemical shift deviation from random coil. Our results provide insight into the molecular basis of ice-binding and antifreezing activities of type III AFP isoforms.

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Cell imaging modular toolkits using protein ligation pairs

문효진 강세병[1,*]

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Fluorescence imaging techniques have been wildly developed to study subcellular components and biological process in cells. Especially, targeted cancer cell imaging is highly desirable for early-stage diagnosis and treatment. Affibody is one of the small proteins engineered to selectively and effectively bind to target cancer cell lines as alternatives of antibodies. For effective cell imaging, affibodies were genetically fused to fluorescent proteins as targeting ligands. However, genetic fusions often caused instability and malfunction of resulting proteins. To overcome these limitations, we used simple ligation methods to establish a new type of cell imaging toolkit. We herein prepared two types of proteins, affibodies and fluorescent proteins, individually and connected them using protein ligation pairs. We applied SpyTag/SpyCatcher system as a protein ligation pair. Collagen adhesion domain (CnaB2) from invasive strains of *Streptococcus pyogenes* split into peptide and protein fragments, followed by rational modification of the parts, SpyTag/SpyCatcher system has been exploited. 13 amino acid SpyTag peptide is able to form spontaneous amide bond with its partner 15 kDaSpyCatcher protein. This isopeptide bond formation is rapid, simple and irreversible in diverse conditions of pH, temperature and buffer. We prepared HER2 affibody with SpyTag peptide to target human breast cancer cell, SK-BR-3, and various fluorescent proteins with SpyCatcher to visualize target cancer cells with various colors. To confirm the covalent formation of SpyTagged affibodies and SpyCatcher-fluorescent proteins, we utilized SDS-PAGE and Mass spectrometry techniques. We also checked targeting and detecting ability of ligased fusion proteins with confocal microscopy. Using this simple protein ligation pair, we can design a variety of templates and develop new imaging modular toolkits using mixing-and-matching strategies and apply them as versatile imaging probes which are difficult to achieve with general genetic fusion.

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Developing Enzyme-Mediated Target-Specific Signal Amplifier based on Protein Ligation System

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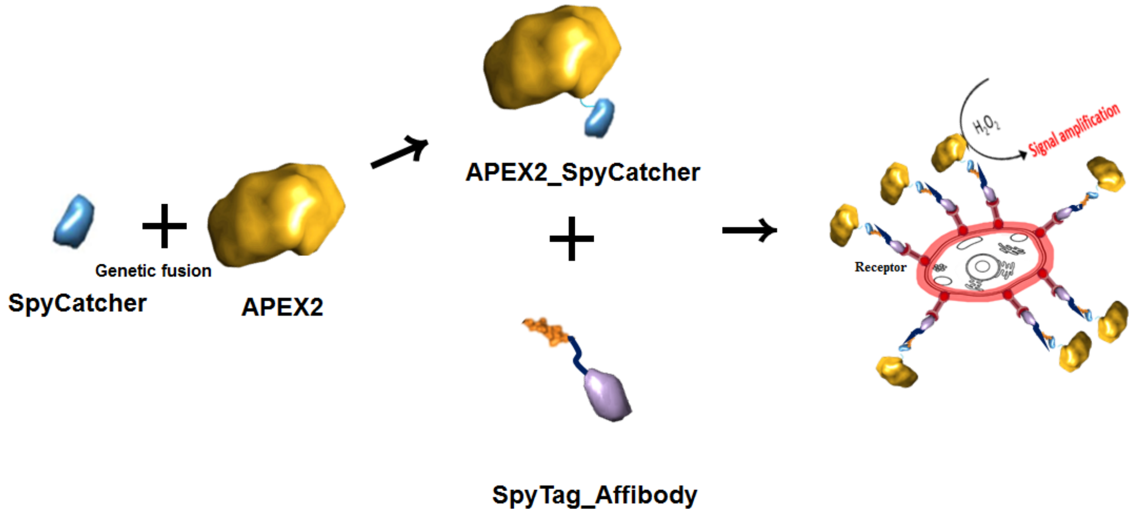
For specific-targeting molecule, the population of target molecules per unit sample volume should be substantial enough to be detected with any given detecting systems. Spatial and temporal variations are also considered within cell. Therefore, signal amplification systems are issue and there are diverse signal amplification strategies. One of the most well-known and well-studied methods is the system which use the enzyme. Recently, enzyme-based assay is based on the inherent properties of the enzymes that selectively recognize and specifically bind their substrates. So those properties allow to be readily detected with significant catalytic activity of the enzymes. For this aim, there are various enzyme-based assay with novel enzymes by enabling to be practically used to colorimetric or fluorometric detection and signal amplification. One of novel enzymes is peroxidase, which catalyzes reduction of hydrogen peroxide and also oxidizes various target substrates. Peroxidases can generate singlet oxygen which affects surrounding molecules. Among them, ascorbate peroxidase 2(APEX2) was chosen for this experiments with potential for spectrophotometry, fluorometry and electro-analytical chemistry. On the other hand, the tagging of proteins with peptides is one of the most widely used methods in detection, purification and immobilization. Recently, the SpyTag/SpyCatcher tagging system employs the covalent bonding of a peptide tag to its protein partner. Its system is based on *Streptococcus pyogenes* (CnaB2). SpyCatcher can form an irreversible covalent bond between SpyCatcher and SpyTag via a spontaneous isopeptide linkage. The fusion proteins, which have peroxidase activity and targeting moieties, have been developed to be used in target-specific signal amplification assay.


SpyCatcher
Genetic fusion
APEX2
APEX2_SpyCatcher
SpyTag_Affibody
Receptor
H_2O_2
Signal amplification

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Developing a simple fusion protein as an antibody-anchoring adapter in ELISA systems

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ELISA (Enzyme-linked immunosorbent assay) has been widely used as a powerful diagnostic tool because of its high sensitivity and accuracy. It uses antigen-specific antibodies and signal-amplifying enzymes with chromogenic substrates. Especially, sandwich-type ELISA system is most common assay format because it can quantify the amount of target-molecules using both capturing and detecting antibodies simultaneously which have two different epitopes. To obtain best results in sandwich-type ELISA, it is important for capturing antibody to have proper orientation on the ELISA plate to capture available antigens which are usually low abundant in the complex biological samples. We designed and prepared a simple fusion protein which consists of monomeric streptavidin and ABD (Antigen Binding Domain) as an antibody-anchoring adapter in ELISA systems. Monomeric streptavidin derived from tetrameric streptavidin has an extraordinarily high affinity for biotin and the binding of biotin to streptavidin is one of the strongest non-covalent interactions known in nature. Also, ABD can bind F_c region of capture antibodies and it helps expose F_{ab} region to catch antigens more readily. We expect this anchoring system brings high sensitivity and reproducibility in ELISA.

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DEVELOPING VERSATILE NANOCARRIER USING AFFIBODY/POLYMERIC NANOGEL HYBRID COMPLEXES

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Binding specificity and high affinity to any given target molecules are essential features for *in vitro* and/or *in vivo* diagnostics and for many other biotechnological and biomedical applications. Recently, affibody has been widely used as ligands for targeted delivery of therapeutics and/or diagnostics. Affibody, especially, has been used to enrichment of low abundant molecules in complex samples, and specific detections of biomarkers *in vitro* and/or *in vivo*, because they have much smaller size compared with antibody, but it has enough binding affinity and specificity to their target molecules. We developed versatile affibody/nanoparticle hybrid complexes as multifunctional theranostic nanocarriers by combining affibody-GST fusion proteins with highly stable polymeric nanogels (NG) which encapsulate anticancer drug, doxorubicin through thiol-disulfide exchange. These hybrid theranostic nanocarriers (Affibody/NG complexes) show high target specificity and the enhanced efficacy. Furthermore, multifunctional hybrid theranostic complexes will be developed by mixing and matching strategy.

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New Alginate Beads Incorporated by Polydiacetylene Liposomes Containing Pentacosa-10,12-diynoyl Succinoglycan Monomers and Their Applications for Colorimetric Sensor

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Alginates are anionic polysaccharides composed of β-D-mannuronic acid and α-L-guluronic acid linked by 1-4 glycosidic bonds. They are known to have an affinity for calcium ion which leads the gelation of alginate by forming egg box junction to associate divalent metal ions of alginate polymer chain. We made the liposomes containing 10,12-pentacosadiynoic acid (PCDA) derivatized with succinoglycan monomers (SGM) isolated from *Sinorhizobium meliloti* and fabricated novel alginate beads incorporated by those liposomes. Since PCDA has been widely used as sensory applications, various behaviors of those polydiacetylene liposomes containing pentacosa-10,12-diynoyl succinoglycan monomers were investigated. In present study, we suggested the potentials of the alginate beads containing the polydiacetylene-based liposomes for the biotechnological applications of sensor system in response to various target compounds.

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Formation of GUVs coated with ECM proteins

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서강대학교 화학과 [1]성균관대학교 에너지과학과 [2]서강대학교 화학과 및 바이오융합과정

Extracellular matrix (ECM) is a collection of extracellular molecules secreted by cells which provides structural and biochemical support to the surrounding cells. ECM proteins exist as composite fibers in vivo via fibrillogenesis. We mimicked ECM fiber proteins on plasma membrane with giant unilamellar vesicles (GUVs). Phosphatidylserine (PS), negatively charged lipid, was used to induce ECM protein fibrillogenesis through electrostatic interaction and protein unfolding. GUVs were incubated in ECM protein solution to attach ECM proteins to the GUVs. A variety of combinations of two kinds of ECM proteins were tested. Some of them attached to membrane lipid of GUV and the others did not attached to the lipid of GUV. These results reflect the mechanism of fibrillogenesis.

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An Effective Delivery of Antigen-Encapsulin Nanoparticle Fusions to Dendritic Cells Leads to Antigen-specific Cytotoxic T cell Activation and Tumor Rejection

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One of the primary goals of vaccination against cancer is to generate robust and effective cytotoxic T cell immune responses upon tumor generation. Dendritic cells (DCs) are the most potent antigen presenting cells and play a pivotal role in activating antigen-specific cytotoxic T cells. Here, we utilized encapsulin protein cage nanoparticles (Encap) as antigen-delivery nanoplatforms, and evaluated their efficacy in inducing DC-mediated antigen-specific immune responses and subsequent melanoma tumor rejection in vivo. We genetically introduced the peptide SIINFEKL (OT-1 peptide) of ovalbumin (OVA) protein to the three different positions of Encap subunit. Encap and its variants (OT-1-Encaps) were then efficiently up-taken and processed by DCs, that significantly induced the proliferation of OT-1 peptide-specific CD8$^+$ T cells both in vitro and in vivo and activated OT-1 specific functional cytotoxic CD8$^+$ T cells resulting in selective killing of externally introduced melanoma tumor cell line B16 bearing the OVA protein (B16-OVA) in vivo. In a B16-OVA melanoma tumor challenge model, OT-1-Encap-C vaccination significantly suppressed tumor growth, and tumor-infiltrating lymphocytes (TILs) isolated from the OT-1-Encap-C-vaccinated B16-OVA tumor group contained a large number of cytotoxic CD8$^+$ T cells secreting high amount of IFN-γ cytokine. The approaches we describe here in may offer new strategies for developing novel vaccination systems that induce and/or regulate strong and selective cytotoxic T cell immunity in non-pathogenic diseases, such as cancers and neurodegenerative diseases.

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Understanding PI3K in Cancer at the Single-Molecule Level

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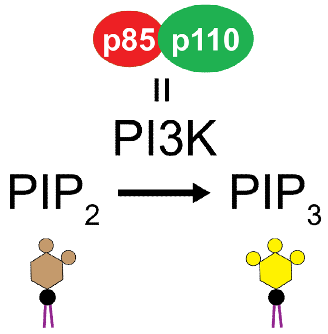
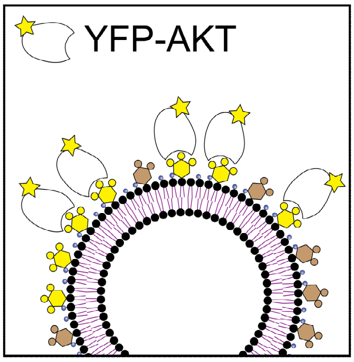
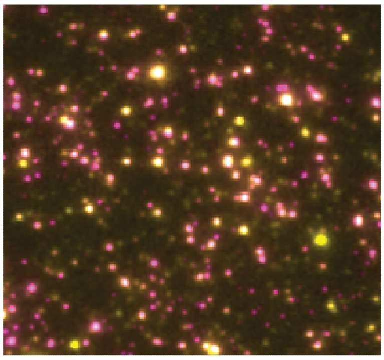
PI3K-Akt signaling pathway controls cell growth, proliferation, and motility, and is frequently deregulated in many types of cancer. PI3K is a lipid kinase that converts PIP2 into PIP3 on membrane, which then recruits downstream signaling proteins such as Akt. Traditionally, the activity of PI3K has been probed indirectly by the phosphorylation of Akt. Here, we developed an assay that directly measures the activity of PI3K by single-molecule fluorescence. In this method, surface-tethered PI3K phosphorylates PIP2 on nearby vesicles, fluorescently-tagged Akt is introduced, and its binding to vesicles is imaged to quantify PI3K activity. After validating the method with fluorescent protein-tagged PI3K, we extend this assay to endogenous PI3K from breast cancer cells to understand the response of cancer cells to PI3K inhibitors. We hope this assay could be useful in screening for PI3K inhibitors or guide selection of cancer patients for PI3K-targeted therapy.







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Measuring mechanical properties of living cell: Micropipette aspiration

이세린 남소정 이길용[1] 신관우[2,*]

서강대학교 화학과 [1]성균관대학교 에너지과학과 [2]서강대학교 화학과 및 바이오융합과정

Studying mechanical properties of living cell is important. It can be helpful to understand cell behaviour under stress, for example, neutrophil change their shape for pass thorough narrow capillary in circulation. Besides, comparing sickle cell mechanical properties and normal cell, we can find factor influencing disease and relationship between mechanical properties and disease. Most tumor cell exhibit lager stiffness compared to normal cell. Micropipette aspiration provided the method for measuring mechanical properties of membrane of various cells such as area expansion modulus. We measured various cell area expansion modulus including cancer cell, fibroblast and normal cell, and compared that. And, We measured mechanical properties of attached cell which cultured on a variety of substrate.

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Preparation of *para*-nitrophenyl-6-azido-6-deoxy-N-acetylglucosaminide and measurement of its kinetic parameters for OGA

김은주* **John Hanover**[1]

대구대학교 과학교육학부/화학교육과 [1]*National Institute of Health*

Modification of Ser/Thr residues of nucleocytoplasmic proteins with O-linked β-D-N-acetylglucosamine (O-GlcNAc) is a highly dynamic post-translational modification. O-GlcNAc “on and off” cycling is regulated by only two enzymes in humans. These two enzymes are a glycosyltransferase termed as O-GlcNAc transferase (OGT) which is responsible for the attachment of GlcNAc and a glycoside hydrolase termed as O-GlcNAcase (OGA) which is responsible for its removal. 6-Azido-6-deoxy-N-acetylglucosamine (6AzGlcNAc) moiety of UDP-6AzGlcNAc was reported to be a substrate for human OGT and label exclusively intracellular proteins. However, it is not currently known if this unnatural sugar is also a substrate for OGA. If 6AzGlcNAc is as good substrates as the natural sugar substrate, GlcNAc, for OGA, 6AzGlcNAc can be considered as an appropriate tool for O-GlcNAc dynamic studies. In order to answer this question, we have synthesized *para*-nitrophenyl-6-azido-6-deoxy-N-acetylglucosaminide (PNP-6AzGlcNAc) and measured its kinetic parameters for OGA.

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Analysis of the lysozyme crystal in PEGDA gel

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서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Almost every biochemical reaction requires a specific protein. Other types of proteins have mechanical and structural functions or mediate cell signaling, immune responses or the transport of small molecules. The function of a specific protein depends on its three-dimensional structure. One of the major challenges in structural biology today is the explanation of the structure, function and interaction of huge macromolecular complexes and membrane protein. To solve these challenges, it is necessary to crystallize the proteins and determine the structure of the proteins.In this study, we selected the lysozyme that is one of the various proteins as crystallized material and observed the lysozyme crystal in poly(ethylene glycol) diacrylate(PEGDA) hydrogels. By using different vol% of PEGDA hydrogels, we are able to limit the growth of lysozyme crystal. Lysozyme crystals made in these hydrogels are observed these morphologies by using microscope. We plan to analyze and determine the structure and function of lysozyme crystals by using X-ray diffraction analysis.

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Binding events of zinc finger proteins

정은미 박소미 정진성[1] 이승재[*]

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Zinc finger proteins are one of the most common families of proteins found in eukaryotes. These proteins utilize zinc to fold into the correct three dimensional structure and mediate a variety of biological functions including transcriptional regulation, post-transcriptional control and protein-protein recognition. This project has focused understanding the consequences of iron substitution in zinc finger proteins (ZFP). Although zinc is typically thought to be the correct metal ion to bind to zinc finger proteins, there is evidence that iron might substitute for zinc in certain types of zinc finger proteins. I am focusing on two zinc finger proteins: Tristetraprolin (Non Classical ZFP) and ST18(Classical ZFP). Tristetraprolin (TTP) uses three cysteine and one histidine residue to bind zinc. TTP regulates the expression of cytokines such as tumor necrosis factor α (TNF- α) by binding to AU-rich sequence elements (AREs) located at the 3' untranslated region (3'UTR) of the cytokines' mRNA. Upon binding, the TTP/mRNA complex is degraded by exosomes. I have discovered that both ferric and ferrous iron will coordinate to TTP and still bind to RNA. In addition, ferrous (Fe(II)) coordinated TTP may be detrimental to the cell because it is redox active and may generate damaging reactive oxygen species (ROS). I have developed a novel spectroscopic assay to measure oxidation rates of zinc finger proteins as a function of metal ion coordination and I have discovered that iron substitution promotes oxidation via the formation of reactive hydroxyl radicals. Future studies are aimed at determining if RNA cleavage is initiated by the hydroxyl radicals that are generated by iron-TTP in the presence of ROS.ZIF-268 is a classical zinc finger protein that uses a Cys_2His_2 ligand set to bind zinc and fold. This protein's DNA binding properties are well understood and it is possible to modify the protein sequence to tune DNA recognition. We hypothesize that iron substituted ZIF-268 may be capable of cleaving target DNA possibly with sequence selectivity. Work to address this hypothesis, we have been over expressed and purified ZIF-268 and characterized its iron (ferric and ferrous) and zinc binding properties. We have learned that ZIF-268 binds DNA with the same affinity when zinc, ferric and ferrous iron is bound. Future studies will examine DNA cleavage initiated by ferrous-ZIF268.

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Characterization of disulfide bonds by tandem mass approaches

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The identification of disulfide bonds provides critical information regarding the structure and function of a protein and is a key aspect in understanding signaling cascades in biological systems. Recent proteomic approaches using digestion enzymes have facilitated the characterization of disulfide-bonds and/or oxidized products from cysteine residues, although these methods have limitations in the application of MS/MS. For example, protein digestion to obtain the native form of disulfide bonds results in short lengths of amino acids, which can cause ambiguous MS/MS analysis due to false positive identifications. In this study we propose a new approach, termed planned digestion, to obtain sufficient amino acid lengths after cleavage for proteomic approaches. Application of DBond software to planned digestion of specific proteins accurately identified disulfide-linked peptides. RNanse A was used as a model protein in this study because the disulfide bonds of this protein have been well characterized. Application of this approach to peptides digested with Asp-N/C (chemical digestion) and trypsin under acidic hydrolysis conditions identified the four native disulfide bonds of RNase A. Missed cleavages introduced by trypsin treatment for only 3 hours generated sufficient lengths of amino acids for identification of the disulfide bonds. Analysis by MS/MS successfully showed additional fragmentation patterns that are cleavage products of S-S and C-S bonds of disulfide-linkage peptides. These fragmentation patterns generate thioaldehydes, persulfide, and dehydroalanine. This approach of planned digestion with missed cleavages using the DBond algorithm could be applied to other proteins to determine their disulfide linkage and oxidation patterns of cysteine residues.

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Synthesis and anti-melanogenesis activity of natural compounds-peptide derivative

이혜숙 김한영*

애경산업(주) 중앙연구소

Peptides generally have biocompatibility and high activity, but also have very low stability. Therefore, C-terminal amidation or N-terminal capping using small organic material was used to prevent peptide degradation. In previous study, we developed small molecule-peptide conjugates as potential whitening agents which inhibit tyrosinase activity and antagonize MC1R at the same time. The conjugated small molecules having tyrosinase inhibitory activity were selected using mushroom tyrosinase assay. Through this method, caffeic acid and p-coumaric acid were screened. However, these conjugates were unstable under UV light because of oxidation of their hydroxyl group. In this study, we developed photostabilized small molecule-peptide conjugates, and their potentials as skin whitening agents were investigated.Acknowledgement This study was supported by a grant of the Korean Health Technology R&D Project, Ministry of Health & Welfare, Republic of Korea.(Grant No. HN10C0006)

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Inhibitory Effect of ortho-Substituted Derivatives of Cinnamaldehyde on Melanin Biosynthesis in Murine B16 Melanoma

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동국대학교 화학과

Many natural products have been used as traditional medicine in Korea for the treatment of skin diseases. Natural compounds can be used as good resources for cosmetic agents because they are generally non-toxic and environmentally friendly. To develop effective skin-whitening agents, we screened the effect of 33 kinds of natural compound library on the melanogenesis signaling pathway activated by α-melanocyte-stimulating hormone (α-MSH) through cell based melanin assay. We found that several natural products inhibit melanin production in a dose-dependent manner without causing cytotoxicity in B16 melanoma cells. o-Substituted derivatives of cinnamaldehyde (o-Benzoyloxycinnamaldehyde, o-Hydroxycinnamaldehyde, and o-Acetyloxycinnamaldehyde) were selected from the library. We investigated the changes in protein level of tyrosinase, tyrosinase related protein (TRP) -1 and -2 which are key enzymes of melanin biosynthesis by using western blotting. Also we studied the inhibitory effect on tyrosinase activity which initiates the first step of melanin synthesis. Both studies show o-Substituted derivatives of cinnamaldehyde are effective inhibitors of melanin pigmentation. These results indicated that they inhibit melanin biosynthesis, associated with hyperpigmentation and can be used as skin-whitening cosmetic for skin care.

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Development of a Biosensor by Metal Ion Quenchable Fluorescent Protein

황광연 남기현[1,*]

고려대학교 생명공학부 [1]포항가속기연구소 PAL-XFEL

Fluorescence of fluorescent proteins (FPs) is often quenched by specific transition metal ions. Based on this molecular property, FPs can be utilized as highly selective biosensors for metal ions. Nevertheless, the exact mechanism by which divalent metal ions behaves at the atomic level during the fluorescent quenching is still unclear. Here we show the cobalt and copper-induced fluorescence quenching of a green fluorescent protein (GFP) and its mode of action through determining the crystal structures of metal-complexed GFP. Crystal structure revealed that Co^{2+} and Cu^{2+} bind to unique histidine residues on the external region of the β-can surface. In FP-Co^{2+}, the first Co^{2+} ion was tetragonally coordinated by His194, His212 and water molecules, whereas the second metal ion was imperfectly coordinated by His200. In FP-Cu^{2+}, the first Cu^{2+} ion was tetragonally coordinated by His210, His212, and the other metal ion was in unstable coordination with His200. Structural comparisons conducted in this study reveal that FP-based biosensor for metals share the common histidine residues in external region of the β-can. Our results will be helpful for the better understanding of the metal-induced fluorescence quenching of FPs by metal ion, and pave the way for the development of metal biosensors.

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Development of peptide based in-vitro diagnostic system for pre-symptomatic of Alzheimer's disease

김상헌 이상춘 하나름 이아영 윤문영*

한양대학교 화학과

Amyloid-bata 42 (Aβ42) which is produced from proteolytic cleavage of the amyloid precursor protein (APP) is the main composition of amyloid structures such as amyloid oligomers, fibrils and plaques. Due to these amyloid structures induce and aggravate the Alzheimer's disease, the Aβ42 as a biomarker represents one of the main molecular hallmarks of AD. We screened 7 cyclic peptides (7mer) and 4 linear peptides (12mer) which bind to Aβ42 via phage display screening. The binding affinity (K_d) of peptides are estimated on the micromolar (~10^{-6} mole L^{-1}) level. In order to develop a diagnostic system, we utilized a sandwich assay using two different peptides substituted for current antibody based diagnostic system and to enhance the sensitivity, we developed a polyvalent directed peptide polymer (PDPP). Finally, This approach represents a promising strategy to potential probe for pre-symptomatic diagnosis of neurodegenerative diseases.

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Development of diagnostic ssDNA aptamer against endocrine disruptor (bisphenol A)

김아루 문지영 윤문영*

한양대학교 화학과

Endocrine disruptor is a major public health problem to people throughout the world. In human body, the compounds functionalize same as sexual hormone with inducing a precocious puberty, gynecomastia, etc. The one of endocrine receptor, bisphenol A, is widely used in making plastic stuffs such as water bottles, sports equipment, CDs and DVDs. It analogous of estrogen and could bind to estrogen receptor. When it exists on hot or warm water, the chemical compound can melt out. Therefore, to prevent taking the bisphenol A such from daily supplies, it should detect easily with fast.Herein, we developed a novel single strand DNA (ssDNA) aptamer for detection of bisphenol A. We used N-oxysuccinimide (NOS) coated well-plate to immobilize the bisphenol A and tris as a first linker to connect between epoxide and NOS group. Afterward, we coated the surface with diepoxybutane as a second linker to interact between hydroxyl group of tris and bisphenol A. To screen a bisphenol A binding ssDNA aptamer, we performed 10 rounds of SELEX and obtained 60mer ssDNA library by asymmetric PCR and “crush and soak” method. In this process, we changed the probe binding time, buffer and salt concentration to give a harsh condition at every round to find more specific probe. After SELEX process, we identified one ssDNA aptamer with high binding efficiency and specificity towards target. We expect this aptamer based biosensor system will be a good for detecting bisphenol A in industrial products for people’s health.

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Quantitative structural analyses of the intermediate complex during protein-induced B?Z transition induced by Z-DNA binding domain of PKR-like protein kinase (PKZ)

이애리 이준화*

경상대학교 화학과

Z-DNA binding proteins (ZBPs) specifically bind to Z-DNA and play important roles in RNA editing, innate immune response, and viral infection. Despite extensive structural studies, a comprehensive understanding of molecular mechanism about their Z-DNA binding affinities and B?Z transition activities, including structures of intermediate complexes, is lacking. Here we scrutinize the B-DNA and Z-DNA binding and B?Z transition steps of the Zα domain ($caZ\alpha_{PKZ}$) of goldfish ZBP-containing protein kinase, through systematic NMR measurements. Solution structure shows that free $caZ\alpha_{PKZ}$ exhibits unique conformational change of DNA binding surface that is modulated by varying salt concentration. We find that increasing [NaCl] from 10 to 100 mM reduced the binding affinities of $caZ\alpha_{PKZ}$ for both B-DNA (600-fold) and Z-DNA (25-fold) and its B?Z transition activity (4.6-fold). Our results highlight the importance of the structural feature of the intermediate complex formed by $caZ\alpha_{PKZ}$ and B-DNA, which determines degree of B?Z transition in DNA.

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Structural features Important for its Antimicrobial Activities in Papiliocin

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건국대학교 생명공학과

A novel 37-residue, cecropin-like peptide, papiliocin, isolated from the swallowtail butterfly Papilio xuthus, possesses high bacterial-cell selectivity, particularly against gram-negative bacteria. Since Trp2 and Phe5 is the highly conserved residues in cecropin-like peptides, we investigated the role of these two aromatic residues. Substitution of Trp2 and Phe5 in papiliocin with Ala revealed that Trp2 is the key residue in antibacterial and anti-inflammatory activities of papiliocin.. In order to gain further insight into the structural requirements for papiliocin function and to design potent and short peptide antibiotics, we made papiliocin short constructs, PapN (residues Arg1-Ala22 from the N-terminal amphipathic helix). PapN exhibits significant antibacterial and anti-inflammatory activities without cytotoxicity, suggesting that PapN can be a potent peptide antibiotic. Bactericidal kinetics of peptides against *E.coli* show that papiliocin completely and rapidly killed E.coli in less than 10 minutes at concentration of 2 x MIC levels while papiliocin analogs without Trp2 or Phe5 kill more than 4 times slowly compared to papiliocin at 2 x MIC. All PapN series peptide without C-terminal helix show much weaker membrane permeabilization ability compared to papiliocin and have no comparable time-killing antibacterial activities in an hour. The results imply that highly conserved Trp2 and Phe5 in amphipathic N-terminal helix are important in rapid permeabilization of the gram-negative bacterial membrane. Then, hydrophobic portion of the C-terminal helix permeabilize into the hydrophobic bacterial cell membrane synergistically with the aromatic rings of the N-terminal helix, providing selectivity against gram-negative bacteria.

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Anti-Tuberculosis and Anti-inflammatory Activity of a Naturally Occurring Flavonoid, Isorhamnetin

전다솜 박영근 김양미*

건국대학교 생명공학과

Isorhamnetin (1) is a naturally occurring flavonoid that has been reported to possess anti-cancer and anti-inflammatory activities. The present study demonstrated for the first time that 1 produced antimycobacterial effects on *Mycobacterium tuberculosis* H37Rv, as well as multi-drug- and extensively drug-resistant clinical isolates, with minimum inhibitory concentrations of 50 and 100 ?g/mL, respectively. To explore the potential therapeutic efficacy of 1, we investigated its anti-inflammatory activity and mode of action in mouse macrophage-derived RAW264.7 cells stimulated with interferon (IFN)-γ. A non-toxic dose of 1 reduced the levels of mRNAs encoding mouse tumor necrosis factor-a, mouse interleukin (mIL)-1β, mIL-6, mIL-12, and mIL-18, mouse inducible nitric oxide synthase, mouse monocyte chemoattractant protein-1, and mouse macrophage inflammatory proteins 1 and 2 in IFN-γ-stimulated macrophages. We found the anti-inflammatory effects of 1 are mediated by actions on the extracellular signal-regulated kinase (ERK), and c-Jun N-terminal kinase (JNK) signaling cascade with Toll-like receptor (TLR)-2 pathway in IFN-γ-stimulated macrophages. Furthermore, the *in vivo* effect of 1 was examined in a mouse lipopolysaccharide-induced lung inflammation model. A non-toxic dose of 1 reduced the levels of pro-inflammatory cytokines, such as IL-1β, IL-6, IL-12, and INF-γ. These data provided the first evidence that 1 could be developed as a potent agent for the treatment of tuberculosis.

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E. faecalis ACP has only one acyl chain binding sub-pocket due to F45-mediated hydrophobic packing

박영근 정민철 송희상 김양미*

건국대학교 생명공학과

Fatty acid synthesis is essential for cell growth and viability. The Acyl Carrier Protein (ACP) is a key element in the biosynthesis of fatty acids being responsible for the acyl group shuttling and delivery within a series of related enzymes. In this study, to understand the origin of high thermal stabilities of E. faecalis ACP (Ef-ACP), solution structure was investigated for the first time. CD experiments showed that the melting temperature of Ef-ACP is 78.2°C, which is much higher than that of Escherichia coli ACP (67.2°C). The overall structure of Ef-ACP shows the common ACP folding pattern consisting of four α-helices (helix I (3-17), helix II (39-53), helix III (60-64), and helix IV (68-78)) connected by three loops. Unique Ef-ACP structural features include a stacking interaction between F45 in helix II with F18 in the α1α2 loop and a hydrogen bonding between S15 in helix I and I20 in the α1α2 loop, resulting in its high thermal stability. Furthermore, S58 in the α2α3 loop in Ef-ACP, which usually constitutes a proline in other ACPs forming a rigid bent structure, exhibited slow conformational exchanges, resulting in the movement of the helix III outside the structure to accommodate a longer acyl chain in the acyl binding cavity. These results might provide insights into the fatty acid synthesis and thermal tolerance of E. faecalis.

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Flexibility of *E.coli* ACP is essential for the Ability of ACP to interact with Enzyme Partner, KAS III

정민철 박영근 송희상[1] 김양미[*]

건국대학교 생명공학과 [1]건국대학교 특성화학부 생명공학과 구조화학실험실

Acyl carrier protein (ACP) plays important role in numerous biosynthetic pathways that depend upon acyl transfer. *E.coli* ACP (*Ec*-ACP) is a highly acidic protein, therefore, the binding of divalent cations at discrete sites on the protein can neutralize the repulsive effects of the 20 acidic residues in *Ec*-ACP and stabilize the structure. In the presence of divalent cation, *Ec*-ACP has two conformers in dynamic equilibrium. We investigated the structures and backbone dynamics of *Ec*-ACP in dynamic equilibrium and confirmed two metal-binding sites of *Ec*-ACP. We found that the Tm of *Ec*-ACP in the presence of Ca2+ was 67.2°C, much higher than 54.9°C, the Tm of *Ec*-ACP in the absence of metal ions. Backbone dynamics study showed that *Ec*-ACP is a flexible protein and metal binding increased the structural rigidity near two metal binding sites. Flexibility is believed to be essential for the ability of ACP to interact with multiple enzyme partners and undergo conformational changes as it reversibly directs acyl groups to the active sites for these enzymes.Since multi-drug resistant gram-negative bacterial infections are threatening worldwide, we tried to discover new antibiotic compounds that have novel mechanisms toward target enzyme, ß-ketoacyl-acyl carrier protein synthase III (KAS III), a condensing enzyme in FAS systems. We determined the pharmacophore maps from receptor-oriented pharmacophore-based in silico screening of *E. coli* KAS III protein. We identified potent *Ec*-KAS III inhibitors with broad-spectrum antibacterial activity with strong binding affinity to *Ec*-KAS III. Further optimization of this compound is required to improve its antimicrobial activity.

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Synthesis of Novel compounds having Ceramide structure and it's application

김유미 김한영[1,*]

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피부 각질층은 피부 고유의 보습기능을 발휘하는데 매우 중요하며, 특히 각질세포간 지질은 세포사이에서 라멜라 구조를 형성하여 단단한 시멘트와 같은 역할을 함으로서 피부장벽기능의 근원이 된다. 이중 세라마이드는 지질 전체의 약 40% 이상이 될 정도로 매우 중요한 성분이며, 피부장벽기능의 필수적인 성분이라고 할 수 있다. 이러한 지질 성분은 어려운 제조방법으로 인한 단가 문제로 범용적인 사용이 어려운 단점이 있다. 이에 제조가 용이하여 범용적인 사용이 가능한 신규 유사 세라마이드 소재를 합성하였다. 이는 서로 다른 두 화합물의 개환 반응으로 보다 편리하고 경제적으로 합성하였으며, 합성한 소재의 구조 및 반응의 종결은 NMR 과 HPLC 분석을 통해 진행하였다. 소재의 효능을 평가를 위해서 보습력 실험과 모발내부평가, 인장강도 실험을 실시하였다. 보습력 평가는 tape stripping 으로 피부 각질층을 손상 시킨 뒤 corneometer 를 사용하여 측정하였으며 손상 전, 후, 3 시간, 6 시간, 24 시간, 48 시간, 72 시간 측정하여 보습력 향상률을 계산하였다. 또한 모발 내부평가를 통해서 모발 끊어짐이 개선됨을 확인하였으며, 모발의 인장강도를 평가함으로 모발이 보다 단단하게 유지됨을 보았다. 소재의 안전성 데이터 확보 및 신규 소재의 세포독성 수준을 파악하기 위해 세포독성 실험을 하였다. 그리고 무좀균과 여드름균에 대한 항균활성을 알아보기 위해 MIC 측정 시험을 진행하였다.

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Discovery of Novel Slingshot Protein Tyrosine Phosphatase Inhibitors

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동국대학교 화학과

In conjunction with protein tyrosine kinases (PTKs), protein tyrosine phosphatases (PTPs) regulate the reversible phosphorylation of tyrosine residues in proteins thereby controlling fundamental physiological processes such as cell growth and differentiation, cell cycle, metabolism and cytoskeletal function. Slingshot protein tyrosine phosphatases (SSHs), consist of SSH-1, -2 and -3, dephosphorylate phospho-cofilin, leading to activate cofilin. Cofilin is an actin-depolymerizing factor and its phosphorylation inactivates its actin severing activity. Moreover, SSHs are overexpressed in tumor cells and appear to be a relevant target for anticancer therapy. In this study, we have screened natural product library consisting of 658-purified single compounds for potent and selective inhibitors of SSHs. As a result, we identified three natural products as SSHs inhibitors which were determined type of inhibition and Ki values. Furthermore, two of three natural products were evaluated for cofilin phosphorylation, by SSHs deactivation in cells.

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ATP-independent catalytic activities of the DEAD-box protein CshA from Staphylococcus aureus

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DEAD-box proteins play important roles in many RNA processes ranging from RNA synthesis to RNA decay. Furthermore, it has been reported that some bacterial DEAD-box proteins known to be components of the RNA degradosome such as CshA do not cleave RNA substrates directly. However, the role of DEAD-box proteins in RNA degradation is poorly understood. We demonstrated that the DEAD-box protein CshA from the vancomycin-resistant Staphylococcus aureus strain Mu50 possesses RNA degradation activity, endoribonuclease activity, and complementary RNA strand annealing activity as well as RNA helicase activity that was common in DEAD-box proteins. Despite CshA contains duplex RNA unwinding activity, it has a poor processivity which shows unwinding of duplex RNA with shorter than 15 base pairs. Moreover, the helicase activity of CshA requires single-stranded RNA tails for its activity. Interestingly, the helicase activity of CshA does not require ATP hydrolysis. In the presence of ATP, CshA instead catalyzed the degradation of single-stranded RNAs at phosphodiester bonds. In addition, we observed that CshA possesses RNA strand annealing activity, which converts complementary single-stranded RNA substrates into double-stranded RNA duplexes. Thus, we suggest that the endoribonuclease and RNA strand annealing activities of the DEAD-box protein CshA may contribute to RNA remodeling in the bacterial RNA degradosome. To our knowledge, this study is the first to report that a DEAD-box protein from a pathogenic bacterium is implicated in multiple ATP-independent activities on RNA, such as RNA degradation, annealing, and duplex RNA unwinding with low processivity.

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Galactosylated Themperature Sensitive Polymer as a Three Dimensional Culture Scaffold for Hepatogenesis of Human Tonsil-Derived Mesenchymal Stem Cell

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이화여자대학교 화학나노과학과

A 3 dimensional cell culture system to achieve the differentiation of tonsil-derived mesenchymal stem cells (TMSCs) toward hepatocytes with high efficiency is crucial in providing a cell source for the medical application. In this study, we investigate the effect of Lactobionic conjugated poloxamer-poly (L-alanine) (galatosylated thermogel) as 3D matrix for hepatogenic differentiation. The cell-encapsulated 3D matrix was prepared by increasing the temperature of the cell-suspended galactosylated polymer aqueous solution (6.0 wt. %) to 37^{o}C. The gel modulus at 37^{o}C was about 1000 Pa, which was similar to that of decellularized liver tissue. In 3D system using a galatosylated thermogel, TMSCs expressed elevated level of liver specific genes, protein and functions together. The 3D system uses a galatosylated thermogel as an extracellular matrix for enrichment of mesenchymal stem cell derived hepatocyte with adequate homogeneity and functionality.

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Detection of EGFR exon 19 deletion in plasma of non-mall cell lung cancer (NSCLC) patients using graphene oxide and quencher-free fluorescent DNA probe

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Mutations in epidermal growth factor receptor (EGFR) have been known as biomarker that can be used to monitor the tumor response against drugs such as tyrosine kinase inhibitors in NSCLC. About 50 % of NSCLC patients possess deletion of several sequences in exon 19 of EGFR gene. As less invasive method for detection of EGFR exon 19 deletion mutation is required, we developed a simple PCR-based detection of EGFR exon 19 deletion gene in plasma of NSCLC patients by using quencher-free fluorescent probe DNA and graphene oxide (GO). In the presence of the exon 19 deletion mutation, which is fully complementary to the probe DNA, the probe anneals to the junction sequence (mutant type). The fully annealed DNA probe was then degraded by the 5′ to 3′ exonuclease activity of Taq DNA polymerase during PCR, releasing the fluorophore from the probe DNA. In contrast, wild type of exon 19 gene would allow the probe DNA to be annealed partially to the template DNA. The partially annealed probe DNA would be digested by Taq polymerase, releasing a fragment of probe DNA. When GO was added to each reaction solution, it produced different fluorescence signals; enhanced fluorescence was observed due to the released fluorophore from the probe DNA that was not adsorbed onto GO, whereas fluorescence was quenched with fragmented single stranded probe DNA that was easily adsorbed onto GO. The fluorescence signal caused by the exon 19 deletion mutation gene was also quantitatively correlated with amount of the mutant gene. Thus, we believe that the GO-based fluorometric assay can be applicable for diagnostic detection of the exon 19 deletion in EGFR gene.

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A small molecule that has potential drug activity on cystic fibrosis by inhibition of ATPase domain of HSC70

서원일 신인재*

연세대학교 화학과

Cystic fibrosis transmembrane conductance regulator (CFTR) is a cell-surface anion channel that permeates chloride and bicarbonate ions. The most frequent mutation of CFTR that causes cystic fibrosis is the deletion of phenylalanine at position 508 (ΔF508), which leads to defects in protein folding and cellular trafficking to the plasma membrane. The lack of the cell-surface CFTR results in a reduction in the lifespan due to chronic lung infection with progressive deterioration of lung function. Hsc70 plays a crucial role in degradation of mutant CFTR by the ubiquitin?proteasome system. To date, various Hsc70 inhibitors and transcription regulators have been tested to determine whether they correct the defective activity of mutant CFTR. However, they exhibited limited or questionable effects on restoring the chloride channel activity in cystic fibrosis cells. Herein, we show that a small molecule apoptozole (Az) has high cellular potency to promote membrane trafficking of mutant CFTR and its chloride channel activity in cystic fibrosis cells. Results from affinity chromatography and ATPase activity assay indicate that Az inhibits the ATPase activity of Hsc70 by binding to its ATPase domain. In addition, a ligand-directed protein labeling and molecular modeling studies also suggest the binding of Az to an ATPase domain, in particular, an ATP-binding pocket. It is proposed that Az suppresses ubiquitination of ΔF508-CFTR maybe by blocking interaction of the mutant with Hsc70 and CHIP, and, as a consequence, it enhances membrane trafficking of the mutant.

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The Immobilized Metal Affinity Chromatography Enrichment Method for Nitropeptides by Using CupriSorb™

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Protein tyrosine nitration (PTN) is a post-translational modification which is addition of nitro group (NO_2) on the ortho position to phenolic ring of tyrosine residue. 3-nitrotyrosine is formed by action of nitrating agent such as peroxynitrite anion ($ONOO^-$) from the radical reaction of nitric oxide (NO) with superoxide anion (O_2^-). The analysis of 3-nitrotyrosine are very important in biologically and clinically because PTN affects in many pathological events such as neurological disorders and several cancers. However, little is known about the mechanisms and the target proteins involved in the modification because of the low stoichiometry of nitrotyrosine in vivo. Mass spectrometry has been proven to be a very sensitive equipment for analyzing post-translational modification of proteins. However, only a relatively small portion of the population for a specific protein may be modified, which makes its analysis difficult. Therefore, it is necessary for efficient enrichment methods to identify nitrated proteins from biological samples. In this study, We performed IMAC using CupriSorb resin loaded Cu^{2+} ion as a enrichment method of nitrated proteins. CupriSorb is a powerful copper specific chelating resin and the ligand directly forms a chelate complex with amine group of *o*-aminophenol. As a result, we expect that CupriSorb resin can become a rapid and exceptional enrichment method of nitrated peptides without tagging steps.

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Anti-obesity effect of green tea in high-fat diet-induced obese C57BL/6J mice

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Green tea is a widely consumed beverage brewed from the fresh leaves of Camellia sinensis and has been previously shown to reduce body weight and fat. The aim of this study is to evaluate the efficacy of green tea at the lipid level. In this study, using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q TOF MS), we performed lipid profiling of liver in obesity mice induced by high-fat diet (HFD) for 12 weeks. C57BL/6J mice were randomly divided into three groups: normal diet (ND) group, HFD group and HFD plus green tea (GT) group (all groups n=10). The acquired data was analyzed by principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA). The results showed a difference among the groups and revealed that green tea changed the levels of lipid which are involved in obesity. Levels of lysophospholipids such as lysophosphatidylcholine (lysoPC), lysophosphatidylethanolamine (lysoPE) and lysophosphatidylserine (lysoPS) significantly decreased in HFD group compared to ND group and GT group showed recovery of lysophospholipids levels. Our study suggests that global lipid profiling could practically evaluate therapeutic efficacies of green tea on obesity.

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Comparison of Anti-cancer Drug Delivery Efficiency: Doxorubicin Encapsulated in the RNA aptamer-conjugated Liposome vs. the One Intercalated in the RNA aptamer

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건국대학교 생명공학과

Combination of drug delivery and specific targeting has a potential for treating cancer diseases. To achieve this goal, specific ligands targeting cancer cells and bioconjugate vehicles for drug delivery are necessary. Liposomes are one of successful drug-delivery materials because they can reduce toxicity and enhance stability of drugs by encapsulation. Aptamers are single stranded nucleic acid molecules that can bind target molecules such as proteins and peptides, which can be used as targeting ligands. Previously, we have developed a RNA aptamer-conjugated liposome (named as aptamosome) that specifically targets the prostate cancer cells expressing prostate-specific membrane antigen (PSMA). Using the aptamosome, anti-cancer drug doxorubicin (Dox) was specifically and efficiently delivered to the prostate tumors. The PSMA-specific RNA aptamer by itself has been also recognized as tumor specific drug delivery material by intercalating Dox. In this study, we compared two different methods for Dox delivery to PSMA-positive cancer cells, which are intercalation of Dox into the aptamer (Apt-Dox) and encapsulation of Dox in the aptamosome (Apm-Dox). We observed that the Apm-Dox was superior to Apt-Dox in specificity and Dox delivery efficiency toward PSMA (+) cancer cells.

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Distinct modulation of hepatic metabolites by non-alcoholic fatty liver disease

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Non-alcoholic fatty liver disease are rapidly increased worldwide and recognized as a risk factor for diabetes, cardiovascular disease, obesity and renal disease. To investigate metabolic changes by NAFLD in obese mice, we performed metabolic profiling and biological analysis of liver tissues. In this study, we used diabetes models; db/db mice (C57BL/6J-db/db). Twenty-week-old male db/db and wild type (WT) mice were fed normal standard diet chow (ND). Then, we applied metabolic profiling based on ultra-performance liquid chromatography/quadrupole time-of flight mass spectrometry (UPLC/Q-TOF MS) and nuclear magnetic resonance (NMR) to find metabolic differences between two groups. Both of multivariate statistical analysis derived from MS and NMR data of liver tissue extracts showed clear metabolic differences between WT and db/db mice. This study identified features of hepatic metabolism of mice which induced NAFLD, and demonstrated that a combined approach based on MS and NMR analysis is a useful method to investigate the metabolic changes induced by NAFLD and understand their metabolism.

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Lipid profiling of human atherosclerotic aorta based on liquid chromatography/mass spectrometry

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Atherosclerosis is the main cause of mortality in industrialized countries. However, only a limited number of studies on atherosclerosis was proceeded in lipid profiling of human tissue. In the present study, we performed the lipid profile of atherosclerotic aorta extracts and normal aorta extracts of human using ultra-performance liquid chromatography/quadrupole time-of flight mass spectrometry (UPLC/Q-TOF MS). Partial least squares-discriminant analysis (PLS-DA) plots showed a clear differentiation between atherosclerotic aorta extracts and normal aorta extracts. Significantly altered lipid metabolites were ceramide (Cer), lysophosphatidylcholine (lysoPC), phosphatidylcholine (PC), phosphatidylethanolamines (PE), phosphatidylinositol (PI), sphingomyelin (SM), diacylglycerol (DG) and triacylglycerol (TG) species and those lipid metabolites were elevated in atherosclerotic aorta. Particularly, lysoPC and Cer species were highly increased in atherosclerotic aorta. These results showed that lysoPC and Cer were associated with development of atherosclerosis. This study demonstrated that UPLC/Q-TOF MS based lipid profiling can be useful tool to understand lipid distribution of human atherosclerotic aorta and may provide the insight for pharmacotherapeutic intervention.

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NMR Structural Analysis of Antimicrobial peptides, LPcin analogs, with Enhanced Activities in membrane environments

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Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of bovine proteose-peptone PP3. LPcin analogs were designed and modified to enhance antibacterial activity using mutation, shorten sequence, and sequence shuffling for better amphipathic characteristics. Three candidates with enhanced antibacterial activity were chosen among 12 LPcin analogs, the name of LPcin-YK1, LPcin-YK2 and LPcin-YK3 respectively, via agar hole diffusion test. To understand the correlation between their structures and antibacterial mechanism, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using various biophysical techniques. We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with several biophysical techniques. We performed MALDI-TOF MS and CD spectrometry for structure refinement. In order to investigate the structures and dynamics, we use various solution and solid state NMR techniques using the purified peptides with micelle and especially bicelle samples to mimic membrane environments. Finally we use structural calculations and MD simulation by using Discovery Studio 3.1 to compensate for solid state NMR data for structural refinement.

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Identification of alterations in metabolite profiles in plasma from patients with atrial fibrillation

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Atrial fibrillation (AF) is the most common cardiac arrhythmia, and its incidence is increasing worldwide. The important treatment method for AF is direct current cardioversion (DCC). Although AF recurrence was generally incurred in half of the patients who underwent cardioversion in a month, well-known predictors for AF recurrence are mainly structural factors.In this study, we applied metabolic profiling to identify altered metabolites in plasma from patients with AF. Metabolic profiles of plasma from patients with AF were investigated using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF MS) coupled with multivariate statistical analysis.The multivariate statistical analysis showed a clear separation between patients with AF and healthy controls. The levels of several metabolites decreased in plasma from patients with AF compared to that from healthy controls. In addition, these changes were detected between recurrence and non-recurrence AF patients.Metabolic profiling of plasma by UPLC/Q-TOF MS could be useful approach for understanding AF pathogenesis and predicting AF recurrence.

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Development of robust and rapid manner for the inhibitor screening of Amyloid-ß peptide aggregation

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동국대학교 화학과

Fibrillar aggregates of amyloid-β peptide in the brain is signs of Alzheimer's disease (AD). Amyloid fiber formation of extracellular amyloid-β peptide deposits is associated with the interactions of high concentration metal ions in the brain. Especially, the rate of amyloid-β aggregation is promoted by high level of zinc ion (Zn2+) that is formed the coordination with histidine and aspartic acid of amyloid-β peptide.[1] Based on this mechanism, development of the inhibitor for preventing amyloid-β peptide aggregation is important. The current aggregates detection and inhibitor screening manner are ELISA, Western blot (WB) and immunoprecipitation (IP).[2, 3] These conventional manners have the limitation such as time consuming, cost and reproducibility. To overcome this weakness, rapid and robust detection manner is designed. Our strategies are based on fluorescence detection manner that observe the increased or decreased fluorescence intensity by amyloid-β aggregate formation as zinc ion concentration. This manner is identified by small molecule Lb-2 that is known to inhibit amyloid-β aggregation in the cell.[4] The strategy may be efficiently applied to drug screening of amyloid-β. Furthermore, we are testing several natural compounds to perform a key role of amyloid-β aggregate inhibition.

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In vivo tissue regeneration of ECM protein sticker

김유환 안승국[1] 신관우[2,*]

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

In the body, for self-healing system of injury, protein fibrillogenesis is the key process of self-assembly that leads to formation of the extracellular matrix (ECM), which well known as fibronectin (FN), collagen (COL), laminin (LAM), and elastin (ELAS). So, considerable efforts[1] have been devoted to manufacturing FN fibers and fabrics in vitro which is model after in vivo healing process. The research achieved that forming protein networks on, polysterene, polymer film. In order to apply to living things, We re-apply about biocompatible materials like a polycaprolactone (PCL), poly(lactic-co-glycolic acid) PLGA and so on. And we're planning to primary culture the stem cell on the biodegradable polymer film. We just identify the generation probability of networks on PCL film. But, Biodegradability of the film is also big issue. So now we use PLGA which can control biodegradability. By using those networked biodegradable film primary culture the stem cell on the film. After the cell settle on the FN networks, we're planning to apply to skin and expect that improvement of tissue regeneration because of fabricated ECM. Further, Its can be usable to the other organ like heart, stomach, liver, and so on.

References

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Effects of Pore size of Nanostructured Aluminium Oxide on the Viability of Cells

김근오 이호연[1] 박현욱 강철훈[1,*] 권영욱[*]

성균관대학교 화학과 [1]경희대학교 동서의학대학원

Interest in the research of nanostructured surfaces for biological field such as implant materials, biomedical studies has increased recently. Therefore, the interaction between nanostructured materials and cells has been studied extensively, but the effect of nanostructured surfaces on the cell viability has received less attention. In this study, we report that we could control the cell growth and viability by adjusting the pore size of the solid surface. We prepared vertically oriented anodic aluminum oxide (AAO) membranes with different pore sizes ranging from 18 to 150 nm. We found that cell response such as morphology, proliferation and viability of HeLa cells to this highly aligned AAO membranes is strongly dependent on the pore size. Cell proliferation and viability on 18 nm sized pore were significantly enhanced compared to those on glass for control. In contrast, cell proliferation, viability and activity were dramatically decreased with the increase of pore size. On AAO of 150 nm of pore size a high degree of cell death was observed. In conclusion, we demonstrate that nanoscopic physical morphology of AAO could affect the cell viability.

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Peptidomimetics with Antimicrobial Activities Using Facile Amphiphilic Scaffold

김현수 임현석*

포항공과대학교(POSTECH) 화학과

Antimicrobial peptide is considered as a potential replacement of an antibiotics. Natural antimicrobial peptides, including magainins , appear commonly in nature, and defend their organism against bacteria by interaction with cytoplasmic bacterial membrane. They tend to adopt amphiphilic character caused by hydrophobic and cationic side chains, many of which consist of α-helical structure.1,2Recently, Lee et al. developed a novel α-helical mimetics using triazine-piperazine-triazine scaffold to target α-helical motif.3 This scaffold mimics α-helical structure with its functional groups at i, i+4, i+7. Herein we designed this scaffold based on hydrophobic backbone with positively charged functional groups mimicking helical amphiphilic structure of antimicrobial peptides. As a result, the triazine-piperazine-triazine scaffold with amphiphilic structure shows low micromolar antimicrobial activity against gram-positive bacteria as well as gram-negative bacteria.

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Carcinogenic activity of PbS quantum dots screened using exosomal biomarkers secreted from HE K293 cells

김혜림 인수일*

대구경북과학기술원(DGIST) 에너지 시스템 공학 전공

Lead sulfide (PbS) quantum dots (QDs) have been applied in the biomedical area because they offer an excellent platform for theragnostic applications. In order to comprehensively evaluate the biocompatibility of PbS QDs in human cells, we analyzed the exosomes secreted from cells because exosomes are released during cellular stress to convey signals to other cells and serve as a reservoir of enriched biomarkers. PbS QDs were synthesized and coated with 3-mercaptopropionic acid (MPA) to allow the particles to disperse in water. Exosomes were isolated from HEK293 cells treated with PbS?MPA at concentrations of 0 µg/mL, 5 µg/mL, and 50 µg/mL, and the exosomal expression levels of miRNAs and proteins were analyzed. As a result, five miRNAs and two proteins were proposed as specific exosomal biomarkers for the exposure of HEK293 cells to PbS?MPA. Based on the pathway analysis, the molecular signature of the exosomes suggested that PbS?MPA QDs had carcinogenic activity. The comet assay and expression of molecular markers, such as p53, interleukin (IL)-8, and C-X-C motif chemokine 5, indicated that DNA damage occurred in HEK293 cells following PbS?MPA exposure, which supported the carcinogenic activity of the particles. In addition, there was obvious intensification of miRNA expression signals in the exosomes compared with that of the parent cells, which suggested that exosomal biomarkers could be detected more sensitively than those of whole cellular extracts.

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Structural anlaysis of ORF49 in Murine herpesvirus 68

김준수 **황광연**[1,*]

고려대학교 바이오시스템공학과 [1]고려대학교 생명공학부

Gamma-herpesviruses such as Epstein Barr virus (EBV) and Koposi’s sarcoma-associated herpesvirus (KSHV) are important human pathogens as they are associated with various tumors. Murine gamma-herpesvirus 68 (MHV-68) is genetically and biologically related to human gamma-herpesviruses and provides a tractable model system to study virus-host interactions. The Open Reading Frame 49 (ORF49) protein is well conserved among gamma-herpesviruses and shown to cooperate with replication and transcription activator (RTA) in regulating virus lytic replication. To date, it is unclear in cellular and structural function. Here, we report the first crystal structure of ORF49 of MHV-68 at 2.2 ?. The crystal belonged to space group $p3_221$, with unit cell parameters a = b = 134.179 ?, c = 157.158 ?, α = β = 90 °, γ = 120 °. The structure consists of an almost α-helix and contains two domains, a dimerization domain (DD) and leucine rich domain (LRD). Our structural and biochemical studies provide us for understanding of the molecular mechanism between ORF49 and RTA in KSHV lytic cycle.

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Crystal structure of Triosephosphate Isomerase from Clonorchis sinensis

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고려대학교 바이오시스템공학과 [1]고려대학교 생명공학부

Clonorchis sinensis is a parasitic flatworm that can cause clonorchiasis in East Asia [1]. In 2009, International Agency of Cancer Research reclassified C. sinensis as a group 1 biological carcinogen because this trematode is known to cause cholangiocarcinoma [2]. Triosephosphate isomerase (TIM), a key enzyme in glycolysis, catalyses the reversible isomerization of dihydroxyacetone phosphate (DHAP) to D-glyceraldehyde 3-phosphate (GAP). Since its role in energy metabolism is considerable, it has been regarded as a major drug target [3]. Recent study has been reported that many parasitic flatworms have a similar tripeptide insert (SXD/E) in TIM [4]. Here, we determined the crystal structure of TIM from Clonorchis sinensis (CsTIM) at 1.75 Å resolution. Interestingly, inserted tripeptide of CsTIM was exposed to the surface and formed a short rigid-helix in contrast to a loop of the corresponding portion in chicken TIM. It might be plausible to develop a vaccine against C. sinenesis based on the insert of tripeptide that does not exist in TIM of host such as human.

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Selective detection and quantification of hOGG1 by real-time PCR

김은택 홍인석*

공주대학교 화학과

It is important to detect the DNA repair enzymes to understand the role of their activity in our body. Human 8-oxoguanine DNA N-Glycosylase 1 (hOGG1) is an 8-oxoguanine DNA glycosylase which acts both as a N-glycosylase and an AP-lyase. The N-glycosylase activity releases damaged purines from double stranded DNA, generating an apurinic (AP) site. The AP-lyase activity cleaves 3´ to the AP site leaving a 5´ phosphate and a 3´-phospho-α, β-unsaturated aldehyde. Using the activity of hOGG1, we designed the specific single strand DNA (8-oxodG ssDNA), which has a 8-oxoguanine nucleotide (located at the center of sequence) and primer annealing sequences (located at the each terminal sites of sequence). After addition of short complementary ssDNA to the 8-oxodG ssDNA solution, the aliquot of hOGG1 was added to the dsDNA. In the presence of hOGG1, the target DNA was cleaved to the short oligomer, which can not be efficiently amplified by real-time PCR. We monitored the Ct values of amplified DNA in the range of concentration of hOGG1. The Ct values were well correlation to the added amount of hOGG1. This correlation curves can be used to detect hOGG1 in unknown specimen.

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Unbiased Proteomic Profiling Strategy for Discovery of Bacterial Effector Proteins Reveals that Salmonella Protein PheA Is a Host Cell Cycle Regulator

나하나 이준석[1,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 분자인지연구센터

Salmonella can survive inside macrophages through injecting effector proteins into the host cell cytosol and cause various diseases. It is not easy to identify effector protein because of low throughput issue of GFP tagging-based genetic manipulation. Herein, we demonstrate that off-the-shelf fluorescent probes, especially, Flu-NHS that contain N-hydroxysuccinimide functional groups with a negatively charge state can tag salmonella proteins including effector protein in RAW264.7 macrophage cells infected with salmonella in the unbiased way. We use competitive chemical proteomic profiling method and bioinformatics analysis such as cross-species BLAST analysis, sequence analysis and draw one top among 29 potential candidates. That is chorismate mutase-P/prehenate dehydrates, PheA. PheA is a Salmonella enzyme known for phenyl alanine biosynthesis and metabolic processing of chorismate. This protein exhibited significant sequence similarity to an area near the DNA binding domain of E2F transcription factor 7, E2F7. The functional similarity such as cell cycle alteration promoting G1/S cell cycle arrest is discovered using FACS and electrophoretic mobility shift assay. Based on our results, we have demonstrated the power of an unbiased tagging approach for the discovery of host cell regulators from pathogens.

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Global landscape of miRNA target sites reveals regulation of the Wnt pathway by miRNA in human embryonic stem cells

권영수

세종대학교 바이오융합공학과

miRNAs in association with AGO2 protein bind partially complementary target sites on mRNAs to regulate target mRNA expression. A vast number of mRNAs harbor potential miRNA target sites, yet most of mRNAs are still devoid of experimental evidence for direct binding of AGO proteins. To address this issue, we generated a knock-in human embryonic stem cell (hESC) line that expresses flag-tagged AGO2 protein from its native genomic locus and carried out crosslinking-immunoprecipitation coupled with next-generation sequencing (CLIP-seq) for AGO2 with an unprecedented sensitivity and specificity. Consistent with the generally accepted model, complementarity between mRNA and 5' nucleotides 2 to 7 or 8 of miRNA were an important determinant for AGO2 binding. In this study, I identified known and novel targets of miRNAs. Unexpectedly, a large number of genes in canonical and non-canonical Wnt pathways were targets of miRNAs in hESCs. The data presented here may provide a framework for computational and biological studies on miRNA functions.

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Displacement phenomena in Serial Affinity Chromatography Set (SACS)

조원련

원광대학교 바이오나노화학부

Displacement phenomena in Serial Affinity Chromatography Set (SACS)

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Fluorescence characteristics of biological materials in ultraviolet light

정영수

국방과학연구소 5본부 3부

Recently, public environmental interests are quickly growing as increase of hazardous substance due to formation of various hazardous substances in the surroundings by industrial development. Some airborne biological particles are important in infection of diseases of humans, animals, and plants. An ambient aerosol consists of fine dusts and microorganisms and if people are affected by those particles for a long period it can cause severe diseases. In fact, certain bacteria, rickettsia, viruses, toxins, and microbial neurotoxins have been feared as potential airborne biological warfare agents. All of these biological cells contain fluorescent molecules. The fundamental fluorescent materials in most bacterial cells are the same; fluorescent amino acids such as tryptophan, tyrosine, and phenylalanine (excitation/emission maxima ~280/350 nm), which are constituents of proteins; reduced nicotinamide-adenine dinucleotides (NADH, NADPH) (excitation/emission maxima ~340/450 nm); and flavin compounds (e.g., flavin adenine dinucleotide, flavoproteins, riboflavin) (excitation/emission maxima ~450/520 nm). Even bacterial spores contain significant amounts of flavins and nicotinamide compounds. In this research, we measured fluorescence of various biological compounds and investigated the fluorescence characteristics of them. This endeavor is part of an effort to determine useful fluorescence excitation and emission wavelengths for discrimination between biological and nonbiological particles and among different types of biological particles such as cells, spores, and toxins. These results can assist in selecting excitation and emission wavelength to allow partial discrimination among aerosol particle types.

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DNA Nanoparticles for a Tumor-Specific Anticancer Drug Carrier; Application of Rolling Circle Amplification

안형준

한국과학기술연구원(KIST) 테라그노시스스

A rolling circle amplification (RCA) technique has been widely used for biomedical applications, but it is yet challenging to rationally design RCA products for a simple target-selective delivery of drugs to cancer cells. Here, we devise a doxorubicin nanocarrier composed of RCA products, cholesterol-DNA, and folate-DNA conjugates. RCA products, designed to contain multiple tandem repeats of short hairpin DNA, employ the repeated sequences complementary to both DNA conjugates, and thus RCA products/cholesterol-DNA/folate-DNA complexes, generated via sequential base pairing processes, acquire the amphiphilic properties that facilitate self-assembly into the highly condensed nanoparticles (RCA nanoparticles) in an aqueous environment. RCA nanoparticles cannot only accommodate doxorubicins with high cargo capacity, but also release them to the environment by the aid of acidity. Particularly, the highly condensed structures enable RCA nanoparticles to be resistant to nuclease attacks in the blood. Furthermore, doxorubicin-loaded RCA nanoparticles have specificity for folate receptors and thus show the selective cytotoxicity on the cancer cells, while minimizing their side effects on the normal cells. These results show that our strategy provides an alternative tool to exploit RCA technique on drug delivery systems and also RCA nanoparticles have great potential as a doxorubicin carrier for the targeted cancer therapy.

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Enhanced cancer therapy by delivering self-assembled RNAi nanoparticles against multiple targets and chemotherapeutic agent to overcome chemoresistance

장미희 안형준[1,*]

한국과학기술연구원(KIST) 테라그노시스연구단 [1]한국과학기술연구원(KIST) 테라그노시스

Chemoresistance is a major obstacle in an effective treatment of chemotherapy. We have developed an enhanced cancer therapy to overcome multi-drug resistance (MDR) by using combinatory strategy that delivers multiple siRNA which can co-silence the expression of efflux transporter and anti-apoptotic protein, as well as treats anticancer drug. Here, we report that folate -decorated RNAi nanoparticles (Dsi RNPs) via self-assembly system, synthesized by rolling circle transcriptions (RCT) and sequence-specific hybridization with folate-DNA-Cholesterol (FA-DNA-CHOL) without aids of polycationic reagents, resulting in efficiently delivering multiple siRNA, which directed against P-glycoprotein (P-gp) and B-cell lymphoma 2 (BCL-2) mRNA, into MDR cancer cells (KB-V1 cells). Dsi RNPs exhibited effective multi- gene silencing efficiency within single nanoparticles with 93% of high siRNA loading capacity, given by multi-tandem of RNA hairpins generated by RCT into condensed RNA nanoparticles. Furthermore, Dsi RNPs allow to enable size-controllable construction and active-targeting uptake to drug-resistance cancer cells. In addition, our combination therapy demonstrated to increase the intracellular DOX concentration and induce remarkably enhanced cellular apoptosis particularly when administrated with Dsi RNPs and doxorubicine (DOX) sequentially in specific order of exposure than administrated simultaneously. Our Dsi RNPs platform showed to restore drug sensitivity in KB-V1 cells by overcoming pump and nonpump resistance. Taken together, our current study demonstrates the potential of combination therapy as an emergence of siRNA delivery and chemotherapy, resulting in synergistic cell killing effect and restorement of drug sensitivity to KB-V1 and enhanced efficacy of chemotherapy. Therefore, our study suggest a promising strategy to improve therapeutic potentials in MDR cancer therapy.

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Systemic Delivery of siRNA to Tumors Using Rolling Circle Transcription; Dual Function of Carrier and Cargo

안형준* 장미희[1]

한국과학기술연구원(KIST) 테라그노시스 [1]한국과학기술연구원(KIST) 테라그노시스연구단

For the rapeutic applications of siRNA, there are technical challenges with respect to targeted and systemic delivery. We here report a new siRNA carrier, RNAtrNPs, in a way that multiple tandem copies of RNA hairpins as a result of rolling circle transcription (RCT) can be readily adapted in tumor-targeted and systemic siRNA delivery. RNAtr NPs provide a means of condensing large amounts of multimeric RNA transcripts into the compact nanoparticles, especially without th aid of polycationic agents such as polyethylenimine, and thus reduce the risk of immunogenicity and cytotoxicity by avoiding the use of synthetic polycationic reagents. The highly condensed RNAtr NPs showed resistance to nucleases and polyanions, facilitated high cargo capacity, and finally resulted in robust gene silencing in vivo. This strategy allows the design of a platform-technology for systemic delivery of siRNA to tumor sites and also provides an alternavtive optical imaging probe for tumor visualization. Therefore, RNAtr NPs suggest great potentials as the siRNA therapeutics and imaging probes for cancer treatment.

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Time-dependent Metabolomics' Analysis of Traditional Nuruk Starters with Different Raw Materials and Water Content During Fermentation

김범태* <u>김준영</u>[1] 이상화[1]

전북대학교 생리활성물질연구소, 생리활성소재과학과 [1]전북대학교 생리활성소재과학과

As our ongoing work for the investigation of the metabolomics of traditional Nuruk starter fermentation in the time-dependent manner, the preliminary work was performed on Nuruk starter (named as TN-1 and 2) prepared from whole wheat as an raw material, and the primary metabolites including sugars and sugar alcohols, amino acids, several organic acids and fatty acids, were analyzed in terms of the variation of kind and the amounts of metabolites. In the present poster, as a further work, the effects of the raw materials and the water contents of traditional Nuruk starter at initial preparation step on the metabolomics were investigated and compared with the primary data obtained from the fermentation of whole wheat Nuruk starter. The raw materials used in preparation of Nuruk disks were barley, green gram, and whole wheat, and two types of composition were prepared, i.e. the one is composed of barley and green gram (3.3:0.52, by weight, named as TN-D), the one is composed of barley, green gram, and whole wheat (3.3:0.52:3.3 by weight, named as TN-C). The water contents on preparation were maintained as 20, 26, and 30%. The Nuruk disks were incubated at 36 oC under 70% of humidity for 30 days. The time-dependent Nuruk samples were collected at 0, 3rd, 6th, 10th, 20th, 30th day after start of fermentation. All samples were chemically modified via oximation and subsequent in-situ silylation, and analyzed with GC-MS. The general features is that the metabolites observed in each Nuruk starters were same in their kinds, and this was shown to be same as results of our preliminary work with whole wheat Nuruk starter. Comparing variation in amounts of organic acids, amino acids with the laps of time metabolites, in TN-C the hyperbolic curve pattern was observed with two maxima at 6 and 20 days. The higher the water content was, the large amount of metabolite was. In sugars, most of sugars including xylose and fructose were following same pattern, but sucrose and maltose showed no definite tendency like other sugars. In

sugar alcohols such as glycerol and arabitol were shown similar pattern to sugars, but the amounts xylitol and mannitol increased to maximum at 20 days and decreased after that. The amounts of fatty acids increased continuously in time-dependent manner and reached maximum at 20 days. In TN-D, however, that kind of pattern observed in TN-C was not observed clearly, and it was notable that the water content did not show any correlation with the variation of metabolites in amounts. The observation in TN-C was similar to TN-1 and 2.

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An alternative mode of gene regulation by microRNAs

권영수

세종대학교 바이오융합공학과

MicroRNAs(miRNA) in association with Argonaute (AGO) family proteins regulate gene expression by repressing translation or reducing mRNA stability. There are 4 different AGO proteins in humans and these proteins are largely equivalent in gene regulation function. Interestingly, endonuclease activity of Argonaute protein in animals are well conserved although the activity is apparently not required for miRNA-mediated gene regulation. In mammals, only AGO2 has endonuclease activity and it was demonstrated that nucleolytic activity is essential for perinatal viability in mice. Although it was shown that the activity is essential for biogenesis of miR-451, it is questionable that for biogenesis of a single miRNA species catalytic activity of AGO2 is conserved in vertebrates. Here, I present an alternative mode of gene regulation by miRNA that requires catalytic activity of AGO2. Based on AGO2-CLIP-seq data, we identified target sites were cleaved by AGO2 in a miRNA-dependent manner. miRNA-dependent endonucleolytic cleavage does not require extensive base pairing like siRNA-mediated cleavage. This finding provides a novel mechanism of miRNA-mediated gene regulation. Further studies are needed for biological and pathological relevance of gene regulation by target cleavage.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Organic solar cell fabricated from conjugated polymers consisting of BTI Unit as Acceptor unit

김동준 서홍석*

부산대학교 화학과

Organic solar cells are attracting much attention for years because there are many advantages such as easy-processing and low cost. Bithiophene imide (BTI) units have the low steric hinderance because imide group is located at center of BTI units, so this could enable a planar structure to have extended conjugation realized. We report the synthesis and properties of new N-alkyl-2,2′-bithiophene-3,3′-dicarboximide derivatives containing as the acceptor. The polymers have good solubility in common types of organic solvents. PBTIBDT-7, PBTIBDT-5 and PBTIBDT-3 were synthesized by palladium-catalyzed Stille polymerization. The polymers have good thermal stability and good solubility in common types of organic solvents. PBTIBDT-7, PBTIBDT-5 and PBTIBDT-3 containing bithiophene imide units show λmax at 649, 652 and 675 nm. HOMO energy levels at -5.6, -5.5 and -5.7 eV, LUMO energy levels at -3.9, -3.4 and -3.9 eV. The best performance of device with PBTIBDT-5:PC61BM layer showed VOC of 0.76 V, JSC of 3.28 mA/cm2, and FF of 0.51, giving the PCE of 1.26%.

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6-(2-Thienyl)-4H-thieno[3,2-b]indole (TTI) based D-A type copolymers with low band gap and application for organic solar cells

김동준 서홍석*

부산대학교 화학과

Organic solar cells (OSCs) are promising devices to use the limitless solar energy effectively. 6-(2-Thienyl)-4H-thieno[3,2-b]indole (TTI) was transformed by replacing the benzene ring with thiophene unit. Replacing the benzene ring with thiophene unit is expected to enhance the intermolecular charge transfer and we designed novel D-A type copolymers. TTI is modified from carbazole and for that reason TTI unit has strong electron donating ability. Because of facilitation of π-electron delocalization and presence of high charge transport, TTI unit is expected to have planar structure. The PTTIDTBT-h, PTTIDTMBI and PTTIDPP were synthesized through Stille coupling reaction and estimated in OSC. PTTIDTBT-h, PTTIDTMBI and PTTIDPP containing TTI unit show λmax at 423,594, 446,682 and 430, 759 nm. The HOMO energy levels at -5.31, -5.20 and -5.09 eV, the LUMO energy levels at -3.66, -3.77 and -3.71 eV. The best performance of device with PTTIDTBT-h:PC71BM layer showed VOC of 0.81 V, JSC of 8.19 mA/cm2, and FF of 0.51, giving the PCE of 3.35%.

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Fluoro, Cyano-Substituted Conjugated Polymers with Deep HOMO Energy Level for Polymer Bulk Heterojunction Solar Cells

김동준 김주애[1] 서홍석*

부산대학교 화학과 [1]부산대학교 화학관 427호

Polymer solar cells (PSCs) have been studied caused by their advantages of compatibility with flexible. We designed conjugated polymers consisting of 2-pyriminecarbonitrile and 2-fluoropyrimidine with flexible side-chains and used for the PSCs. We synthesized the new conjugated polymers, PTTICN, PTTICNR and PTTIFR, which were synthesized by Stille polymerization. The optical band gaps from UV-vis absorption onset of PTTICN, PTTICNR and PTTIFR were about 2.0 eV. The HOMO energy levels of four polymers (PTTICN, PTTICNR and PTTIFR) were at -5.26 ~ -5.34 eV, their LUMO energy levels were at -3.47 ~ -3.50 eV, corresponding to the electrochemical band gap of around 1.8 eV. The device comprising PTTICN and PC71BM (1:4) with DIO showed a VOC of 0.65 V, a JSC of 7.27 mA/cm2, and a fill factor (FF) of 0.48, giving a power conversion efficiency of 2.29%. The device comprising PTTICNR and PC71BM (1:4) with DIO showed a VOC of 0.82 V, a JSC of 6.38 mA/cm2, and a fill factor (FF) of 0.54, giving a power conversion efficiency of 2.81%. The device comprising PTTIF and PC71BM (1:4) with DIO showed a VOC of 0.64 V, a JSC of 7.38 mA/cm2, and a fill factor (FF) of 0.55, giving a power conversion efficiency of 2.61%.

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Syntheses of 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI) based polymers for organic solar cells with low bandgap

김동준 서홍석*

부산대학교 화학과

Organic solar cells (OSCs) as candidates for alternate renewable energy sources are extensively attracted interest caused by cost-effective processing, easy fabrication, low cost and light weight. Polymer consist of electron-pushing unit as a donor and electron-pulling unit as an acceptor. We report on two conjugated polymers, PTTIBT and PTTIMBI. 6-(2-thienyl)-4H-thieno[3,2-b]indole (TTI), transformed from carbazole moiety, used for electron-pulling unit and BT/MBI used for electron-pulling units. The PTTIBT and PTTIMBI were synthesized by stille reaction and estimated in OPVs. The absorption of film state of PTTIBT and PTTIMBI show maximum peaks at about 500-800 nm. The HOMO?LUMO energy bandgaps of this material shows 1.69 eV and 1.57 eV for PTTIBT and PTTIMBI respectively. especially, PTTIMBI of the polymer achieved the high PCE values, 2.60%.

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Specific detector for Ozone using luminogenic probe in biological and atmospheric samples

김범석 신인재[1,*]

연세대학교 이과대학 화학과 [1]연세대학교 화학과

In recent years, a variety of non-invasive imaging methods have been developed and utilized to study biological processes. Bioluminescence and fluorescence imaging methods are considered to be more advantageous than other imaging methods for their higher sensitivity and ease of handling. In particular, bioluminescence imaging boasts of having almost no background noise in the normal cells as they do not express the enzyme. This point enables the luminescence based probes to have higher sensitivity than fluorescence analysis during imaging. As a part of our group's on-going interest in research of non-invasive imaging probes, we turned our attention to expand the scope and utility of bioluminescence based probes. Current study describes our effort towards the development of distinct bioluminescence-based probes for detection of ozone, which are thus far unpresedented. This probe design hinges on installation of functional moiety that gets selectively cleaved in the presence of ozone. Herein, we showed that a luminogenic ozone probe has selectivity for the ozone and gives an luminescence in vitro. Furthermore, we applied this compound to variety of experimental condition such as transfected cell line and atmospheric environment. The results indicate that this probe is not apposite for cell-based system due to its low cell permeability and slow activity, however, proved to be a useful material for detection of ozone in ambient air samples.

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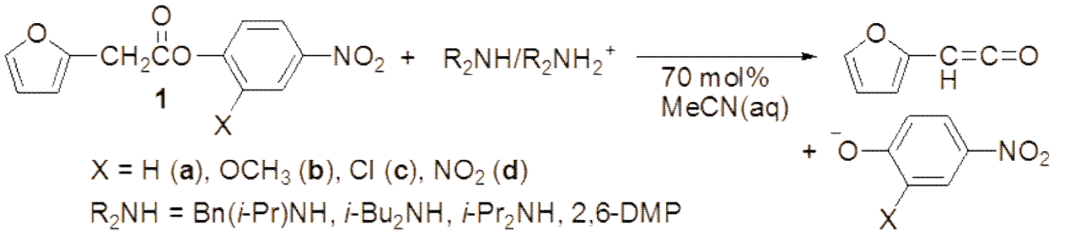
Elimination Reactions of Aryl Furylacetates Promoted by R_2NH-R_2NH^{2+} in 70 mol% MeCN(aq). Effects of β ?Aryl on the Ketene-Forming Transition-State

변상용 조봉래[1,*]

부경대학교 화학과 [1]고려대학교 화학과

Ketene-forming elimination from 2-X-4-nitrophenyl furylacetates (1a-d) promoted by $R_2NH_2^{2+}$ in 70 mol% MeCN(aq) has been studied kinetically. When X = Cl and NO_2, the reactions exhibited second-order kinetics as well as Br?nsted β = 0.37-0.54 and |βlg| = 0.31-0.45. The Br?nsted β decreased with a poorer leaving group and |βlg| increased with a weaker base. The results are consistent with an E2 mechanism. When the leaving group was changed to a poorer one [X= H (1a) and OCH_3 (1b)], the reaction mechanism changed to the competing E2 and E1cb mechanisms. A further change to the E1cb mechanism was realized for the reaction of 1a with i-Pr_2NH/i-Pr_2NH^{2+} in 70 mol% MeCN-30 mol% D_2O. By comparing the kinetic results in this study with the existing data for $ArCH_2C(O)OC_6H_3$-2-X-4-NO_2 ,the effect of the β-aryl group on the ketene-forming elimination was assessed.



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Transition metal and base-free synthesis of 3,3-diaryl-2-oxindoles *via* an intramolecular oxidative coupling between sp^{2}C-H and sp^{3}C-H bonds

임진우 문혜란 김재녕*

전남대학교 화학과

Various 3,3-diaryl-2-oxindoles have been synthesized in good yields from 2,2,*N*-triarylacetamides in the presence of montmorillonite K-10 in 1,2-dichlorobenzene under O_2 balloon atmosphere. The intramolecular oxidative coupling between sp^{2}C-H and sp^{3}C-H bonds might proceed *via* a radical mechanism of the benzylic hydroperoxide intermediate.

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Synthesis of benzo[*a*]carbazoles from 2-arylindoles *via* a sequential propargylation, propargyl-allenyl isomerization, and 6π-electrocyclization

임진우 문혜란 김재녕*

전남대학교 화학과

An efficient two-step synthetic approach of benzo[*a*]carbazoles from 2-arylindoles has been developed. The first step is a propargylation of 2-arylindoles at the 3-position catalyzed by montmorillonite K-10 in benzene. The second step is DBU-catalyzed sequential propargyl-allenyl isomerization and a concomitant 6π-electrocyclization process involving two aromatic π-bonds.

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Synthesis of pyrazolo[1,5-*a*]quinolines from 1-aryl-5-styrylpyrazoles *via* intramolecular Friedel-Crafts reaction/aerobic oxidation

문혜란 임진우 김재녕*

전남대학교 화학과

Various pyrazolo[1,5-*a*]quinolines were synthesized *via* the intramolecular Friedel-Crafts (IMFC) reaction of 1-aryl-5-styrylpyrazoles and the following base-catalyzed aerobic oxidation process. The required 1-aryl-5-styrylpyrazoles were readily prepared from the corresponding conjugated dienones and arylhydrazines in a one-pot process.

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An expedient synthesis of pyrrolo[3,2,1-*ij*]quinolone-1,2-diones *via* intramolecular Friedel-Crafts cyclization protocol

문혜란 김수연 김재녕*

전남대학교 화학과

The first successful intramolecular Friedel-Crafts (IMFC) cyclization of *N*-cinnamylisatin derivatives in polyphosphoric acid (PPA) provided pyrrolo[3,2,1-*ij*]quinoline-1,2-diones in good to moderate yields. The electron-deficient benzene ring of isatin could be used effectively in IMFC reaction in PPA, although some restrictions are still present.

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Synthesis of 1,3,4-trisubstituted benzenes from Morita-Baylis-Hillman adducts of α-bromocinnamaldehydes *via* [5+1] annulation strategy

김수연 임진우 김재녕*

전남대학교 화학과

An efficient synthetic method of 1,3,4-trisubstituted benzenes has been developed starting from Morita-Baylis-Hillman adducts of α-bromocinnamaldehydes *via* a formal [5+1] annulation strategy. The method involved a sequential nucleophilic substitution (SN_2') reaction, and intramolecular 1,6-conjugate addition, and E2 elimination process.

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Structure of N,N,N'-tribenzylthiourea : X-ray and NMR study

도희진 송재희[1] 허정석 김영준*

충남대학교 화학과 [1]순천대학교 화학과

N,N,N'-tribenzyl thiourea was obtained by aminolysis of 1,3,5-triazinyl dithiocarbamates. Two C-N bond lengths of N,N,N’-tribenzyl thiourea were different and compared with urea and thiourea by X-ray crystallography. Restricted C-N bond rotation in N,N,N’-tribenzyl thiourea was investigated by using variable-temperature ^{1}H NMR spectroscopy in Toluene-d_8. The Gibbs free energy of N,N,N’-tribenzyl thiourea was calculated approximately 10.3 kcal/mol from the coalescence temperature.

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Synthesis and reactivity of substituted 1,3,5-triazines

도희진 송재희[1] 김영준[*]

충남대학교 화학과 [1]순천대학교 화학과

Substituted 1,3,5-triazines were synthesized by the reaction of cyanuric chloride, potassium alkylcarbamodithioate, and amines in anhydrous THF in the presence of base. Dibenzylcarbamodithioate reacted very well with 2-dibenzylamino-4,6-dichloro-1,3,5-triazine whereas benzylcarbamodithioate did not in the same reaction condition. This results show that the nucleophilicity of dibenzylcarbamodithioate is greater than benzylcarbamodithioate. Other experimental results will be reported and the reactivity of substrates and nucleophiles will be discussed.

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Hole Transporting Materials Based on Triphenylamine Cores End-capped with Carbazole And Triarylamine Dervatives

김후희 김보미[1] 정성훈[2] 김미진[3] 채규윤[1,*]

원광대학교 바이오 나노 화학부 [1]원광대학교 화학과 [2]원광대학교 바이오나노화학과 [3]원광대학교 화학

Organic light emitting diodes (OLEDs) have recently received intense research interest due to their low power consumption, high contrast and brightness, easy fabrication, and ability to render a wide range of colors in flat panel displays and lighting fixtures. in this study, a series of novel HTMs based on triphenylamine cores end-capped with carbazole and triarylamine derivatives has been synthesized and investigated with very high Tg and Td values. The devices demonstrated good performance that was comparable to that of NPB overall

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Formal Synthesis of Isoindolobenzazepine alkaloids

김동화 김건철*

충남대학교 화학과

Isoindolobenzazepine alkaloids were isolated from the plants of the Chilean Berberis species.Their structure, five- and seven- membered rings with aromatic moiety has drawn the synthetic interest of many group. In this synthetic study has been designed to be carried out by Friedel-Crafts reaction and intramolecular Heck reaction for cyclization.

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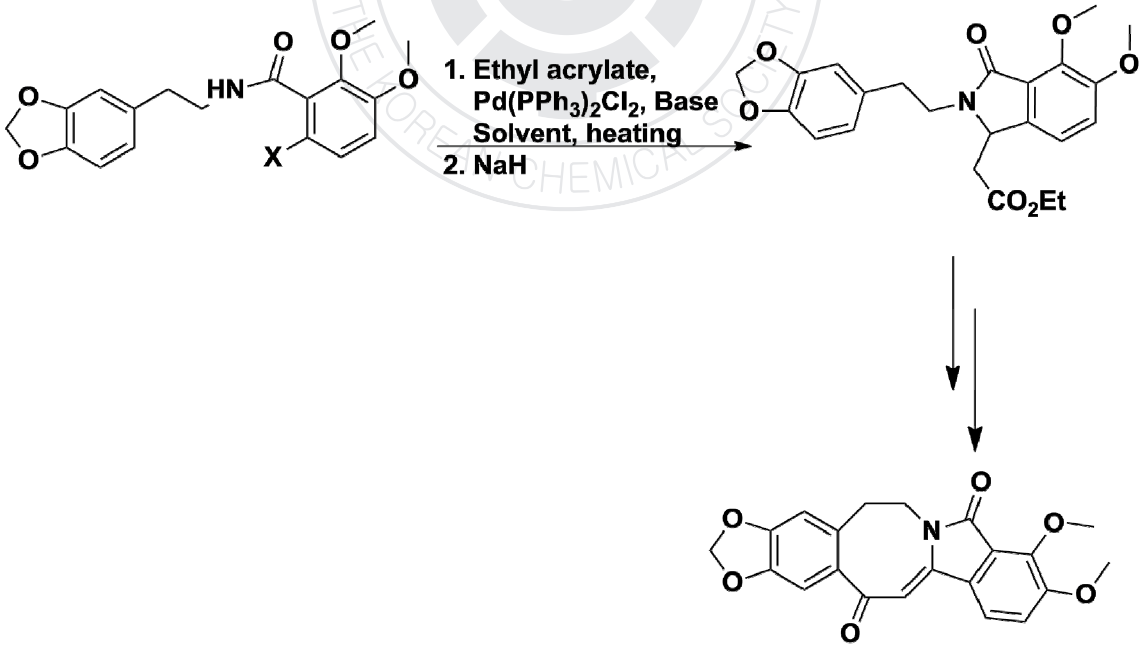
Formal synthesis of magallanesine through tandem Heck reaction and aza-Michael reaction

홍길표 김건철*

충남대학교 화학과

Magallanesine, the first known isoindolobenzazocine alkaloid, was isolated from Beberis Darwinii. In this study a isoindolobenzazocine derivative has been synthesized by inter-molecular Heck reaction and intra-molecular aza-Michael reaction. Using this method, we are going to synthesize magallanesine.



madallgallanesine

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Detection of Ga^{3+} and Al^{3+} ions based on pyrene sulfonamide functionalized inorganic/organic hybrid magnetic network

Ashwani Kumar Anup Pandith 김홍석*

경북대학교 응용화학과

Pyrene sulfonamide derivatives functionalized inorganic/organic hybrid magnetic network was prepared for detection of Ga^{3+} and Al^{3+} among alkali, alkaline, and different transition metal ions. Pyrene sulfonamide functionalized $Fe_3O_4@SiO_2$ nanoparticles easily detected Ga^{3+} and Al^{3+} ions with switch on monomer emission intensity in acetonitrile. The minimum detection limit for Ga^{3+} and Al^{3+} was found to be 1 ?M and 50 nM, respectively. Further sequential recognition of anions will be discussed.

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Imidazole appended 9,10-anthracenedicarboxamide probe for selective descrimination of picric acid in aqueous ethanol

Anup Pandith 김홍석*

경북대학교 응용화학과

A novel and simple imidazole appended 9,10-anthracenedicarboxamide probe was designed for sensing of nitrophenols. Designed probe detected nitrophenols through "*switch off*" response and selectively descriminated picric acid (PA) by ratiometrically among the nitrophenols in ethanol-water mixture (1:1). Probe efficiently detected the nitrophenols synergic interactions such as hydrogen bonding as well as π-π interactions sensing ability of probe was examined by UV-Vis, fluorescence and ^{1}H-NMR studies. Further experimental details were supported through DFT based computational studies.

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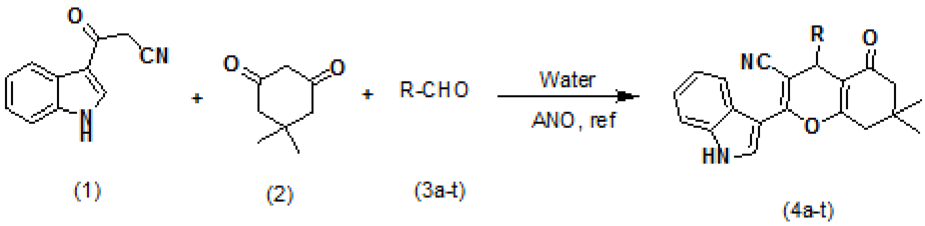
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ammonium niobium oxalate (ANO)-Catalyzed green synthesis of tetrahydro-2-(1H-indol-3-yl)-7,7-dimethyl-5-oxo-4-subtituted-4H-chromene-3-carbonitriles

Mudumala Veeranarayana Reddy 정연태*

부경대학교 이미지시스템공학과

We have reported a green and efficient method for the synthesis of a series of tetrahydro-2-(1H-indol-3-yl)-7,7-dimethyl-5-oxo-4-subtituted-4H-chromene-3-carbonitriles in excellent yields via one-pot multi-component reaction by using a catalytic amount of Ammonium niobium oxalate (ANO) in water. The environmental acceptability, economic viability, less reaction time, high product yields, and easy purification of products, cleaner reaction profile, higher atom efficiency and reusability of ANO qualify this method as the best one for the synthesis of these compounds.



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발표코드: **ORGN.P-245**
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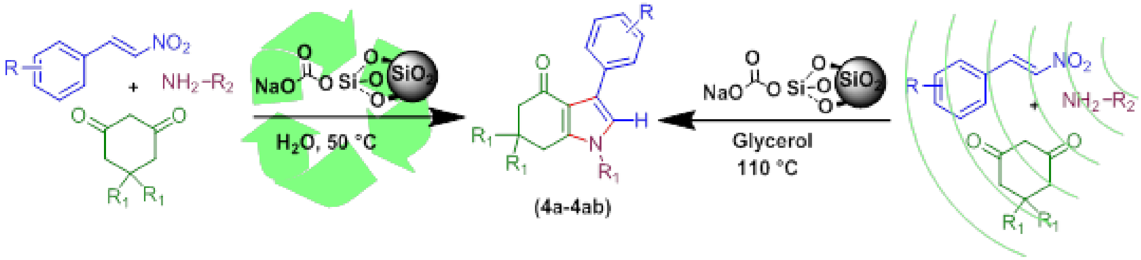
Ultrasound assisted synthesis of diversely functionalized dihydro-1H-indole-4(5H)-one catalyzed by Silica sodium carbonate (SSC)

ShindeVijayVilas 정연태[1,*]

부경대학교 융합디스플레이공학과 [1]부경대학교 이미지시스템공학과

A green and efficient procedure has been developed for the synthesis of dihydro 1H-indol-4(5H)-one using silica sodium carbonate (SSC) as a basic heterogeneous catalyst and water or glycerol as the solvent. Products were obtained in good to excellent yields under conventional heating (water, 50 °C) or under sonication (glycerol, 110 °C). In the reaction in water, the catalyst was easily reused for further reactions without loss of activity. Ambient reaction conditions, wide scope, simple purification and the reusability of the catalyst for five consecutive runs have improved the practical utility of this multicomponent reaction protocol manifold.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of high Tg hole transport layer materials based on triphenylamine derivatives for organic light-emitting diode

김수현 임효[1] 양두리[2] 주미라[1] 김보미 채규윤*

원광대학교 화학과 [1]원광대학교 바이오나노화학부 [2]원광대학교 바이오나노화학과

A series of novel star-shaped hole transporting materials (HTMs) based on triphenylamine core end-capped with carbazole and triarylamine derivatives have been readily synthesized by Suzuki coupling reactions. The synthetic compounds [4-(3,5-Bis-carbazol-9-yl-phenyl)-phenyl]-diphenylamine, {4-[(Naphtanlene-1-yl-(naphtalene-2-yl)amino)]-phenyl}-diphenylamine, Tris-[4-(3,5-Bis-carbazole-9-yl-phenyl)-phenyl]amine, 9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl-9H-carbazole. With the star shaped structures, compounds Tris-[4-(3,5-Bis-carbazol-9-yl-phenyl)-phenyl]amine and 9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazol exhibit very high glass transition temperatures () of 216℃ and 181℃, respectively and high thermal decomposition temperatures (>500℃). Among the designed HTMs, the device performance based on HTM {4-[(Naphthalen-1-yl-(naphyhalene-2-yl)amino]-phenyl}-diphenylamine is the best and comparable to that of the commom N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine(NPB) based device.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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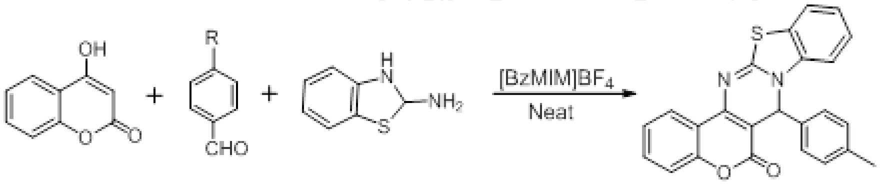
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An efficient green chemical synthesis of benzo[4,5]thiazolo[3,2-a]chromeno[4,3-d]pyrimidin-6(7H)-one catalyzed by reusable [BzMIM]BF4 ionic liquid

AVUTHU VIDYA SAGAR REDDY 이상동* 정연태*

부경대학교 융합디스플레이공학과

Structurally diverse benzo[4,5]thiazolo[3,2-a]chromeno[4,3-d]pyrimidin-6(7H)-one derivatives incorporating medicinally privileged heterosystems have been synthesized by an environmentally benign, efficient and convenient synthesis involving the [BzMIM]BF4 ionic liquid catalyzed multicomponent domino reaction of 4-hydroxy-2H-chromen-2-one with aromatic aldehydes and 2-aminobenzothiazole in solvent-free medium.



(1) (2a-u) (3) (4a-u)

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장소: 대구 EXCO
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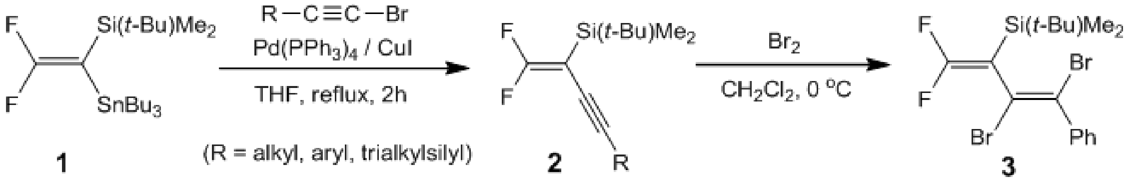
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of 2-(*t*-butyl)dimethylsilyl-1,1-difluoro-1-en-3-ynes and their bromination reaction

안혜진 진영현 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

Alkynylation of 1-(*t*-butyl)dimethylsilyl-2,2-difluoroethenylstannane 1 with alkynyl bromides in the presence of 10 mol% $Pd(PPh_3)_4$ and CuI in THF at reflux temperature for 2h afforded 2-(*t*-butyl)dimethyl-silyl-1,1-difluoro-1-en-3-ynes 2 in good yields. Bromination of 2 with Br_2 in CH_2Cl_2 at 0 ℃ resulted in the formation of dibrominated 1,3-butadiene 3 in good yields. Further reactivity of 3 with arylboronic acid or arylstannane in the presence of Pd catalyst will be presented.



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Encapsulation of Cobalt Oxide in Conjugated Network Polymer as a Catalyst for Hydrogen Evolution

김석진 정선민[1] 백종범*

울산과학기술대학교(UNIST) 에너지공학부 [1]울산과학기술대학교(UNIST) 에너지공학과

In the hydrogen evolution field, cobalt oxides have been recognized as a promising non-precious transition metal catalyst. In addition, two-dimensional (2-D) network polymer supported cobalt oxide catalysts with good crystallinity are highly anticipated to enhance catalytic performance. Here, we report the fabrication of a 2D nitrogenated network polymer-encapsulated cobalt oxide (Co@C_2N) catalyst via an in-situ solvothermal synthesis. Co@C_2N exhibits outstanding catalytic activities for hydrogen (H_2) generation from the hydrolysis of alkaline sodium borohydride ($NaBH_4$) solutions. The rate of maximum hydrogen generation is comparable to the best reported values for catalysts containing other noble metals in alkaline solutions. Furthermore, Co@C_2N can also catalyze the in-situ reduction of a nitro group into an amino group (4-nitrophenol to 4-aminophenol) in the presence of $NaBH_4$. The origin of high catalytic activity with enhanced stability could be due to the strong interaction between cobalt oxide nanoparticle and C_2N framework, which contains large portion of nitrogen.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of light emitting N-methyl phenothiazine substituted methyl and phenyl quinoline

형도성 권태우*

경성대학교 화학과

N-Methyl phenothiazine is a well known electron donor material having electron-rich sulfur and nitrogen hetero atoms. It has been used as electron donor component due to their low reversible oxidation potentials by virtue of the sulfur atom, which can facilitate the hole transport of the carrier. Methyl or phenyl substituted quinolines are long known to be a good electron acceptor materials. In this study, we reported the synthesis of new electron transfer material based on N-methyl phenothiazine and methyl or phenyl substituted quinoline via Grignard, Friedlander and Suzuki reactions. Products were determined by using ^{1}H, ^{13}C, FT-IR, GC/MS, Uv-vis and photoluminescence. Detailed synthetic routes and characterization of novel phenothiazine derivatives will be discussed.

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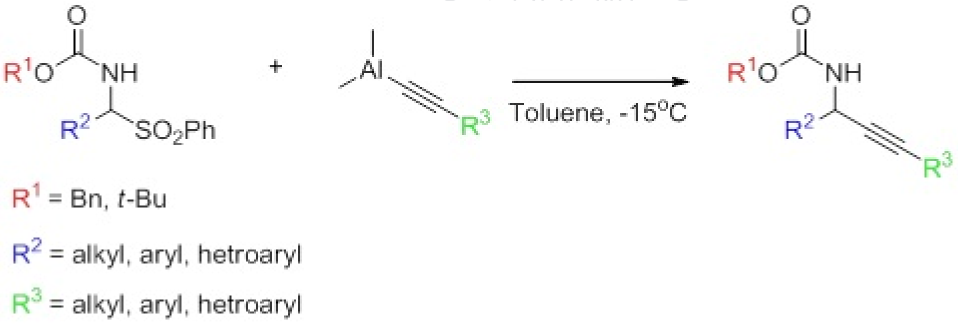
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Efficient synthesis of α-Amidoalkyl sulfone trimethyl aluminum reagent

이보미 이상협[1,*]

대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

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). As a latter example, Micouin et al. developed the alkynyldimethylaluminum reagent from the reaction of alkynes with trimethylaluminum using a catalytic amount of Et3N. We have utilized alkynylaluminum reagents for the synthesis of N-carbamoylpropagylamins.



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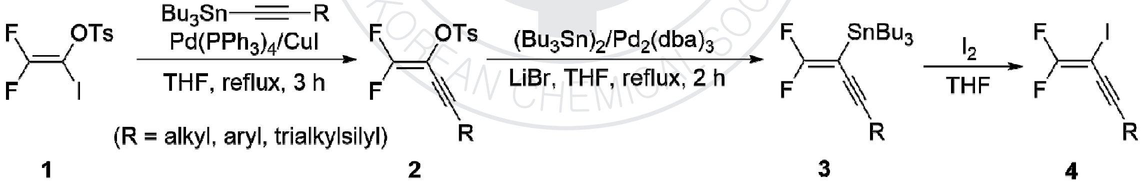
장소: 대구 EXCO
발표코드: **ORGN.P-252**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of 1,1-difluoro-2-iodo-1-en-3-ynes and their cross-coupling reactions

김수진 원성용 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

Coupling reaction of 2,2-difluoro-1-iodoethenyl tosylate 1 with alkynyl stannane reagents in the presence of 10 mol% $Pd(PPh_3)_4$ and CuI in THF at reflux temperature for 3 h provided 1,1-difluoro-1-en-3-ynyl tosylate 2 in good yields. Stannylation reaction of 2 followed by iodination afforded 1,1-difluoro-2-iodo-1-en-3-ynes 4 in moderate yields. Cross-coupling ractions of 3 with alkenylboronic acids or arylboronic acids under the Suzuki-Miyaura condition will be presented.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tandem Neopentyl glycol-based Maltosides for Membrane Protein Study

배형은 채필석[1,*]

한양대학교 바이오나노학과 [1]한양대학교 생명나노공학과

Membrane proteins, also known as cell gatekeeper, play crucial roles in many cellular functions. Accordingly, research on membrane proteins has brought tremendous attention in scientific community. Due to the amphipathic character, membrane proteins tend to denature and aggregate after extraction from the native membranes. Thus detergent molecules require working with these bio-macromolecules. However, many membrane proteins solubilized by conventional detergents often lose their activity rapidly, particularly in the case of fragile membrane proteins. In this study, we synthesized several tandem neopentyl glycol-based maltosides, designated TNMs, and characterized their physical properties in terms of critical micelle concentrations and micelle sizes. Some of these agents tend to form micelles while the others appeared to form liposomes. These agents will be evaluated for their efficacy with regards to protein solubilization and stabilization in a near future.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

A Practical Method for the Synthesis of Non-Symmetrical Ureas Utilizing Zirconium (IV) Chloride

김희권

전북대학교 의학전문대학원/핵의학교실

Urea structure is one of the common structures found in a variety of natural compounds and biologically active compound, and urea unit are widely used for many practical areas such as pharmaceutical drugs, agriculture, and materials science. Herein, we demonstrated a facile synthetic method for the preparation of unsymmetrical ureas from amines. The carbamoylimidazole compounds were prepared by the reaction of 1,1-carbonyldiimidazole with the primary or secondary amines, with further activation via treatment with zirconium (IV) chloride for generating desired urea structure. This reaction protocol was applied for the synthesis of trisubstituted and tetrasubstituted ureas with high yield.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of novel prostate specific membrane antigen inhibitors with 2-nitroimidazole moiety

권영도 김희권[1,*]

전북대학교 의과학과 [1]전북대학교 의학전문대학원/핵의학교실

Prostate cancer is one third of new cancer diagnoses in men and common cause of cancer death. Prostate-specific membrane antigen (PSMA) is significantly unregulated in prostate cancers and metastases, which is recognized as a molecular imaging target. Therefore, many group have studied about PSMA inhibitor to image and diagnosis prostate cancer. The effect of hypoxia on prostate cancer has been not studied extensively, even thought prostate cancer is associated with hypoxia. 2-nitroimidazole moiety have been used as hypoxia imaging derivatives and shown interesting results. In this study, novel prostate cancer imaging agents are prepared with a strategy containing hypoxic sensitive molecule structures and PSMA inhibitor structure to investigate the relationship between hypoxia and prostate cancer.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

A Class of Amphiphiles with High Lipophobic Density for Membrane Protein Manipulation

이호진 채필석[1,*]

한양대학교 바이오나노학과 [1]한양대학교 생명나노공학과

Amphipathic molecules, called detergents, are popularly used for membrane protein study. Membrane proteins solubilized in conventional detergents often have high propensity to denature and aggregate, rendering the further characterization of these biomolecules impossible. Accordingly, it is of great interest to develop a new class of amphiphiles with high protein stabilization efficacy. Previously, we developed maltose neopentyl glycol (MNG) amphiphiles with a central quaternary carbon between the head and tail groups. These agents showed remarkable properties in membrane protein solubilization, stabilization and crystallization compared to conventional detergents. As an attempt to further enhance detergent property, we designed new amphiphiles with two quaternary carbons closely located to each other within the central part of the molecules. The resulting architecture has four alkyl chains in close proximity, endowing their lipophilic groups with a high hydrophobic density. Such high hydrophobic density would increase detergent binding affinity to protein surface, thereby increasing both membrane protein solubility and stability. Therefore, these new agents could be a promising tool for membrane protein structural study.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Benzene-derived Facial amphiphiles for Membrane Protein Study

고주연 채필석[1,*]

한양대학교 바이오나노 [1]한양대학교 생명나노공학과

Membrane proteins play key roles in a variety of cellular processes. More than half of pharmaceutical drugs target membrane proteins. Despite such biological and pharmaceutical importance, a number of membrane proteins with known structure are far smaller than that of soluble proteins. This discrepancy illustrates the difficulty associated with membrane protein manipulation. Membrane protein solubilization and stabilization are challenging mainly due to the amphipathic character of these bio-macromolecules. As a membrane-mimicking system, detergent micelles are popularly used to study a target membrane protein. However, conventional detergents have serious limitations and thus we have developed a new class of facial amphiphiles, designated benzene-derived facial amphiphiles (BFAs). These novel agents were characterized in terms of critical micelle concentration (CMCs) and micelle size, measured by using a fluorescent dye and dynamic light scattering (DLS), respectively.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

LC-ESI-MS/MS analysis of polyphenolic compounds from leaves and stems of Rumex nervosus Vahl and their comparative antioxidant activities

DestaKebedeTaye 신성철*

경상대학교 화학과

Rumex nervosus Vahl is a perennial shrub in polygonaceae family which is widely distributed in Arabian Peninsula and east Africa, where its young leaves are edible. A wide range of pharmacological activities of the plant including antibacterial, anti-inflammatory, antioxidant, and antiviral activities were reported. In our recent study, 19 flavonoids from the flowers of R. nervosus were characterized for the first time using LC-ESI-MS/MS along with their anti-inflammatory activities. In this study, 14 flavonoids including one hydroxycinnamate were characterized from stems and leaves of R. nervosus along with their comparative antioxidant activities. External standard based quantification showed r2 in excess of 0.998. Both leaf and stem were rich in flavonols followed by flavones. Quercetin rutinosdie (7) was the highest component in both tissues contributing 55.5 % and 56.3 % in leaf and stem, respectively while component 2 contributing the least. The DPPH. and ABTS.+ scavenging activities and Fe2+ chelating activity increased dose dependently. EC50 of leaf and stem extracts to scavenge DPPH. was much lower than BHT indicating maximum activity. Both tissue extracts showed lower ABTS.+ scavenging activity than BHT. The Fe2+ chelating activity of EDTA was much higher than leaf and stem extracts. The results strengthen the fact that the plant could be used as a potential source of functional food.

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The fullerene recognition of 3D-organic zeolite supramolecular architectures

이재철 백경수* 박연실 구혜린

숭실대학교 화학과

The fullerene recognitions of 3D-organic supramolecular architecture 5 were investigated. The formations of self-assemblies of 3D-organic supramolecular architecture 5 by stepwise additions of dimeric copillar[5]arene 1_2, porphyrin connector 2, Zn 2, and bridge 3 in solution were monitored by ^{1}H NMR and 2D-NOESY experiments. 3D-organic supramolecular architecture 5 displays complexation selectivity for C_{70} over C_{60}, which was confirmed by ^{13}C-NMR, UV-Vis spectrometer, PL spectrometer, and HPLC analysis. Especially, the solvent polarity-driven reversible associations and dissociations of fullerene-3D organic supramolecular architectures would enable an easy and efficient separation of fullerenes.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

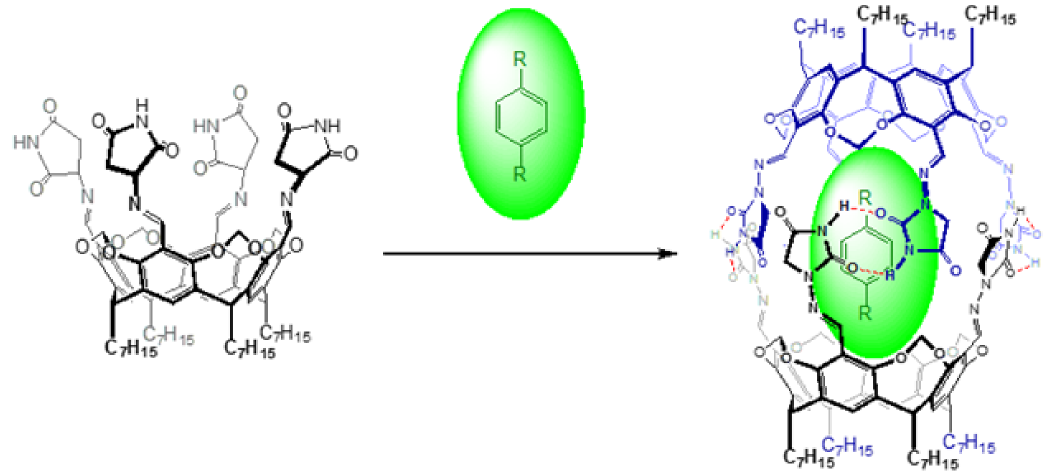
Guest selectivity of molecular capsule based on hydantoinyliminocavitand

김조원 박연실 유선호 백경수*

숭실대학교 화학과

Resorcin[4]arene-based tetrakis(N-hydantoinylimino)cavitand 1 forms a stable molecular capsule in the presence of suitable neutral guests such as 1,4-diiodobenzene, 1,4-dimethoxybenzene and 4-diethoxybenzene. Molecular capsule G@1_2 is stabilized by the eight intermolecular imidyl N-*H*C=O hydrogen bondings, two from each four paired hydantoinyl units on two cavitands. The formations of molecular capsules were confirmed by solvent titration, VT ^{1}H-NMR, 2D-NOESY, and 2D-DOSY NMR.

2



R=I, OCH$_3$, OCH$_2$CH$_3$

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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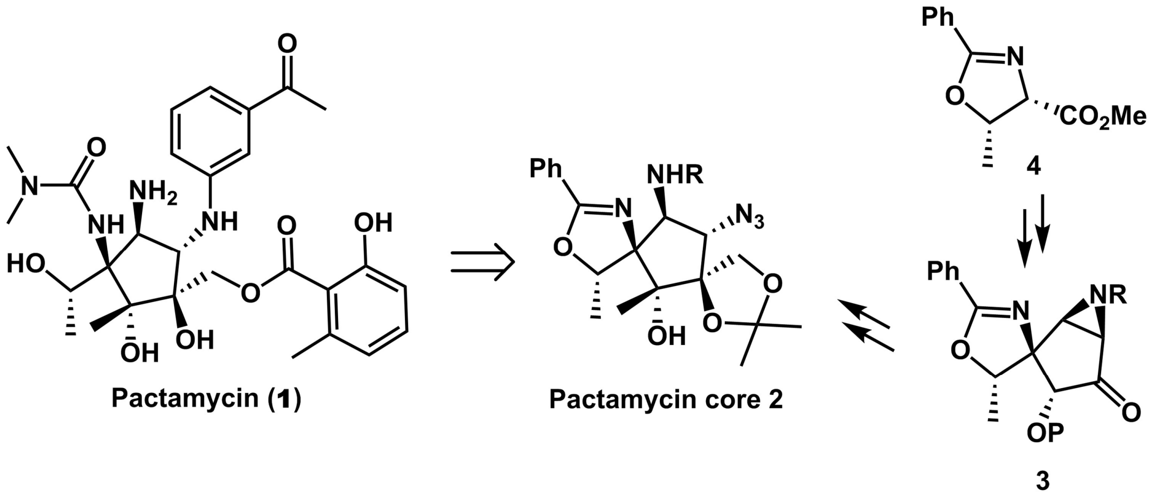
발표코드: **ORGN.P-261**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Studies toward the total synthesis of pactamycin, multi-functionalized aminocyclitol natural product

김태정 이윤서[1] Masaya Nakata[2,*] 함정엽[*]

한국과학기술연구원(KIST) 천연물연구소 [1]강릉원주대학교 해양자원육성학과 [2]Department of Applied Chemistry, Keio University, Japan

Pactamycin (1), an antitumor antibiotic produced by *Streptomyces pactum var pactum*, was isolated in 1962 and is one of the most potent cytotoxic agents *in vitro* against KB human epidermoid carcinoma cells and inhibits the synthesis of specific proteins. Pactamycin (1) has a unique multi-functionalized cyclopentane ring in which all carbons are substituted by heteroatoms. As a part of a project directed toward the total synthesis of pactamycin (1), we designed aziridine 3, potentially functionalized for further conversion into pactamycin core 2.The construction of the pactamycin carbon framework started with oxazoline 4, which was converted into azidirine 3 in 12 steps including ring-closing metathesis and stereoselective aziridine formation. Reproducible chemical methods enabling the synthesis of pactamycin core 2 containing an octa-substituted cyclopentane skeleton have been developed. Further studies toward the total synthesis of pactamycin from core 2 are now in progress and results will be disclosed.


Pactamycin (1)
Pactamycin core 2
Ph
NHR
N_3
OH
4
CO_2Me
3
NR
OP

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Synthesis and fluorescence properties of dimeric rhodamine derivatives containing pyromellitic dianhydride

최재영 장승현*

대구대학교 화학과

In this research, we synthesized new kinds of fluorescent sensors by rhodamine derivatives. Compound 1 was synthesized from rhodamine 6G derivative and pyromellitic dianhydride. Compound 2 was synthesized from rhodamine B derivative and pyromellitic dianhydride. These synthesized compounds were confirmed by measurement of ^{1}H-NMR and FAB-Mass. These compounds were found selectivity for metal cation by fluorescence titration using various metal cations.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

synthesis and fluorescence properties of rhodamine 6G derivatives containing formyl coumarin

박성호 장승현*

대구대학교 화학과

In this research, we synthesized fluorescent sensors from rhodamine 6G derivatives and formyl coumarin. The synthetic routes for rhodamine 6G derivatives containing formyl coumarin was outlined at scheme 1. Two derivatives were synthesized of imine reaction. The structures of new compounds were confirmed by ^{1}H-NMR and Mass. The compounds were found to selectivity by fluorescence titration using various metal cations.

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Synthesis of Benzimidazo[1,2-*a*]pyridines, Benzimidazo[2,1-*a*]isoquinolines and Benzimidazo[2,1-*a*]isoindolones from 2-(2-Bromovinyl)benzimidazoles and 2-(2-Bromoaryl)benzimidazoles

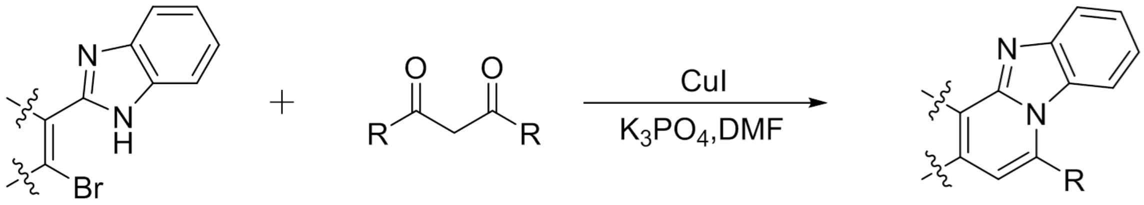
양병우 유재명 조찬식*

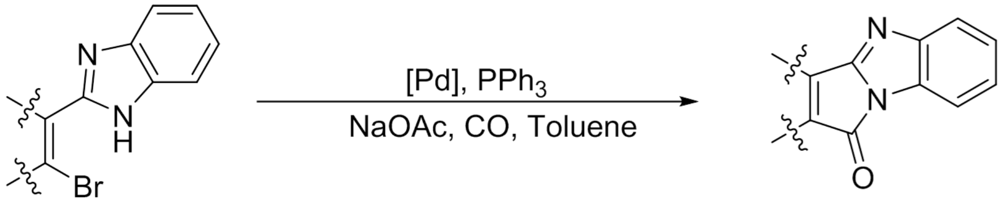
경북대학교 응용화학과

2-(2-Bromovinyl)benzimidazoles and 2-(2-bromoaryl)benzimidazoles are coupled and cyclized with 1,3-diketones in DMF at 130 ^{o}C in the presence of a catalytic amount of a copper(I) salt along with a base to give the corresponding benzimidazo[1,2-*a*]pyridines and benzimidazo[2,1-*a*]isoquinolines in good yields.[1]

2-(2-Bromovinyl)benzimidazoles and 2-(2-bromoaryl)benzimidazoles are carbonylatively cyclized under carbon monoxide pressure in toluene at 110 ^{o}C the presence of a catalytic amount of a palladium catalyst along with a base to give benzo[*d*]pyrrolo[1,2-*a*]imidazolones in good to high yields.[2]

1.(a) Ho, S. L.; Cho, C. S. *Synlett* **2013**, 24, 2705. (b) Ho, S. L.; Cho, C. S.; Sohn, H.-S. *Synthesis* **2015**, 47, 216. (c) Jiao, Y.; Ho, S. L.; Cho, C. S. *Synlett* **2015**, 26, 1081.
2.Bae, Y. K.; Cho, C. S. *Synlett* **2013**, 24, 1848.


CuI
K_3PO_4,DMF
N
NH
Br
O
O
R
R
N
N
R


[Pd], PPh_3
NaOAc, CO, Toluene
N
NH
Br
N
N
O

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Synthesis of Indolo[1,2-*c*]quinazolines and Isoindolo[2,1-*a*]indolones from 2-(2-Bromophenyl)-1*H*-indoles

유재명 양병우 조찬식*

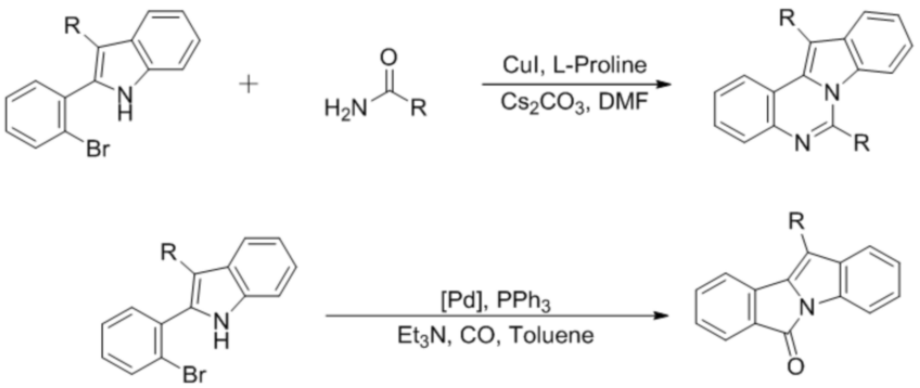
경북대학교 응용화학과

2-(2-Bromophenyl)-1*H*-indoles are coupled and cyclized with primary amides in DMF at 130 °C in the presence of a catalytic amount of a copper(I) salt along with a base to give the corresponding indolo[1,2-*c*]quinazolines in good yields.[1]

2-(2-Bromophenyl)-1*H*-indoles are carbonylatively cyclized under carbon monoxide pressure in toluene at 110 °C in the presence of a catalytic amount of a palladium catalyst along with a base to give isoindolo[2,1-*a*]indolones in good to high yields.[2]

1. (a) Ho, S. L.; Cho, C. S. *Synlett* **2013**, *24*, 2705. (b) Ho, S. L.; Cho, C. S.; Sohn, H.-S. *Synthesis* **2015**, *47*, 216. (c) Jiao, Y.; Ho, S. L.; Cho, C. S. *Synlett* **2015**, *26*, 1081.

2. Bae, Y. K.; Cho, C. S. *Synlett* **2013**, *24*, 1848.


R
NH
Br
+
O
H2N
R
CuI, L-Proline
Cs2CO3, DMF
R
N
N
R
R
NH
Br
[Pd], PPh3
Et3N, CO, Toluene
R
N
O

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Synthesis and Characterization of Novel Diketopyrrolopyrrole Copolymer for OTFTs

장용주 이상경* 박민주 송동진 강훈민 한진희 정용원 **SHAIK BAJI**

경상대학교 화학과

Diketopyrrolopyrrole (DPP) based copolymers are promising candidates for high ambipolar charge carrier mobilities, they have low optical energy band gap and high absorption coefficient and high molecular weight. Recently many DPP based compounds have been synthesized and they have shown good mobility. In order to exhibit high mobility planarity is one of the important requirement. Based on this the planar donor group containing central thiophene and lateral phenyl group derivatives synthesized. The DPP acceptor was copolymerized with the donor group. The novel conjugated copolymer based on DPP synthesized compound was confirmed by FT-IR, NMR spectroscopy and elemental analysis. The thermal properties of the compound were analyzed by thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC). Optical and electrochemical properties of the compound were analyzed by UV-vis absorption spectroscopy and cyclic voltammetry.

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Synthesis of Novel PDE5 Inhibitors Based on Tetrahydro-β-carboline

박민주 이상경* 송동진 장용주 **SHAIK BAJI** 강훈민 한진희 정용원 이다현

경상대학교 화학과

Phosphodiesterase type 5 inhibitors (PDE5 inhibitors) are the major kinds of pharmacological compounds. The first clinical use of these compounds was in the treatment of male erectile dysfunction. Sildenafil, vardenafil and tadalafil were known for commercial PDE5 inhibitors. In these three PDE5 Inhibitos, tadalafil was selected to improve the pharmacological effect. The synthesis of tadalafil derivative compounds was described in here. The structures of synthesized compounds as tadalafil derivatives were confirmed by ^{1}H-NMR, ^{13}C-NMR and EI-Mass spectrum. These novel tadalafil-like compounds can be expected to exhibit good pharmacological effect. So, the biological activity test will be researched in the future.

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New Conjugated Copolymer Containing Diketopyrrolopyrrole and Thiophene units for Organic Thin Film Transistors

송동진 강훈민 장용주 박민주 정용원 한진희 SHAIK BAJI 이상경*

경상대학교 화학과

Diketopyrrolopyrrole based material have been more researched for organic thin film transistors and solar cell. Diketopyrrolopyrrole are used as a strong electron acceptors in order to lower the LUMO energy level and more efficient electron injection and transport. By considering the above properties, diketopyrrolopyrrol flanked with pyridinyl group was synthesized as an acceptor and copolymerized with donor group. The compound was confirmed by FT-IR, ^{1}H-NMR spectroscopy, gel permeation chromatography and elemental analysis. The optical properties were determined by uv-vis absorption spectrum. The compound has shown absorption value at 680 nm wavelength in the solution. In the thin film state the absorption value is red-shifted due to intermolecular interactions. In the film state the compound has absortion value at 690 nm in UV-visible absorption spectrum. The electrochemical properties were determined by cyclic voltammetry. The HOMO-LUMO energy gap of the molecule was calculated to give 1.71 eV. The HOMO and LUMO values were -5.55 and -3.79 eV, respectively. The thermal properties were determined by thermo gravimetric analysis and differential scanning calorimetry. The compound has shown the decomposition temperature with 5% weight loss at 367 °C. The compound has shown glass transition temperature at 214 °C. The OTFT characterization for 3 in under process

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Leuco-Malachite Green derived Haptens

<u>정용원</u> 이상경* 박민주 송동진 장용주 강훈민 한진희 SHAIK BAJI

경상대학교 화학과

Malachite green (MG) is a triphenylmethane dye that exhibits antimicrobial and antiparasitic properties. When absorbed by during waterborne exposure, MG is easilyand rapidly metabolized into leucomalachite green (LMG). In addition to its use in dye industry, MG has been used in food industry despite the negative impact when accumulated in fish. Hapten synthesized from small units of aromatic rings were used to develop antibodies and immunoassays for the detection of MG and LMG. In this study, LMG derived series of hapten are synthesized. Spectroscopic techniques including ^{1}H-NMR, ^{13}C-NMR, and FT-IR were used to characterize each structure.

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Study for structure property`s change of α/β peptide oligomers containing cis-APiC

최성림 최수혁*

연세대학교 화학과

Generally, we can study various helical secondary structures for synthesis of many peptide oligomers containing various residues. This research focus on α/β-peptides oligomers containing 6-membered ring β-residues because , from the previous study, we researched that α/β-peptides oligomers containing cis-ACHC ((1R,2S)-2-Aminocyclohexanecarboxylic Acid) and L-Ala have two intramolecular hydrogen bonds: C=O(i) ??? H-N(i+3) and C=O(i) ??? H-N(i-1).But in this molecule structure, we thought that axial carbonyl group at C4 in ACHC has steric hinderance because of the axial hydrogen at C6 in ACHC. Therefore using cis-AiPC ((3R,4R)-4-Aminopiperidine-3-carboxilic acid), we remove steric hinderance and expect that α/β-peptides oligomer`s helix property is raised.for This research, we study with CD, IR, 2D NMR data and single crystal structure and compare with on α/β-peptides oligomers containing ACHC and Cis-AiPC protected Tosyl group in N6.

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Condensation of p-Cresol with Ketones

한인숙* <u>정은정</u>

강원대학교 과학교육학부

In order to explore the possible bis-arylation of ketones with phenoles, the condensations of p-cresol with various ketones were studied. For example, acetone reacts with p-cresol in the presence of p-TsOH at reflux for 24 h to yield 2,2-di(2-hydroxy-5-methylphenyl)propane. Similarly, 2-butanone gave 2,2-di(2-hydroxy-5-methylphenyl)butane. The yields are 30-40%. But acetophenone gave di(2-hydroxy-5-methylphenyl)methane. On the other hand, benzaldehyde gave the same compound in addition to di(2-hydroxy-5-methylphenyl)phenylmethane. The formation of the diarylmethane compound is quite unusual because the yield was about 50%. The arylalkane derivatives show significant effect on several tumor cells.

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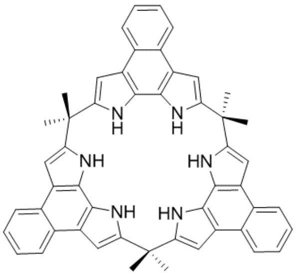
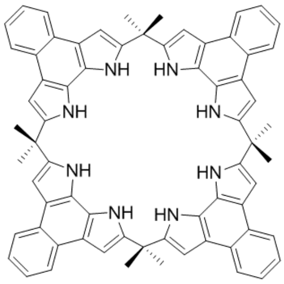
Calix[n]naphthobipyrrole (n = 3, 4) as Novel Macrocyclic Multi-oxoanion Receptors

이창희* **SILTEABEJEABEBAYEHU**

강원대학교 화학과

We have synthesized and characterized a new class of macrocyclic anion receptors utilizing naphthobipyrrole as a building block. Condensation of naphthobipyrrole with acetone in the presence of acid catalyst afforded new macrocyclic compounds; calix[3]naphthobipyrroles and calix[4]naphthobipyrroles. The synthesized compounds were characterized by spectroscopic means. The computer-generated model indicated that the compounds are nonplanar geometry and have potential for anion recognition especially for multi-oxo anions such as sulfate, phosphate, pertechnitate and nitrate. The anion recognition properties were carried out by 1H NMR and Uv-Vis spectroscopy and the results indicate that the synthesized hosts exhibit higher binding affinity towards tetrahedral shaped multi-oxoanions over halides or nitrate. The studies also indicate the 1/1 (host/guest) binding stoichiometry for both hosts. Red shifted absorption were observed upon binding with multi-oxoanions whereas other anion binding did not induce appreciable change in absorption. The detailed binding studies will be presented.


N
H
N
H
NH
HN
NH
HN


NH
HN
NH
HN
NH
HN
NH
HN

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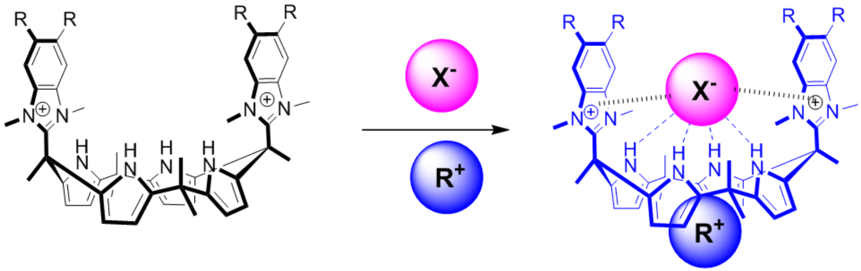
Guest Recognition Properties of Calix[4]pyrrole Carrying Benzimidazoloim Moieties at the Diametrical meso-Positions

이창희* **bezaendalemulugeta**

강원대학교 화학과

Calix[4]pyrroles bearing a dicationic benzimidazolium ions at diametrically crossing meso-positions have been synthesized and characterized by standard spectroscopic methods. The synthesized receptors display strong affinty with various anions. The anion binding studies carried out in organic solvent indicate that the anion reside in the binding pocket created by the two imidazolium moieties. The counter cation resides in the electron-rich, bowl-shaped cavity created by four pyrrole rings resulting a receptor-shared ion-pair formation. Cation selectivity is also observed. The synergistic effects of the coulombic interaction, anion-pi interactions as well as hydrogen bonding are attributed to the high binding affinity. The results clearly suppport . The cooperative interactions of anion-pi interaction, hydrogen bonding and coulombic interaction are attributed to the unusually high selectivity and affinity. The detailed binding studies including 1H NMR titration and UV-vis spectroscopic changes will be presented.



R =H, Cl

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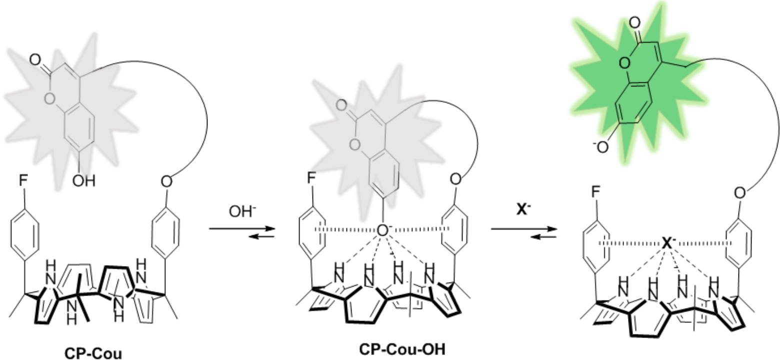
Probe-Calix[4]pyrrole Ensemble Bearing Covalently Linked Single-Armed Fluorophore as a Sensitive 'Turn On' FDDA Anion Sensor

이창희* <u>SAREEN DIVYA</u>[1]

강원대학교 화학과 [1]강원대학교

The anions play a ubiquitous role in various chemical and biological processes, thereby emphasizing the need for their facile recognition which could eventually be applied to a host of applications. The anion recognition chemistry of calix[4]pyrroles has attracted considerable attention. There are reports where meso-aryl picket calix[4]pyrroles have been utilized for recognition of these anions in conjunction with chromenolate anion, wherein the coumarin moiety aids in the sensing process by participating in the displacement assay. In line with this, we have synthesized a meso-aryl picket calix[4] pyrrole CP-Cou in which the coumarin unit is covalently linked to the macrocycle through a five carbon alkyl bridge. The receptor undergoes deprotonation upon treatment with a base (tetrabutylammoinum hydroxide, TBAOH) and forms an nofluorescent, intramolecular host-guest complex. However, exposure of this ensemble to suitable anionic substrates leads to the full recovery of fluorescence due to the displacement mechanism. The proposed system has a potential to be explored as an ideal molecular logic gate as well as highly sensitive FDDA senor application.


CP-Cou
OH-
CP-Cou-OH
X-
F
O
OH
NH

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Expanded porphyrin analogues bearing alkylidenyl double bonds at meso-positions (II)

이창희* 황선아

강원대학교 화학과

The novel meso-alkylidenyl porphyrinoids are non-aromatic and conformationally flexible macrocycles that display unusual prototropy and unique protonation. Most of the reported compounds display site-selective protonation and pyrrole inversion. The protonation selectivity ujsually depend on the number of N-H present in the core. As a part of our continuing efforts for the construction of the novel expanded version of the meso-alkylidenyl porphyrinoids macrocycles, we here report the synthesis, characterization, chemistry and conformational characteristics of the meso-alkylidenyl benzipentaphyrins bearing alkylidenyl double bonds at meso-positions. When the bispyrryl benzene derivative was condensed with pyrrole and aromatic aldehydes, three different stereoisomers are formed. All three isomers are identified charaterized by proton NMR spectroscopy. The pyrrole inverted conformation are also determined by spectroscopic means. The p-benzipentaphyrin adopts only one pyrrole inverted geometry while m-benzipentaphyrin adopts two pyrrole inverted geometry. The intramolecular hydrogen bonding between carbonyl and pyrrole N-H is attributed for these conformational diversity. The structural characteristics and protonation selectivity as well as chemical reactivity will be discussed.

일시: 2015년 10월 14~16일(수~금) 3일간
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel calix[4]pyrrole-based, Fluorescence Dye Displacement Assay (FDDA); Effect of meso-αααα-tetraaryl groups on the binding affinity

이창희* 김보람

강원대학교 화학과

Calix[4]pyrroles possessing four aryl group at meso-positions have been synthesized and the four possible isomeric compounds was identified. The α,α,α,α-aryl isomers containing various substituents at p-positions were isolated and characterized. The binding pocket created by four meso-aryl groups and four pyrrole N-Hs are expected to exhibit various affinity and selectivity depending on the nature of the anionic guests. The anion binding studies carried out in acetonitrile confirmed that the receptors form stable complex with various anions. The binding affinities toward coumarin anion was strong with 1/1 binding stoichiometry. These results indictae that the system could be ideal model system for Fluoresence Dye Displacement Assay (FDDA) for anions. The fluorescence of guest was completely quenched upon supramolecular host-coumarin complex formation. This systems could be excellent model systems for the turn-on type, FDDA sensor for anionic guests. The anion binding and sensing chemistry of the titled compounds will be presented.

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Highly selective detection of cyanide through the cyanide-catalyzed imine-to-oxazole transformation

박석안 김해조*

한국외국어대학교 자연과학대학 화학과

Cyanide anions (CN?) are extremely toxic to living organisms by inhibiting their respiratory system, and thus intake of a trace amount of the cyanide anions can result in death. Hence, we report a fluorogenic probe of latent fluorescence based on 2-hydroxyphenylsalicylimine for selective detection of cyanide. The probe has shown a highly selective and sensitive response to cyanide over other various anions with a micromolar limit of detection (LOD = 9.4 ?M) with exhibited a strong blue fluorescence through the cyanide-catalyzed imine-to-oxazole transformation.References1. K.W. Kulig, Cyanide Toxicity, U.S. Department of Health and Human Services,Atlanta, 19912. Agency for Toxic Substances and Disease Registry, Toxicological Profile for Cyanide, Atlanta Department of Health and Human Services, 2006.3. Y.H. Cho, C.-Y. Lee, D.-C. Ha, C.-H. Cheon, Cyanine as a powerful catalyst for facile preparation of 2-substituted benzoxazoles via aerobic oxidation, Adv.Synth. Catal. 354 (2012) 29924. E.V. Anslyn, D.A. Dougherty, Modern Physical Organic Chemistry, University Science Books, 2006.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Impact of temperature-dependent molecular packing of disubstituted polythiophene thin films on electrical and photovoltaic characteristics

고상원* **Zhenan Bao[1,*]**

한국철도기술연구원 교통환경연구팀 [1]Stanford University Department of Chemical Engineering

We demonstrated that electrical and photovoltaic characteristics of disubstituted polythiophene depend on molecular packing in thin films accompanied by a transition from a random orientation to an ordered lamellar phase via a nearly-hexagonal lattice upon annealing. While the maximum mobility was observed in an edge-on lamellar packed structure, the broad orientation distribution of polymer crystallites is more effective to disubstituted polythiophene/C60 bilayer photovoltaic characteristics than hexagonal or ordered lamellar phase. This observation corresponds to the enhanced dark current density (JD) and the decreased exciton diffusion length (LD) upon annealing. We believe that above findings provide insight into the tuning electrical and photovoltaic properties depending on polymer packing structures, which is crucial for the management of charge and energy transport in a range of organic optoelectronic devices.

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A fluorescence turn-on probe for a catalytic amount of cyanides through the cyanide-mediated cinnamate-to-coumarin transformation

나상윤 김해조[1,*]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

We report a latent fluorescence probe based on 2-hydroxycinnamate for selective detection of cyanide. The probe underwent a rapid cyanide-catalyzed cinamate-to-pyrone transformation reaction and displayed strong fluorescence selectively to the cyanide anion over other various anions in 5% water-acetonitrile solvent, which could be easily detected under the naked eye.Keywords: Cyanide-catalyzed cyclization; Fluorogenic probe; Cinnamate-to-coumarin transformation; Latent fluorescence

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Substituent effects on the C-N bond rotation energy in dibenzylamino-1,3,5-triazines

이주연 김영준*

충남대학교 화학과

Dibenzylamino-1,3,5-triazines were synthesized from cyanuric chloride and the electron donation groups (OMe, $N(C_4H_8)_2$) or the electron withdrawing groups (CN, Cl) were introduced to the triazines.Dibenzylamine has double bond character, because it has lone pair electron of the nitrogen atom.For this reason, ^{1}H-NMR spectra showed two benzyl signals at room temperature and two peaks coalesced at higher temperature. We obtained the free energies ($\Delta G‡$) of C-N bond rotation of dibenzylamino-1,3,5-triazines from the Dynamic NMR experiments. Electronic effects of the subsituents will be discussed using Hammett plot.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis and photophysical properties of fluorescein-labeled 2’-deoxyuridines for detection of pH-sensitive microenvironment

이정연 황길태*

경북대학교 화학과

Monitoring intracellular pH is important for better understanding of physiological and pathological processes in living cells. Many cellular events in the microenvironment and various methods for monitoring pH in a cell have been proposed. Among these, fluorescent probes are very attractive because they are simple, highly sensitive and non-destructive to cells. Fluorescein is the most common fluorescent reagent and has a pKa of 6.4, and its ionization equilibrium leads to pH-dependent absorption and emission over the range of 5 to 9. Herein, we synthesized fluorescein-based 2’-deoxyuridines by using Sonogashira coupling reaction. The fluoresent probe exhibit change in fluorescence intensity when they dissolve in various pH buffers (pH 3.0-9.3). This probe emitted increased fluorescence emission in basic solution with pKa of 6.3. Synthetic procedures and fluorescence properties will be described in detail.

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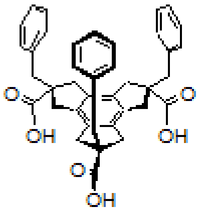
C_{3V}-symmetric trindane based tripodal anion receptors with Guanidine as recognition groups

김기동 김규진 최홍진*

경북대학교 응용화학과

Design and synthesis of artificial receptors for selective recognition of anions have been received considerable interest recently. Receptor molecules with preorganized binding motifs are useful for the effective and selective binding of guest species. Most anions interested in biological, environmental measurement are F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, HSO_4^-, NO_3^-, HCO_3^- ions which have C_3-symmetric element. The C_{3v}-symmetric anionic receptors have shown good binding affinity for such oxoanions and spherical halide anions due to their preorganized structure and complementarity. The C_{3v}-symmetric trindane-triol 1 was derivatized by extending the lower arm to obtain the anion receptors 2 and 3 by introducing suitable anion recognition motifs i.e. guanidine. The selectivity of 2 towards various anions was also determined by UV-Vis absorbance and fluorescence spectroscopy, which showed spectral responses selectivity in presence of F anion due to the deprotonation of guanidine proton. The receptors 3 with electron-donating groups showed similar fluoride selectivity in UV-Vis and fluorescence study. Finally, the 3D structures of the receptors and their complexes with anions were determined by performing the DFT calculations.References 1. Park, Y. S.; Bang, S.-H.; Choi, H.-J. *Tetrahedron Lett.* 2013, 54, 6708.2. Kim, W.; Sahoo, S.K.; Kim, G.-D.; Choi, H.-J. *Tetrahedron*, 2015, doi:10.1016/j.tet.2015.08.043.3. Park, J.-O.; Sahoo, S.K.; Choi, H.-J. *Spectrochim Acta A*, 2016, 153, 199.



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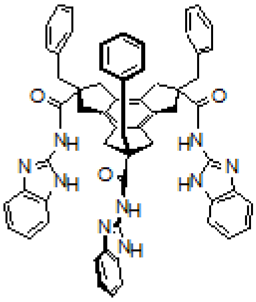

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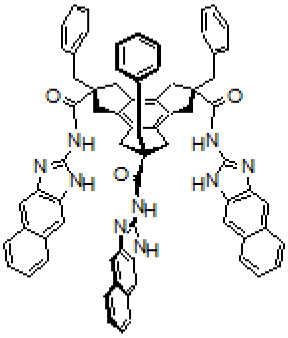

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일시: 2015년 10월 14~16일(수~금) 3일간
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발표코드: **ORGN.P-283**
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Photophysical Properties of the pH-Sensitive 2’-Deoxyuridine Labelled with BODIPY Unit

손예슬 황길태*

경북대학교 화학과

세포 내 pH 는 많은 세포 소기관의 기능을 조절하고 세포 증식, 세포자살, 엔도시토시스 등의 세포 대사 과정에서 중요한 역할을 한다. 따라서, 세포 내의 pH 변화를 모니터링 하는 것은 세포의 기능을 연구하고 생리학적, 병리학적 과정을 이해하는 데 매우 중요하다. 최근 많은 형광 probe 가 세포 내 pH 를 모니터링 하는 수단으로 개발되어 왔지만, pH 를 감응하는 형광 뉴클레오시드는 아직 많이 알려져 있지 않다. 형광 뉴클레오시드는 핵산을 둘러싸고 있는 미세 환경의 변화를 관찰할 수 있어 pH 변화를 감지하는 센서로 개발된다면 여러 가지 질병을 진단하는 데 유용한 도구가 될 수 있다. 우리는 meso- 위치가 dimethyl amine 기로 치환된 BODIPY 유도체를 합성하였고, sonogashira coupling 을 통해 2’-deoxyuridine 을 도입하여 BODIPY 유도체가 라벨된 2’-deoxyuridine 을 합성하였다. 합성한 BODIPY 유도체는 BODIPY core 가 excitation 되면 전자 donor 인 amino 기의 질소 원자에 의해 PET 가 일어나게 되어 형광이 quenching 되고, amino 기의 질소 원자가 protonation 되면 PET 가 일어나지 않아 형광이 회복되는 원리로 작동한다. 이러한 원리를 토대로 우리는 다양한 pH 조건에서 형광의 변화를 조사하였다. 우리는 이 형광 뉴클레오시드가 생체 내의 pH 를 모니터링하여 다양한 질병 진단에 유용한 도구가 될 수 있을 것이라 기대하고 있다.

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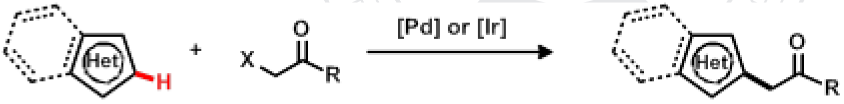
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of α-heteroaryl acetic acid derivatives by C─H bond functionalization

장하림 주정민*

부산대학교 화학과

We describe a general strategy for the synthesis of α-heterocyclic acetic acid derivatives. Depending on the electronic nature of heterocycles, one of three distinctive reactive species derived from α-haloacetates and α-haloacetamides can be adopted. A variety of five-membered heteroarenes can be employed, providing rapid access to C─H alkylated products.



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발표종류: 포스터, 발표일시: 목 11:00~12:30

A metal-catalyst-free addition of zinc enolates derived from esters and amides to tosylimines: A facile synthetic protocol for the synthesis of 3-amino esters and amides

임평원 주성류 김승회*

단국대학교 화학과

A facile synthetic route for the preparation of 3-amino esters and amides was developed by the addition reaction of zinc enolates derived from α-halo ester and amide to tosylimines. It was of great interest that the reactions took place efficiently in the absence of any transition-metal-catalyst under mild conditions and provided the resulting products in moderate to good isolated yields.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 2',3'-dideoxy-3'-fluoronucleoside containing the 2-pyridone as an unnatural base

정수진 황길태*

경북대학교 화학과

DNA 의 이중나선은 Watson-Crick 모형에 따라 아데닌과 티미딘 (dA:dT), 구아닌과 시토신(dG:dC)이 각각 수소결합을 통해 구조를 형성하며 구성성분인 핵산은 모든 생물을 구성하는 필수적인 유전물질로 알려져 있다. 지금까지 암을 조기진단하고 , 더 효과적인 치료를 위한 설계를 목적으로 PET(Positron Emission Tomograpy)가 가장 많이 사용되고 있으며, 뉴클레오시드를 변형한 방사성추적 물질들은 매우 다양하게 개발되어 왔다. 본 연구에서는 분자수준에서 유전자수준에 이르기까지 더 효율적인 분자 영상화를 위해 뉴클레오시드를 변형한 방사성추적 물질을 디자인하였다. 천연염기(natural base)와 같이 소수성 상호작용을 기본으로 하는 비천연염기(unnatural base)인 N-글리코시드계의 기초물질인 Pyridone 을 도입하여 3'-Fluoronucleoside 를 합성하였다. 11C(t1/2=20min) 보다 더 긴 반감기를 가진 18F(t1/2=110min)을 표지한 물질들은 더 좋은 해상도, 화학적 안전성을 보이며 , 종양이 발생한 부위에 대해 높은 선택성을 지니므로 생체 내의 의약품 농도 변화의 측정을 용이하게 하는 등 생리 화학적으로 뛰어난 장점들을 가지게 된다. 본 연구에서는 합성 마지막 단계에서 18F 을 도입하여 기존에 PET 에 사용되던 방사성추적 물질의 반감기 손실을 감소시킬 수 있도록 설계했다.또한 비천연염기(unnatural base)의 도입으로 인해 최근 각광 받고 있는 항암 작용, 항 바이러스 등에 작용하는 화학적 치료제로서의 역할이 가능할 것이며, 이는 새로운 연구효과를 창출함과 동시에 산업화에도 큰 도움이 될 것이라 사료된다.

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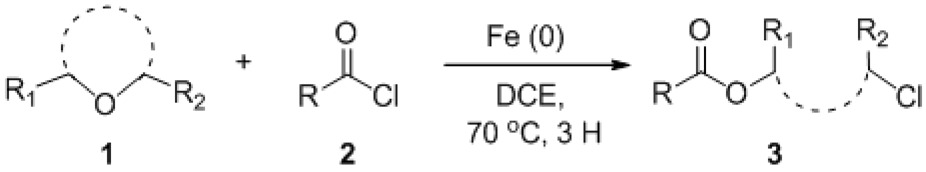
Mild and Efficient Iron(0)-Promoted Regioselective Acylative Cleavage of Ethers: Scope and Mechanism

chirumarrysridhar 강지수 신동수*

창원대학교 화학과

An efficient iron powder catalyzed acylative cleavage of cyclic and acyclic ethers with acyl/aroyl chlorides was studied to produce chloroesters and esters respectively to examine the scope and mechanism. Less electron donating alkyl group in un-symmetric acyclic ethers gave the only isolable ester counterpart. Regioselectivities were also observed with cyclic ethers to give rise primary ester and secondary chloride in the products, chloroesters. Steric hindrance of ethers as well as acid chlorides played a major role on elemental iron mediated C-O bond cleavage. The mechanism of ether cleavage with acyl/aroyl chlorides in presence of mild and green pre-catalyst Fe(0) found to involve in SRN1 via single electron transfer followed by SN1 dissociative pathways.



R = alkyl or aryl; R_1, R_2 = H, alkyl or aryl

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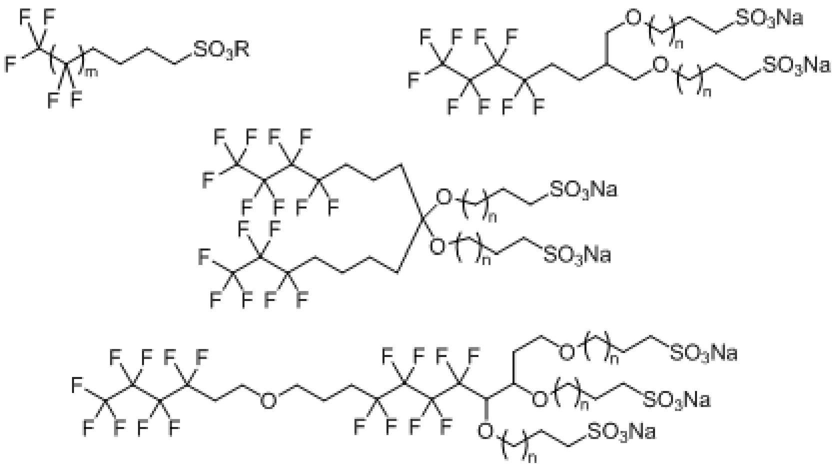
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design and Synthesis of hemifluorinated PFOS alternatives and property studies

VAIDYARAGHAVENDERRAO 고요한 이태균 **chirumarrysridhar** 신동수*

창원대학교 화학과

Perfluoroalkyl sulfonates (PFAS): acids, salts, halides, etc., including perfluorooctyl sulfonate (PFOS), widely used in various applications. Due to toxicity towards health and environment and its non-biodegradability, we focused on synthesis of the different PFOS alternatives by reducing fluorine content. Here, we described design and synthesis of hemifluorinated PFOS alternatives by using Zn/CuI mediated Micheal-type addition reaction in ionic liquids considering environmentally benign reaction conditions as well as products. On the other hand disulfonates and trisulfonates with perfluorobutyl subunit were also synthesized starting from readily available 1H,1H,2H,2H-nonafluorohexyl iodide, diethyl malonate, octafluoro-1,4-diiodobutane and sultones. All compounds were characterized by 1H NMR, 13C NMR, IR and mass and subjected to surface tension reduction measurements and the data were recorded using surface tensiometer. These hemifluorinated PFOS alternatives were found to be more or less biodegradable and showed good surface tension reduction properties.



m = 1, 3, 4; n = 1, 2
R = Li, Na, K, Et_4N^+, $Me_2(C_{10}H_{21})_2N^+$ etc.

일시: 2015년 10월 14~16일(수~금) 3일간
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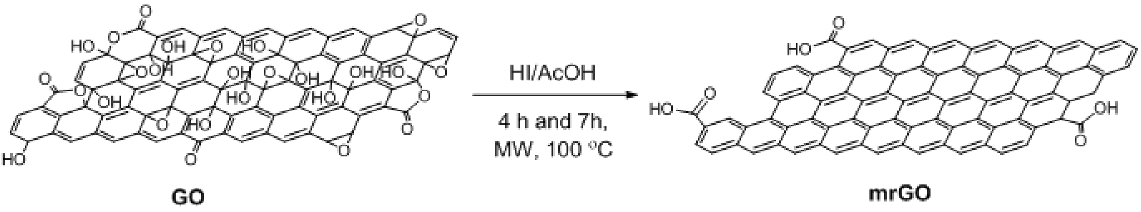
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Microwave-assisted synthesis, characterization of reduced graphene oxide and its antibacterial activity

<u>PATILKALPESHTUMADU</u> 고요한 김한솔 chirumarrysridhar 신동수*

창원대학교 화학과

In this study, a facile, fast and cost effective method for the synthesis of high quality reduced graphene oxide sheets is reported by a microwave-assisted chemical reduction using hydriodic acid/acetic acid as reducing agent. Exposure of GO with microwave irradiation (4 h and 7 h) was found to be more rapid and sustainable reduction as compared to that of the conventional chemical reduction process (48 h). Formation of high quality microwave-assisted reduced graphene oxide (mrGO) was ensured by means of electron microscopies, Raman and infrared spectroscope studies. Furthermore, the antibacterial activity was evaluated for the mrGO, which showed good inhibitory effect against both Gram positive and Gram negative bacteria.



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발표종류: 포스터, 발표일시: 목 11:00~12:30

Pyrrolo[3,4-c]pyrrole-1,3-dione Based Polymers Containing Benzodithiophene for OFETs and PSCs

성지영 조은솔 현명호*

부산대학교 화학과

The polymer solar cells (PSCs) made from the π- conjugated polymer and fullerene derivative have been considered as a most promising solar to electrical energy conversion techniques due to their easy device fabrication to large area at low cost. In this study, pyrrolo[3,4-c]pyrrole-1,3-dione (DPPD)-based new electron acceptor units bearing bi-thiophene and thienothiophene in between the DPPD units were prepared and copolymerized with electron rich benzodithiophene derivatives to offer two new polymers P(BDTT-BTTDPPD) and P(BDTT-BFTTDPPD), respectively. The calculated weight average molecular weight / polydispersity of the polymers P(BDTT-BTTDPPD) and P(BDTT-BFTTDPPD) were 8.46 x 104 gmol-1 / 3.24 and 1.69 x 105 gmol-1 / 3.67, respectively. The estimated optical band gaps P(BDTT-BTTDPPD) and P(BDTT-BFTTDPPD) were 2.10 eV and 2.08 eV, respectively. The determined highest occupied/lowest unoccupied molecular orbital (HOMO/LUMO) energy levels of P(BDTT-BTTDPPD) and P(BDTT-BFTTDPPD) were ?5.44 eV/?3.34 eV and ?5.42 eV/?3.34 eV, respectively. Polymer P(BDTT-BFTTDPPD) displayed red shifted absorption maximum and slightly higher HOMO level than P(BDTT-BTTDPPD). The photovoltaic and charge transport studies of polymers are under progress.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of (5,5'-dinitro-2H,2'H-[3,3'-bi(1,2,4-triazole)]-2,2'-diyl)dimethyanol and its energetic salts

배세원* 이세진[1] 임영권[2]

국방과학연구소 4본부 2부 [1]국방과학연구소 제4기술연구본부 2부 [2]국방과학연구소 4-2

Nitrogen-rich materials play an important role in the design of new energetic compouns and their use as explosives.[1] Among them, one of the promising heterocyclic backbone for the preparation of high performance energetics is considered to be the triazole ring.[2] Bistriazole ring has allowed the preparation of a wide spectrum of energetic compounds from secondary explosives to highly sensitive primary explosives depending on functional groups and ion pairing. In this presentation, we report synthetic methods of dinitrobistriazole and its energetic salts and discuss their physical properties for the potential uses as explosives.References1) L.V. De Yong, J. Hazard. Mater., 1989, 21, 125.2) T.M. Klapotke, Chem. Eur. J., 2011, 17, 13068.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

A Series of Alternating Copolymer Based on Fluorine Substituted Quinoxaline

공민성 진영읍*

부경대학교 공업화학과

The novel series of alternating copolymers (PBDT-DFQx and PBDT-FQx) were synthesized by using Stille coupling reaction. In this polymers, either di-fluorinated quinoxaline (DFQx) or mono- fluorinated quinoxaline (FQx) was used as an electron-deficient unit and alkoxyl substituted benzo[1,2-b:4,5-b']dithiophene (BDT) was used as an electron-rich unit. To check into the impact of fluorine atom, either di- or mono-fluorinated quinoxaline (Qx) unit was introduced to the resulting copolymers. Consequently, the polymer containing mono-fluorinated quinoxaline showed narrow optical band gap compared with di-fluorinated quinoxaline. The properties of synthesized copolymers were checked by TGA, GPC, UV-vis absorption spectroscopy and cyclic voltammetry measurements. Two copolymers had a good thermal stability showing 5% weight loss temperature values (Td) over 300°C. Two polymers displayed maximum peaks at 596 - 602 nm in solution state and maximum peaks were red-shifted 601 ? 606 nm in the film state. Highest occupied molecular orbital (HOMO) energy level of two polymers displayed -5.66 eV and -5.52 eV respectively.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Two Novel Bulk Heterojunction Type Polymer Solar Cells Based on Benzodithiophene and Mono- or Di- Fluorinated Qunioxalines

금상하 진영읍*

부경대학교 공업화학과

Two novel bulk-heterojunction (BHJ) type polymer solar cells (PSCs) based on fluorinated Quninoxaline (Qx) and benzodithiophene (BDT) were designed and synthesized. BDT have widely used as electron rich unit because of its strong electron donating ability and planarity and Qx unit growing in its popularity due to its structure similarity with strong electron deficient unit benzothiadiazole (BT) and enhanced solubility compared with BT. The two new PSCs (PBDT-DT-DFQx and PBDT-DTFQx), which introduced either mono- or di- fluorinated Qx, were designed to investigate the effect of the fluorine atom. These conjugated polymers were measured an optical bandgap of 1.97?2.00 eV, with highest occupied molecular orbital (HOMO) energy around -5.50 eV and lowest unoccupied molecular orbital (LUMO) energy around -3.54eV. All the polymers were observed strong absorption in the range of 400-650nm in film state. As a result, High 5.58% of power conversion efficiency (PCE) was achieved with PBDT-DT-DFQx.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **ORGN.P-294**

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Synthesis of non-natural glycoamino acids via Pd/Au-catalyzed Sonogashira cross coupling

전민호 홍성유[1,*]

UNIST 화학공학부 [1]울산과학기술대학교(UNIST) 나노생명화학공학부

Non-natural glycoamino acids are one of the key targets for synthetic carbohydrate chemistry due to their metabolic and chemical stabilities with potential biological functions. Pd/Au catalyzed Sonogashira cross coupling between alkyne-containing carbohydrates and p-iodophenylalanine with low catalyst loading with 2 mol%. Higher reactivity of Au^{I} compared to Au^{III} is observed from initial rate analysis. The Pd/Au catalytic system is tolerant to both *O*-and *S*-protected sugar derivatives without any signs of epimerization.

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Chain extension method for appocarotenoid

정현욱 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carorenoids are characterized by the long conjugated polyene chain that shows distinctive red color. Carotenoids are used as element of cosmetics, health foods and also plays medicinal role, example, preventing cancer. Chain extension of isoprenoid using Kocienski reaction efficiently provided fully conjugated carotenoid compound. The novel C5 benzothiazolyl(BT) sulfone containing an acetal group was prepared as an element for the chain-extension of apocarotenoids. The Julia-Kocienski olefination of the C5 BT-sulfone with C10 2,7-dimethyl-2,4,6-octatrienedial and deprotection of the acetal groups efficiently produced C20 crocetin dial. The compound of C30 and C40 apocarotenoids were prepared from C20 crocetin dial by the repeated application of the Julia-Kocienski olefination of the C5 BT-sulfone and hydrolysis.

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발표분야: 유기화학
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Efficient Conversion of Carbohydrates into Pyrrole-2-carbaldehydes: Application towards the Total Syntheses of (-)-Hanishin and Related Natural Products

DASADHIKARYNIRMAL 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

A practical conversion method of carbohydrates into *N*-substituted 5-(hydroxymethyl)pyrrole-2-carbaldehydes (pyrralines) was developed by the reaction with primary amines and oxalic acid in DMSO at 90 °C. Further cyclization of the highly functionalized pyrralines afforded the pyrrolefused poly-heterocyclic compounds as potential intermediates for drugs, food flavors, and functional materials. The mild Maillard variant of carbohydrates and amino esters in heated DMSO with oxalic acid expeditiously produced the pyrrole-2-carbaldehyde skeleton, which can be concisely transformed into the pyrrole alkaloid natural products, 2-benzyl- and 2- methylpyrrolo[1,4]oxazin-3-ones and , lobechine , and (-)-hanishin.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Various 2,7-substituted-oct-4-enedial Derivatives for Unnatural Carotenoids

박명남 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids present in nature as natural pigment of yellow and orange, can be classified as the xanthophylls and carotenes depending on the presence or absence of oxygen respectively. Most of the carotenoids are composed of 40 carbon atoms to form a conjugate polyene chain. Carotenoids may exhibit conductivity by the polyene chain present in it and can be used as molecular wire. 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 by our sulfone-mediate coupling and double elimination strategy utilizing 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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발표종류: 포스터, 발표일시: 목 11:00~12:30

Regioselective Synthesis of 1-α-tocopheryl-2-glyceride for the synthesis of self-assembled membrane

김윤지 구상호[1,*]

명지대학교 에너지융합공학과 [1] 명지대학교 화학과

Phosphatihylcholine derivatives of 1,2-diglycerides are the main components of cell membranes. We studied about the preparation of various glycerides for self-assembly installation into cell membranes or liposomes. It would be an interesting topic for intracellular metal ion transporters or drug delivery vehicles to synthesize new functional membranes or liposomes from unnatural glycerides of biologically active alcohols or acids. 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.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Carotenoids Stabilized by Aryl Substituents and Their Biological Activity

ALAMMOHAMMADSHARIFUL 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids are a class of natural pigments found mainly in algae, plants and photosynthetic bacteria. From the several roles of carotenoids, the biological activity as antioxidants is amongst the most important. Here, two types of unnatural carotenoids were synthesized. One, carotenoids with anisyl and tolyl substituents at C-13 and C-13’ position were synthesized by the coupling of allylic sulfone subunit and dialdehyde subunit. Two, carotenoids containing pyrenylene group at middle position that can be synthesized by the coupling of the allylic sulfone and substituted pyrene. The synthesized unnatural carotenoids were selected for biological study of antioxidation based on the stabilizing of substituent groups.

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A study on the synthesis of fully conjugated units for lycopene

강세인 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids of the natural products are medically and biologically important. We studied about synthesis of the natural carotenes using sulfone-mediated coupling reaction, protection of alcohol and double elimination. Lycopene and lycophyll were efficiently produced using Julia-Kocienski olefination by the coupling of C10 geranyl benzothiazolyl(BT) sulfone with C20 crocetin dialdehyde. Julia-Kocienski olefination of C5 BT-sulfone and C10 2,7-dimethyl-2,4,6-octatrienedial was utilized as a chain-extension method for the synthesis natural carotenoid products. The procedure of olefination could be used to synthesize the extended polyene of apocarotenoid.

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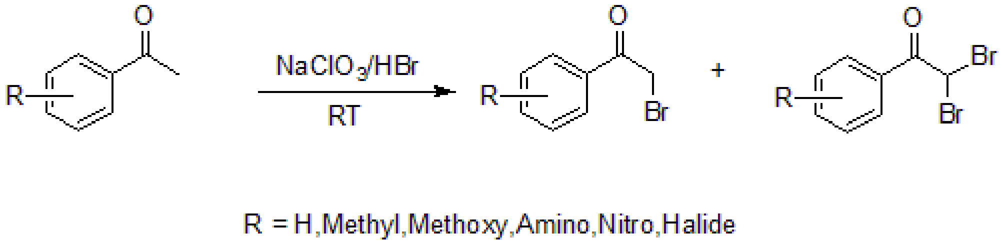
발표종류: 포스터, 발표일시: 목 11:00~12:30

α-Bromination of Aryl Ketones by in situ Formation of Bromine with HBr-NaClO3

고성현 이학준[1,*] 반재영 이경미

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

α-Bromination has been widely employed in organic synthesis as alkyl halides don’t only have their own impact and identity but they also precursors of various biologically and industrially important intermediates. Most of the brominating reagents require careful handling and toxic by-products. Herein, we report a green process for α-bromination by in situ generation of bromine from stable oxidant, NaClO3 with HBr that helps the synthesis of α-bromoaryl ketones from aryl ketones in water.



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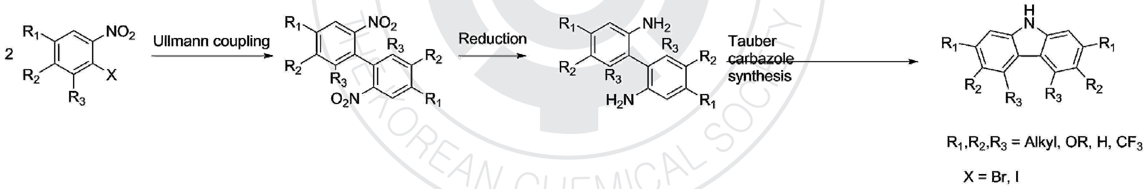
발표종류: 포스터, 발표일시: 목 11:00~12:30

Efficient and Economical Synthesis of Carbazoles II

백정현 이학준[1,*] 반재영 shabbir saira[1]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Previously, we presented about development of synthesizing carbazoles for Organic Light-Emitting Diodes (OLED). The synthetic route was composed of Ullmann cross coupling, Pd/C catalyzed reduction and Tauber carbazole synthesis. In this study, we applied this protocol to various compounds for generalization of the corresponding method.



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발표종류: 포스터, 발표일시: 목 11:00~12:30

Spiropyran-Isoquinoline Dyad as Cation Sensor

신은주* 고용민[1]

순천대학교 화학과 [1]순천대학교 기초의화학부

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.Incorporating isoquinoline ring into SP is expected to lead to excellent light-controlled fluorometric ion sensing system. In this study, isoquinoline-substituted spiropyran derivative was synthesized and cation-sensing ability was investigated using absorption and fluorescence spectroscopy.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Cation Sensing Using Spiropyran-Fluorescein Dyad

신은주* <u>김빛나</u>

순천대학교 화학과

Artificial sensors for sensing and recognition of various metal ions have received considerable attention. Especially, the design and synthesis of sensors for colorimetric and fluorimetric detection of metal ions is a challenge to many chemists. 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 with spiropyran and fluorescein units, was prepared. Their cation-sensing abilities were investigated using absorption and fluorescence spectroscopy.

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Efficient Catalyst for the Synthesis of Styrenated Phenol

신은주* 김빛나 정민철[1]

순천대학교 화학과 [1]순천대학교 화학공학과

The functionalization of arenes is of great importance in the synthesis of pharmaceuticals, agrochemicals, and fine chemicals. These synthetic routes were conventionally performed by Friedel-Crafts alkylation and acylation reactions. Normally, these reactions are catalyzed by different Lewis acid catalysts, however, drastic reaction conditions were employed resulting in lower product selectivity and over-alkylation. Intermolecular hydroarylation reaction of vinyl arenes with various electron rich arenes has attracted considerable importance in both chemistry laboratory and chemical industry in view of the demand for efficient, economic, and environmentally friendly processes. Hydroarylation of alkenes derivatives was successfully catalyzed by various homogeneous Lewis acid catalysts. However, all these catalysts have limitations, such as high amount of catalyst, low recyclability and require tedious workup procedure for the catalyst separation. Thus, identification of an efficient reusable heterogeneous catalytic system for hydroarylation of alkenes remains an intriguing challenge. In the recent years, heteropoly acid catalysts are represented as green solid acid catalysts for various acid-catalyzed reactions. Polyoxometallates (POMs) among heteropoly acid catalysts possess high acidic strength, safe to handle, and non-corrosive solid acid catalysts. In this work, efficient reusable heterogeneous catalysts have been explored for the addition of phenol to the styrene derivatives under solvent-free conditions.

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High Throughput Screening protocol for the coupling reaction of aryl halides

김한성 최진섭 한민수[1,*] 남계춘[*] 이선우[*]

전남대학교 화학과 [1]광주과학기술원(GIST) 화학과

The 4-(2-pyridylazo)-resorcinol mercury (Par-Hg^{2+}) complex, a chemosensor for halide anions, was prepared and studied for the high throughput screening tools in the transition metal-catalyzed coupling reactions. It showed high selectivity towards halide ions such as iodide, bromide and chloride. When this Par-Hg^{2+} complex was applied in the Suzuki coupling reaction, it provided both quantitative and qualitative conversion extent of aryl halides from the change of color in the reaction mixture and the equation of correlation between the concentration of halide and intensity of absorbance of the reaction sample. This halide sensor was employed as a high throughput screening (HTS) tool to find optimized condition for the C-H activated coupling reaction of heterocyclic substrates such as benzoxazole, benzothiazole, N-methylindole and benzothiophene with aryl bromide. The extent of conversion of aryl bromides were easily detected from colorimetric change and obtained from the UV Vis spectroscopy. These results gave the information of the suitable ligand and base in each coupling reaction.

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Isolation and Synthesis of Carboline Derivatives from Bacillus vallismortis strain BS07M

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Bacillus vallismortis strain BS07 originally isolated from near the roots of chili pepper and has been found to be an efficient plant growth promoting and diseases controlling agent. A chemical investigation on the methanol extract of the broth led to the isolation of several β-carboline carboxylic acid derivatives through extraction, C-18 flash column chromatography, silica MPLC, and C-18 HPLC. Structures of these carbolines were determined by spectroscopic methods including IR, UV, specific rotation, HRTOFMS, and 1D & 2D NMR. Those structures were confirmed by chemical synthesis and literature data. In addition, we synthesized several β-carboline carboxylic acids and their carboxylic acid methyl ester derivatives to investigate biological properties. Here, we report structures of the isolates and chemical synthesis.

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Macrolactins and Bacillomycin from solid Bacterial Culture Broth (BS07)

Md.Maniruzzaman Manir 문석식* 박경석[1,*]

공주대학교 화학과 [1]농촌진흥청 국립농업과학원 농업미생물과

Soil microorganism Bacillus vallismortis (BS07) has been used for efficient plant growth promoting and diseases controlling biopesticide. Continued chemical investigation on the solid culture broth resulted in the isolation and identification of several macrolactin macrolides and lipophilic depsipeptide bacillomycin. These metabolites were purified through extraction, C-18 flash column chromatography, silica gel column chromatography, and preparative C-18 HPLC. Their structures were determined by spectroscopic method including HRTOFMS and 2D NMR and confirmed by literature data. Biological activities of these isolates are under investigation. The structures of the isolates will be presented.

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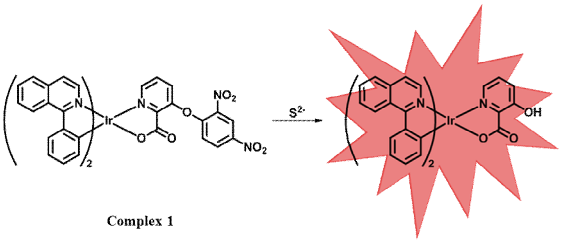
Electrogenerated Chemiluminescent Sulfide Probes based on Cyclometalated Ir(III) Complexes

김서연 홍종인*

서울대학교 화학부

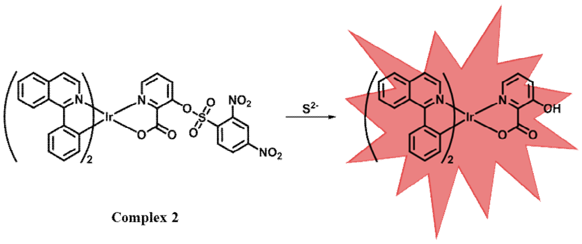
Electrogenerated chemiluminescence (ECL) is the emission of light from the electron-transfer reaction between electrochemically generated precursors at the electrodes. ECL method is different from the optical detection methods because ECL technique does not require the use of complex and expensive light sources, and therefore, provides simple and miniaturized sensing tools. Since ECL has no background optical signal, it can show good detection limit. These features make ECL a highly sensitive and selective analytical method.We designed ECL chemodosimetric and ratiometric sulfide sensors based on cyclometalated Ir(III) complexes. Some Ir(III) complexes are known as good ECL luminophores because they emit bright light at various wavelengths by modulating main ligands. Among them, (piq)2Ir(pic) (piq = phenylisoquinoline, pic = picolinate) exhibits efficient orange-red ECL around 606 nm with TPrA in air-saturated condition. We developed two ECL chemodosimetric probes, based on Ir(III) complexes using piq as a main ligand and pic as an ancillary ligand, for the detection of sulfide anion. While complex 2 shows a low selectivity, complex 1 shows a good “turn-on” ECL sensing property and high selectivity for sulfide anion over the other thiol species. Details of synthesis, photophysical and electrochemical studies will be presented.



Complex 1

PeT Quenching PL & ECL

Turn on Red PL & ECL



Complex 2

PeT Quenching PL & ECL

Turn on Red PL & ECL

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Understanding how different arrangement within the supramolecular complex affects electrical properties of carbon materials

장재규 홍종인*

서울대학교 화학부

Supramolecular architectures have been utilized in many ways (e.g. exciton dissociation, long-range energy transfer, electron or hole transport, stimulus responsive) in the field of organic electronics. Especially, hierarchical structures, where organic molecules are arranged on the surface of carbon materials through intermolecular interactions, have drawn much attention due to its superior electric properties.Recently, Hong et al reported that the nanosheet and nanofiber structures self-assembled from amphiphilic molecules are able to disperse graphene and single-wall carbon nanotube (SWCNT) in aqueous media, respectively.1 In this work, we found that new nanofiber structures self-assembled from two amphiphilic molecules can effectively functionalize SWCNT in aqueous solution. The functionalized SWCNTs were used as the counter electrode of dye-sensitized solar cells instead of platinum. TEM and kinetic studies revealed that the two amphiphilic monomer molecules formed different self-assembled structures on the surface of SWCNTs according to the existence of the alkyl chain moiety in the monomer. The two dissimilar supramolecular structures are expected to exert different influence on the iodide redox couple.

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Structural Characterization of Peptide Oligomers Containing (1S,2R)-2-Aminocycloheptanecarboxylic Acid

서누리 최수혁*

연세대학교 화학과

We synthesized a series of peptide oligomers containing (1S,2R)-2-aminocycloheptanecarboxylic acid and L-alanine. It is predicted that the structure of the oligomers will have 11- and 9-atom ring hydrogen bonds. The crystal structure of the trimer containing (1S,2R)-2-aminocycloheptanecarboxylic acid did not show any intramolecular H-bonds. In contrast, the CD spectra of these oligomers suggested folded conformations in solution. Longer peptide analysis by two-dimentional NMR methods were conducted.

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Practical Synthesis of Pyrrolo[2,1-f][1,2,4]triazin-4(*3H*)-ones

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서강대학교 화학과 [1]한국화학연구원 의약화학연구센터

Pyrrolo[2,1-f][1,2,4]triazin-4(*3H*)-ones have already found a number of bio-applicable uses such as Tankyrase inhibitors, Eg5 inhibitors, phosphoinositide 3-Kinases (PI3Ks) inhibitors. For synthetic aspect, these heterocyclic moieties are the key intermediates of pyrrolo[2,1-f][1,2,4]triazines which showed outstanding biological activities. Based on the reported approaches, however, high temperatures and longer reaction times are required for the preparation of pyrrolotriazinones. To this end, a more practical method for the synthesis of these nitrogen containing heterocycles were investigated. Interestingly, we found that the cyclization using PPh_3-Br_2-Et_3N under mild reaction conditions (at 0 ℃, for 10 min) was provided a mixture of imino-*4H*-pyrrolo[1,2-d][1,3,4]oxadiazines and the desired pyrrolo[2,1-f][1,2,4]triazin-4(*3H*)-ones. Further studies for the oxadiazine-triazinone rearrangement, all reported procedures were unsuccessful. Notably, treatment of lithium trimethyl(phenylsulfido)aluminate (Li[Me_3AlSPh]) has easily provided the pyrrolotriazinones in high yield and with a retained enantiomeric excess (ee).

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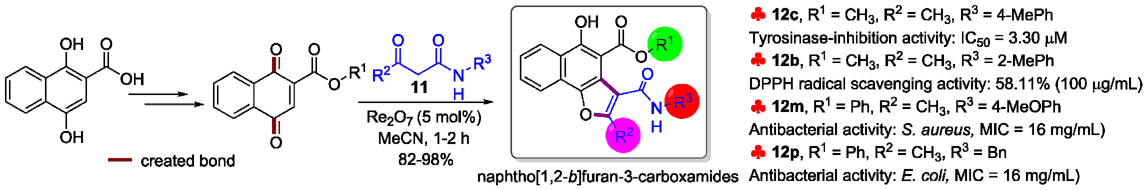
Re$_2$O$_7$-Catalyzed Regioselective Synthesis of Naphtho[1,2-*b*]furan-3-carboxamides and Their Biological Evaluation

하립개 이용록*

영남대학교 화학공학부

Naphtho[1,2-*b*]furans, oxygen-containing aromatic heterocycles, are structural components of biologically active natural and synthetic compounds and exhibit a range of pharmacological properties. For example, rubioncolin A and B were isolated from *Rubia oncotricha* as racemic. They have also been isolated from *Rubia cordifolia*, which is used widely in traditional medicine to treat coughs, bladder and kidney stones, joint inflammation, uterine hemorrhage, and uteritis. Recently, the structure and stereochemistry of these compounds were determined by X-ray crystallography, and the total synthesis of rubioncolin B was accomplished by Traner. Rubicordifolin was isolated as a natural product from *Rubia cordifolia*, and it exhibits potent cytotoxic and antitumor activities. Furomollugin has been isolated from several members of the Rubiaceae family and from *Rubia cordifolia*. The compound exhibits cytotoxic activity to human colon carcinoma cells (HT-29), strongly suppresses HBsAg secretion by human hepatoma Hep3B cells, and exhibits inhibitory activity against DNA topoisomerases I and II. Radermachol was isolated from *Radermachera xylocarpa* K. Schum in India, and has been used as nervine, calmative, antispasmodic, emetic, anthelmintic, abortifacient, as well as a substitute for ipecacuanha. Furomollugin analog and its derivatives significantly inhibited the tumor necrosis factor (TNF)-α-induced inflammatory responses in HT-29 human colon epithelial cells and might be a valuable new drug candidate for the treatment of colon inflammation. Because of their important bioactivities and pharmaceutical applications, a number of synthetic methods have been developed for the synthesis of substituted naphtho[1,2-*b*]furans. Recently, the synthesis of naphtho[1,2-*b*]furans using In(OTf)$_3$ and Fe-Pd bimetallic nanoparticles-catalyzed reactions was reported. Although a number of methods for the synthesis of these compounds have been reported, there have been few biological evaluations of naphtho[1,2-*b*]furans.We herein present a green and efficient process for the construction of diverse naphtho[1,2-*b*]furan-3-carboxamide derivatives 12a-12q via the novel Re_2O_7-catalyzed formal [3+2] cycloaddition of 1,4-naphthoquinones with β-ketoamides as the key step. The synthesized compounds were screened for their tyrosinase inhibitory, antioxidant and antibacterial activities. The results showed that compound 12c exhibited excellent tyrosinase inhibitory activity with an IC_{50} of 3.30 μM, which is comparable to that of kojic acid (IC_{50} = 30.55 μM). Compounds 12a, 12b and 12i displayed moderate antioxidant activities compared to the BHT in a DPPH assay. Compound 12m showed good activity against *S. aureus* (MIC = 16 μg/mL) and compound 12p was highly active against *E. coli* (MIC = 16 μg/mL).



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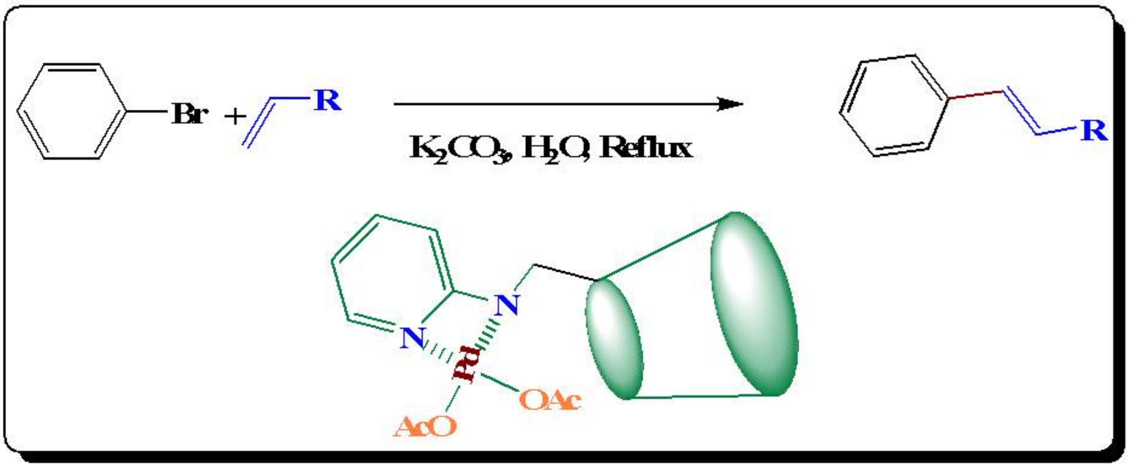
A New β-Cyclodextrin-modified Pyridin-2-amine supramolecular ligands and their Pd(OAc)$_2$ Complex as an Efficient and reusable catalyst for Mizoroki?Heck cross-coupling reactions in water

Dindulkar Someshwar 정다함[1] 조은애[2] 정선호[3,*]

건국대학교 생명공학과 [1]건국대학교 대학원 생명공학과 [2]건국대학교 유비쿼터스정보기술연구원 [3]건국대학교 특성화학부, 건국대학교 대학원 생명공학과

A novel class of β-cyclodextrin-modified pyridin-2-amine/Pd(OAc)$_2$ complex as well as in situ generated complex is an efficient, reusable catalyst and superamolecular platform for phosphane-free Mizoroki?Heck cross-coupling reactions in water. The olefination of iodo- andbromoarenes to the corresponding products was achieved good to excellent yields using catalytic amounts of palladium acetate and β-cyclodextrin-functionalized pyridin-2-amine in aqueous medium. The reaction is compatible with diverse functional groups and without use of an inert atmosphere. This reusability of catalytic system and accessibility in aqueous medium make this protocol green and ecofriendly which can be replaced with metal salts or other heterogeneous catalysts in industrial synthetic procedure.



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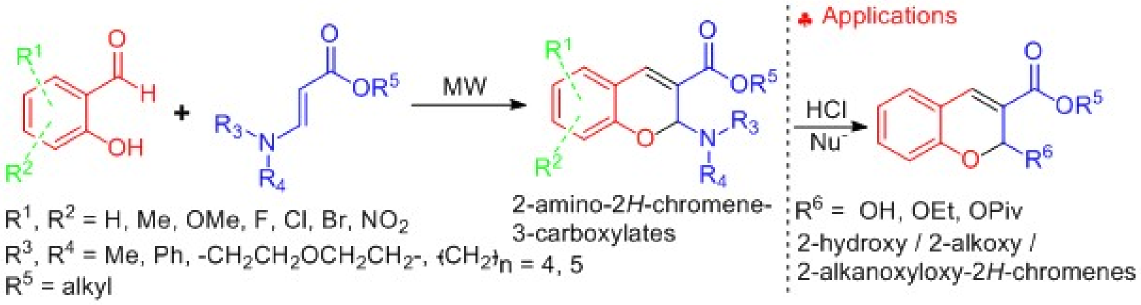
An Environmentally Benign Approach to 2-Amino-2*H*-chromene-3-carboxylates Using Microwave Irradiation

윤상현 하립개 이용록*

영남대학교 화학공학부

Substituted-2*H*-chromenes are important structural motifs found widely in nature and exhibit a wide range of important biological activities, including antifungal, antioxidant, antitumor, anti-HIV, antibacterial, antiviral activities, and others. Molecules bearing these skeletons are also used extensively as selective and sensitive cyanide anion receptors, chromogenic and fluorogenic probes, photochromic materials, and precursor to flavylium dyes. Their importance and usefulness have prompted the development of a number of methods for the synthesis of substituted-2*H*-chromenes in recent years. The typical synthetic methods for substituted-2*H*-chromenes include condensation reactions of phenol/naphthol derivatives with 1,1-diethoxy-2-butenes, 1,1-disubstituted-2-propyn-1-ols, 3-chloro-1-butynes, mesityl oxides, or α,β-unsaturated aldehydes/prenals. Other protocols rely on the construction of benzopyran from salicylaldehydes *via* domino oxa-Michael reactions, tandem Knoevenagel condensations, or Morita-Baylis-Hillman type reactions. For the synthesis of 2-amino-2*H*-chromenes, a few examples are available through the reaction of salicylaldehydes with β-cyanoenamines, β-nitrovinylamines, or *N*-styrylamines and many of them suffer from toxic solvents, tedious work-up, low yields, long reaction time, and harsh reaction conditions. Therefore, efficient and environmentally benign synthetic routes to 2-amino-2*H*-chromenes are in demand. We herein present a facile and environmentally friendly approach to diverse 2-amino-2*H*-chromene-3-carboxylates from salicylaldehydes and β-aminoacrylates under microwave irradiation. This methodology offers several significant advantages, such as economic availability, catalyst-free, low toxicity, ease of handling, high regioselectivity, excellent functional-group tolerance, and environmental benignity under mild reaction conditions. The synthesized compound was also converted to the corresponding derivatives.


MW
HCl
Nu⁻
♣ Applications
R¹, R² = H, Me, OMe, F, Cl, Br, NO₂
R³, R⁴ = Me, Ph, -CH₂CH₂OCH₂CH₂-, (CH₂)n = 4, 5
R⁵ = alkyl
2-amino-2H-chromene-3-carboxylates
R⁶ = OH, OEt, OPiv
2-hydroxy / 2-alkoxy / 2-alkanoxyloxy-2H-chromenes

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Synthesis and CD Spectroscopic Studies of a New Peptoid Foldamer: Oligomers of N-Substituted β^2-Homoalanines

이강주 임현석* 문희조 현유정 서창덕

포항공과대학교(POSTECH) 화학과

Among the unnatural oligomers, peptoids (poly N-substitutied glycines) have been widely studied as a promising class of peptidomimetics. They are easily synthesized, resistant to proteolytic degradation, and far more cell permeable than peptides. However, owing to lack of chirality and hydrogen bonding source, peptoids are too flexible to form folded sturucture without specific side chaines. The α-peptoids with α-chiral side chains were reported to form a helical structure clearly, and the β-peptoid helices with similar side chains were also reported recently. Here, we designed an entirely new peptoid structure (oligomers of N-substituted β^2-homoalanines) as a novel foldamers. Using pre-synthesized monomers, the peptoid oligomers were synthesized on solid-phase efficiently. The purified peptoids were investigated by CD spectroscopy to support their strong probability of folded structure. Importantly, readily available side chains regardless of a-chiral methyl group can be utilized in the peptoids to provide a huge chemical diversity. This new backbone structure will expand the scope of peptoid foldamers and act as a promising scaffold to design biologically potent oligomers.

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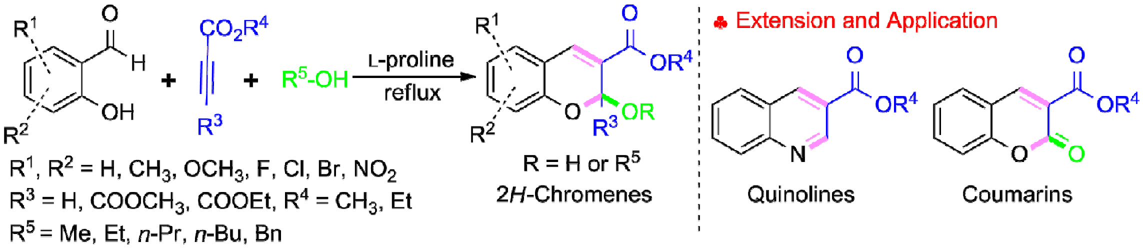
Green Synthesis of Highly Functionalized 2*H*-Chromenes via L-Proline Catalyzed Multicomponent Reactions

CAIHONGYUN 하립개 이용록*

영남대학교 화학공학부

2*H*-chromene is a well-known privileged structural motif, which is present in a number of biologically active natural products as well as drugs, and it also plays a key role in the regulation of various biopolymers. An abundance of well-known bioactive compounds contain a 2*H*-chromene moiety. Importantly, naturally occurring (+)-calanolide A, (+)-pseudocordatolide C, dentatin, and nordentatin exihibit diverse and potent biological activities, such as anti-HIV, antitumor, antiproliferative, anti-inflammatory, and antimycobacterial activities. (+)-Daurichromenic acid has potent anti-HIV activity in acutely infected H9 cells (EC_{50} = 0.00567 ?g/mL), uninfected H9 growth inhibitory activity (IC_{50} = 21.1 ?g/mL), and a therapeutic index (TI) of 3,710. Cannabichromene (CBC) is one of four major cannabinoids in Cannabis sativa and some of its analogs have high therapeutic potential for the treatment of anti-inflammatory diseases. Ageratochromenes, precocene I and II, are well known for their insecticidal activity and for inducing precocious metamorphosis. They also exhibit important properties, such as an antijuvenile hormone by reducing the length of larval life in sensitive species and preventing ovarian development in some adult insects. Because of these important pharmacophoric properties, molecules bearing the 2*H*-chromene moiety have been synthesized and studied extensively. From the viewpoint of synthetic chemistry, MCR is an important strategy to extend the structural diversity of 2*H*-chromenes. In this regard, the development of new multicomponent protocols for the synthesis of new 2*H*-chromenes-incorporating heterocycles have attracted considerable interest in recent years.We herein present a green and efficient one-pot process for the construction of diverse and functionalized 2*H*-chromenes via L-proline catalyzed multicomponent reactions of salicylaldehydes, alkynes (propiolates, acetylenedicarboxylates) and alcohols. As an extension of this method, quinoline derivatives were synthesized in the designed protocol by replacing the salicylaldehyde with 2-aminobenzaldehyde. The synthesized 2-hydroxy-2*H*-chromenes were also transformed successfully into biologically interesting coumarins through the PCC oxidation.



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Chemosensing via Chemoenzymatic Signal Amplification

권오현 정호영 박지효[1] 기정민*

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) 나노생명화학공학부

Specific detection of scarce analytes is extremely important, and many tools such as chemosensors and chemodosimeters have been developed. However, most of classical chemosensors and chemodosimeters are based on stoichiometric molecular recognition or chemical reaction, and are therefore conceptually limited in terms of enhancing the sensitivity. Hence, generation of super-stoichiometric amount signals from small amount of analytes can significantly improve the detection limit of current technologies, with possibilities of naked-eye detection. Herein we describe our design of a signal amplification system for chemodosimeters, based on chemoenzymatic reactions. This system combines chemodosimeters with enzymatic reactions to produce amplified signals. It consists of a sensing module based on classical stoichiometric chemodosimeters and a signal production module based on enzymes to generate amplified output signal. We will also discuss an exponential signal amplification system based on enzymatic autocatalysis.

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Hyper stability of Graphene/Pt catalysts for fuel cell

임윤광 전인엽[1] 백종범[*]

울산과학기술대학교(UNIST) 에너지공학부 [1]울산과학기술대학교(UNIST) 에너지 및 화학공학부

Platinum on carbon based material have come into focus recently for the capture and stability for using fuel cell catalysts. Graphene and carbon nanotube(CNT) are attractive in fuel cell. In this work, a new platinum on graphene catalysts based on ball milling method is presented. Graphene nanoplatelets with selectively functionalized edges are prepared through a simple and attached platinum with ball milling. This catalysts can substitute any other platinum on carbon based material. Platinum not come away from graphene nanoplate because triazine ring captured platinum. So this catalysts get high stability.

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Novel Chemical Tools for High-Energy Phosphoamino Acids

MA WENJIE 박지효[1] 최이건[1] 정형상[2] 오주영 정호영 기정민[*]

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Post-translational modification (PTM) plays important roles in adjusting the biological functions of target proteins. One of the most common and extensively studied PTMs is protein phosphorylation. Protein kinases and phosphatases that install or remove the phosphoryl group are essential in controlling most cellular signal transduction pathways, and their misregulation is linked to many diseases including cancer. Our research is focused on studying phosphohistidine (pHis) and phosphoaspartate (pAsp), which are more elusive and labile forms of protein phosphorylation. In prokaryotes and lower eukaryotes, pHis is essential in signaling processes, and it is becoming more widely reported to be relevant to certain human diseases such as cancer and inflammation. In addition, pAsp is a major component of prokaryotic two-component signaling pathways. Accordingly, investigation of the biological function of pHis and pAsp is becoming increasingly important. While it is relatively straightforward to investigate chemically stable phospho-serine (pSer), phospho-threonine (pThr) and phospho-tyrosine (pTyr), studying the functional role of pHis and pAsp has proved much more difficult. It is because most of conventional chemical and biochemical methods are incompatible with these labile PTMs, due to their chemical instability. In order to address this lack of adequate research tools, we have been developing novel chemical tools for pHis and pAsp through synergistic combination of organic chemistry and protein chemistry. Here we report our recent progress on the development of such tools, particularly chemical probes for pHis and pAsp.

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Scrambling of Oxygen and Sulfur Atoms in Cyclic Thiocarbonate

김보배 남기평*

영남대학교 화학과

O/S scrabmling is common in cyclic thiocarbonate studies. However this scrambling is not completely understood yet. We are going to present the mecahnism of scrambling in details.

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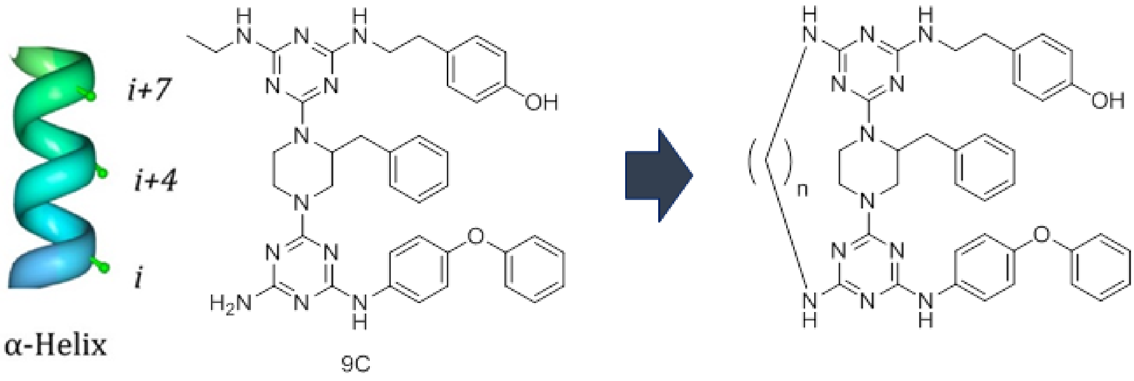
A novel stabilization strategy of α-helix mimetic small molecules using hydrocarbon bridge

이영주 임현석*

포항공과대학교(POSTECH) 화학과

Targeting α-helix mediated protein-protein interaction (PPI) is an important issue for drug discovery. The α-helix mimetic molecules targeting α-helix mediated PPIs can have α-helix structure using hydrogen bonding. However, hydrogen bonding will be disordered in aqueous solution. To overcome this problem, stapling strategy that staples peptide residues covalently and stabilizes the α-helix structure was introduced in peptidic molecules. However, there is no report about stapling small molecules. Previously, our group reported triazine-piperazine-triazine scaffold acts as α-helix memetics. We found 9C compound inhibited the interaction of Mcl-1/BH3 mediated by α-helix structure. Based on this discovery, we designed bridging strategy with triazine-piperazine-triazine α-helical mimetic scaffold. Through bridging this scaffold, we block the rotation of each single bond between each scaffolds and this bridging strategy can compensate entropy loss. Finally, we demonstrated that bridging of the 9C compound using pegylated linker gives much improved binding affinity. From this result, we believe that with this simple bridging strategy of triazine-piperazine-triazine scaffold will be a starting point for development of stapled α-helical mimetic small molecules.



9C

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Asymmetric alkylation of cinchona-based phase transfer catalyst(PTC) ; Theoritical study

<u>김용균</u> 이연지 남기평*

영남대학교 화학과

Cinchona based PTC catalytic reaction has been calculated with DFT method. Experimental data of asymmetric R/S ratio was rationalized with computation results.

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Asymmetric alkylation by Thiophene-derived Cinchona-based Phase Transfer Catalyst (PTC) : Experiment

이연지 김용균 남기평*

영남대학교 화학과

New Chichona-based PTC with thiophene derivatives and their asymmetric alkylation (% yield and %ee) will be presented.

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Synthesis of Terminal Allene via Decarboxylative Coupling Reaction

임정아 **GABRIELCHARLESEDWINRAJA IRUDAYANATHANFRANCISMARIARAJ**
남계춘* 이선우*

전남대학교 화학과

We developed that the copper-catalyzed decarboxylative coupling of paraformaldehyde with aryl-alkynyl carboxylic acid derivatives and dicyclohexylamine to afford the corresponding terminal allene. This coupling reaction proved to work across a various of reagents including functionalized aryl alkynyl carboxylic acids. These decarboxylative coupling reaction is highly environmentally friendly because the reaction was conducted in H_2O and without any additives, releasing only CO_2 and H_2O as the by-products.

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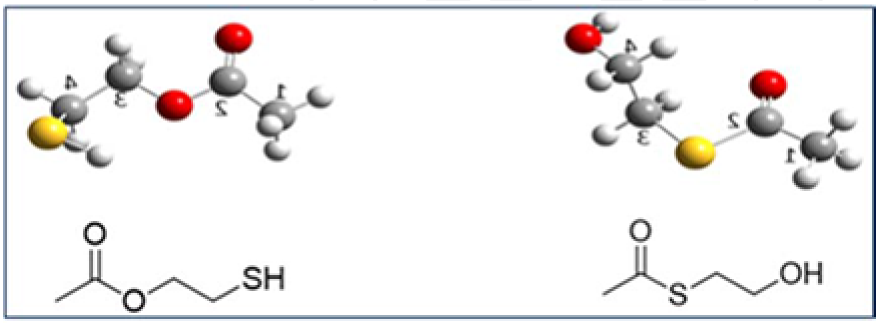
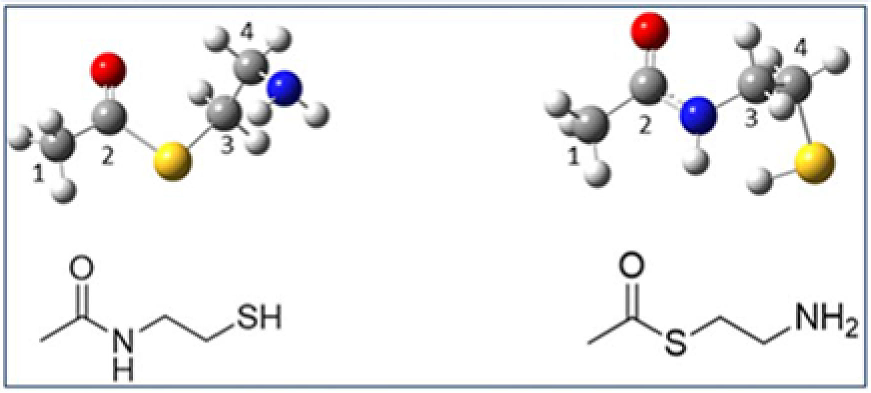
The Investigation of Chemoselectivity in β-mercaptoethanol or β-mercaptoamine with Acid Chloride Derivatives

김미형 이홍섭 정완희 안철진*

창원대학교 화학과

The chemoselectivity in O-acylation of β-mercaptoethanol and N-acylation of β-mercaptoamine are important to prepare the functionalized organic compounds with free-SH. In this paper, we investigated the chemoselectivity in β-mercaptoethanol and β-mercaptoamine with acid chloride derivatives.





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Convergent Synthesis of Unsymmetrical Fr?chet-type Dendrimersusing Double click chemistry

김소연 이재욱*

동아대학교 화학과

A convergent synthetic method for the synthesis of Fr?chet dendrimers will be described. The well-known click chemistry which is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition, is useful tool for synthesis of dendrimers because it was proved as an ideal reaction to obtain very good to excellent yields. Therefore, the click chemistry as a concept of simplifying synthesis is very useful tool to produce functional polymers and dendrimers. 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. Herein we will use the first click reaction (Staudinger/aza-Wittig reaction) leading to the alkyne-functionalized Fr?chet monodendrons containing the benzene at a core, and then will use the second click reaction (1,3-dipolar cycloaddition reaction) with azide-dendrons leading to the formation of unsymmetrical Fr?chet-type dendrimers.

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Axially chiral biaryl dials: A chiral shift reagent for amino esters

김수빈 이기성 이성언 한호규*

고려대학교 화학과

Axially chiral biaryl dials were obtained by the chiral resolution of their racemic mixtures, which were synthesized by Ullmann coupling of aryl aldehydes. These dials were tested as a chiral shift reagent for amino esters.

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Synthesis of the C1-C10 Fragment of Madeirolide A

황성현 백인환 이철범*

서울대학교 화학부

We present studies toward the total synthesis of Madeirolide A. This compound has been isolated from the marine sponge Leiodermatium sp., and has been shown to be a potent inhibitor of Candida albicans, a pathogenic fungus. Madeirolide A has a complicated structure with a 24-membered macrolactone and 16 stereocenters. The bioactivity and structural complexity make madeirolide A an attractive target for total synthesis. Our approach for synthesis is based on the assembly of four fragments. Using reductive cyclization developed from our group, three oxacycles in the compound have been envisioned to be efficiently created under novel photoredox catalysis of an iridium complex. Here we describe the introduction of the synthesis of the C1-C10 part of madeirolide A.

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Phase transition behaviors of the rod-disc liquid crystal by Surface Anchoring Interactions

윤원진 최유진[1] 정광운[2,*]

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

Rod-disk liquid crystal (RD12) was newly designed and synthesized for understanding and characterizing of surface-induced phase transition behaviors of RD12 by changing the surface chemistry and the physical interaction. 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. It was realized that the macroscopically oriented nematic (N) phase of RD12 was obtained by the surface anchoring interaction and the crystallization of RD12 was perfectly suppressed from the cross-polarized optical microscopic observations and analyses. The tailored molecular alignment and anisotropic physical properties of RD12 can allow us to develop the smart optical and electrical thin films for practical applications in electro-optical devices. This work was supported by a grant from the Korea Institute of Science and Technology (KIST) Institutional Program (2Z04320), Basic Science Research Program (2013R1A1A2007238), SW Fusion Components R&D Program (MOTIE-10047806), BK21Plus Program, Korea.

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The Selective Detection of Lysosomal ATP in Live Cells

전용웅 안교한*

포항공과대학교(POSTECH) 화학과

The development of selective recognition systems for organic phosphate anions has received considerable attention due to their diverse activities in biology.1 Among various organic phosphate anions, adenosine-5'-triphosphate (ATP) is particularly important, as it is not only perceived as "molecular unit of currency" for intracellular energy transfer but also a signaling molecule to coordinate responses to energy status, in part by modulating ion channels and activating signaling cascades.2 Recently it was revealed that an abundance of ATP is contained in lysosomes and the release of ATP from lysosomes to the extracellular matrix through lysosomal exocytosis plays essential roles in the signaling for immunogenic cell death, apoptosis and neurotransmission.3 At the moment, however, there is no way to detect and quantify lysosomal ATP selectively, in spite of its huge demand.Although a handful number of fluorescent probes for ATP have been reported, few of them are ATP selective; furthermore most of them are based on a single fluorescent intensity change, which is affected by various factors such as solvents, instruments, concentration and micro-environments (acidity, viscosity and polarity and so on) so that it is impossible to quantify the analyte under unknown conditions by fluorescent intensity measurement. Ratiometric probes showing two different fluorescent emission peaks, however, can be used to quantify the target anlayte by the ratio of the two fluorescent intensities even in a complexed situation. Herein, we disclose the first lysosomal ATP probe that detects ATP only in lysosomes with the ratiometric-emissive property and superb selectivity toward ATP.References1.Chem. Rev. 2011, 111, 6603-6782.2. Science 2001, 294, 1102-1105.3. Nature 2009, 461, 282-286

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Cyclic MPP with Histidine-Ir Coordination as a Novel Therapeutic for Photodynamic Therapy

박재형 유자형[1,*] 권태혁[2,*] LOGANATHANPALANIKUMAR[3]

울산과학기술대학교(UNIST) 화학 [1]울산과학기술대학교(UNIST) 자연과학부 화학과 [2]울산과학기술대학교(UNIST) 친환경에너지 공학부 [3]울산과학기술대학교(UNIST) Environmental Scienc

Mitochondria are an interesting target for cancer chemotherapy and other disease treatments due to their role in energy production, reactive oxygen species production, and apoptosis. There has been a great deal of research over past few decades towards improving the selective delivery and cellular uptake of anti-cancer drugs. However, mitochondrial delivery of drug molecule is difficult due to the intricacies involved in crossing three diverse membranes possessed by mitochondria. Since the vital cell functions are related to mitochondria, development of mitochondria specific targeting can improve the efficiency of cancer treatment with a high integrity. In this present work, We have synthesized mitochondria penetrating peptide with histidin on both ends: HK(FxR)4-H. These Histidin side group is utilized for the formation of complex with Ir and hence generate cyclic peptide with mitochondria penetrating property. The ring size has been varied by changing the number of amino acid sequence to find the optimum ring size for better penetration. The Ir metal is known to produce singlet oxygen upon light irradiation. So this peptide can induce rapid cell death upon photo irradiation and can serve as a novel photodynamic therapeutic agent for cancer therapy. Moreover, most of the mitochondria targeting agent failed to deliver high molecular weight cargo to mitochondria. So our molecular design can be a solution problem as it can carry high molecular weight cargo by conjugation to it.

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Identification and quantitative analysis of detergent Deflux composition using chromatography-mass spectrometry

박나현 김종혁[1] 조성희[1,*]

한국화학연구원 분석센터 [1]한국화학연구원 화학분석센터

Deflux has been widely used in semiconductor industry to remove flux residue or polluted material. Flux, which is composed of rosin and a number of activators, is used for preventing contamination and reoxidation on the surface of metal oxide film. Through the reaction with deflux, the solubility of flux is increased and flux residue cleaning efficiency is enhanced. Therefore, for providing useful information about cleaning efficiency of flux, in this study, unknown deflux compositions were identified and quantified by gas chromatograph-time of flight mass spectrometer(GC-TOF/MS), high resolution GC-TOF/MS and ultrahigh performance liquid chromatograph mass spectrometer(UPLC-MS). Two alkyleneglycol alkylethers, two alkylaminoamines, and a alkylaminoalcohol were predicted as deflux compositions fragmentation patterns and accurate mass using GC-TOF/MS and high resolution GC-TOF/MS, respectively. These compositions were identified by retention time and mass spectrum compared with individual standard. Identified compositions were quantified by UPLC-MS using SIR mode to avoid of matrix effect. Under the optimized conditions, the correction coefficient of each calibration curve was over 0.993. This method could be used to predict individual organic compound in unknown substance.

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Azopyrazoles Formation by Silver-Catalyzed Reaction of Diazo Compounds and Arylhydrazines

PANDIT RAMESHWAR PRA 이용록*

영남대학교 화학공학부

Azopyrazoles are the most important heterocyclic compounds that possess a wide range of biological properties. Azopyrazoles are valuable building blocks and structural motif in the synthesis of natural products. Pyrazoles bearing azo group are also found as the core structure in many food colorings, dyestuffs and bioactive molecules.Herein described is the cascade synthesis of functionalized azopyrazoles in good yields from an efficient one-pot AgOTf-catalyzed cascade reaction of α-diazo-β-ketoesters with two equivalents of arylhydrazines or arylhydrazine hydrochloride. This cascade process involves simultaneous diazopyrazolone formation, N-H insertion and oxidation in the presence of catalytic amount of AgOTf. In addition, AgOTf-catalyzed reaction of 4-diazopyrazol-3-one, prepared by known method, with arylhydrazines to acquire functionalized azopyrazoles with wide range of functionality on the aromatic rings has also been illustrated.

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Traceless C-C bond Formation via Tandem Alkylation and Retro-ene Reactions Using Heterocyclic Sulfones

채영현 최진 이철범*

서울대학교 화학부

Our laboratory has been interested in the retro-ene reactions of allylic sulfinic acid that can be performed in tandem with the Diels-Alder reaction.1 As a follow-up study, we developed tandem alkylation and retro-ene reactions using unusual heterocyclic sulfones. This tandem protocol was aimed to form C-C bonds in a traceless fashion that was distinct from classical C-C bond forming reactions. Diverse allylsulfones as the precursor of the allylic sulfinic acid could be prepared through various C-C bond forming reactions (alkylation, aldol, and Michael reaction etc.). Subsequently, the retro-ene reaction was performed in one-pot under mild conditions and to yield functionalized reductively rearranged alkenes. It was found that thiadiazole substituted sulfones were more suitable precursor of allylic sulfinic acid than previously known heterocylic sulfones. We anticipate that the traceless tandem methodology will be useful to synthesize various functionalized alkenes via allylsulfone substrates that can be prepared through a range of C-C bond forming reactions. The details of our studies will be shown in this poster.

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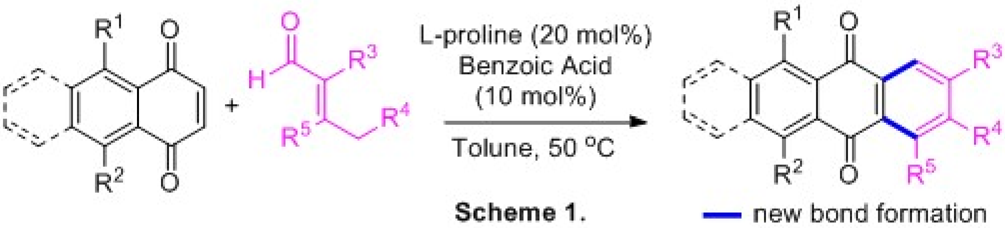
Efficient Approach to Anthraquinones and Tetracenediones *via* Organocatalyzed Benzannulation

소마이마가크리쉬나 하립개 이용록*

영남대학교 화학공학부

Organic compounds possessing an anthraquinone nucleus are widely distributed in natural products. They are also important molecules with many applications in medicinal and pharmaceutical industry as they have been found to exhibit a broad range of biological activities, such as anti-cancer, antibacterial, antineoplastic, anti-tumor, and anti-HIV activities. Additionally, anthraquinone derivatives are used as dyes for coloring natural and synthetic fibers. Similarly, tetracenedione derivatives are also found in natural products and have been used as important building blocks for the manufacturing of organic electronic devices and organic semiconductors. Due to the importance and usefulness of anthraquinone and tetracenedione derivatives, many synthetic protocols have been explored. Some of them include Friedel-Crafts reactions of phthalic anhydride with substituted benzenes, the cyclization of polyketides, Cu-catalyzed intramolecular cyclization of enynes, oxidation of the anthracenes or hydroxyl anthracenes, and ZnI_2-catalyzed Diels-Alder reaction/oxidation/Friedel-Crafts cyclization. Despite their merits, existing synthetic approaches have several drawbacks such as use of expensive catalysts, multiple reaction steps, harsh reaction conditions and low product yields. Therefore, there is still demand for an efficient and facile synthetic approach that can conveniently provide a range of anthraquinones and tetracenediones using L-proline as a catalyst.There are no reports on the construction of anthraquinones and tetracenediones by organocatalyzed benzannulation reaction of 1,4-naphthoquinones or 1,4-anthracenedione with a variety of α,β-unsaturated aldehydes yet. Here, we report a novel and efficient synthesis of anthraquinone and tetracenedione derivatives by L-proline catalyzed benzannulation between 1,4-naphthoquinones or 1,4-anthracenedione and α,β-unsaturated aldehydes in good to excellent yield *via* domino formal diene formation/[4+2] cycloaddition/oxidation (Scheme 1). This methodology was also successfully applied to the synthesis of natural products.


R1
R2
O
O
H
R3
R5
R4
+
L-proline (20 mol%)
Benzoic Acid
(10 mol%)
Tolune, 50 °C
new bond formation

Scheme 1.

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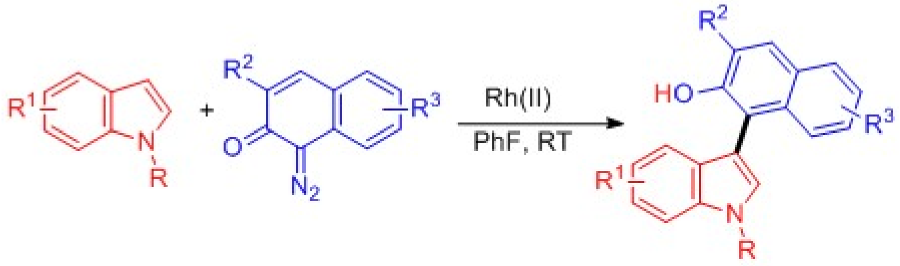
발표종류: 포스터, 발표일시: 목 11:00~12:30

Efficient Synthesis of 3-Naphthylindole by Rhodium(II)-Catalyzed Regioselective Direct Arylation of Indoles with 1-Diazonaphthalene-2-(1*H*)-ones

BARALEKRAJ 이용록*

영남대학교 화학공학부

Indoles are important heterocycles contained in many natural products, agrochemicals, and pharmaceuticals. They are potential drugs and have a wide range of biological activities. Likewise, they are also used widely as the building blocks for the synthesis of functionalized indoles. Specially, C-arylindoles showed a wide range of biological activities, such as anticancer, antibacterial and antifungal, antiapoptotic Mc1-1 protein inhibitors, PPAR-γ partial agonists, AKT-mTOR signaling pathway kinases inhibitors, endothelin antagonists, nonpeptidyl GnRH receptor antagonists, and h5-HT2A receptor antagonists. Owing to their importance and usefulness, a range of synthetic approaches for C-arylindoles have been developed based on the transition metal-catalyzed direct arylation of indoles with activated arenes and some approaches include the oxidative C-H coupling of indoles with nonactivated arenes also. But, there are few reports of direct C-C bond formation to construct functionalized naphthalene derivatives based on the indole nucleus.Here, we present the regioselective synthesis of 3-naphthylindoles by a Rhodium(II)-catalyzed cross coupling of indoles with 1-diazonaphthalene-2-(1*H*)-ones. This procedure provides a range of novel 3-naphthylindoles in high yield. Furthermore, the other direct coupling of benzofuran, pyrrole or furan with 1-diazonaphthalene-2-(1*H*)-ones afforded 2- or 3-naphthyl substituted heterocycles.


R1
N
R
+
R2
O
N2
R3
Rh(II)
PhF, RT
R2
HO
R3
R1
N
R

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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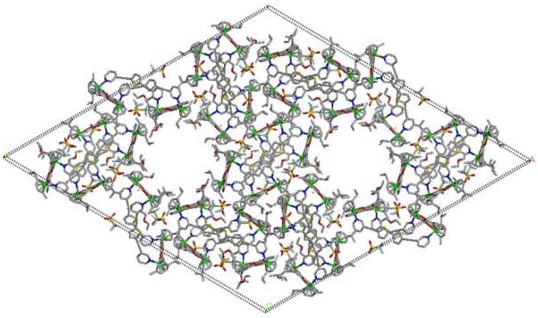
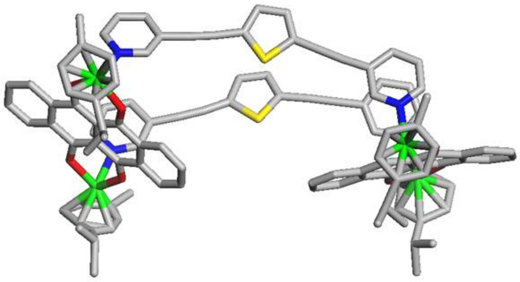
Synthesis and characterization of self-assembled architectures based on Ru(II) acceptors and thiophene-derived donor

김태근 지기환*

울산대학교 화학과

Self-assembly is a spontaneous process in which smaller components combine and rearrange to get a more stable supramolecule. When metal-ligands coordination is involved, it is known as coordination-driven self-assembly. In recent years coordination-driven self-assembly has grown rapidly and many new nanometer-sized supramolecular architectures with various shapes have been reported. Convenient synthesis of catenanes, rotaxanes and molecular knots using self-assembly process is also a hot topic in current research. In this poster we will present the self-assembly of thiophene-derived bidentate ligand and various Ru(II) p-cymene acceptors. All the resulted self-assembled architectures have been fully characterized using various spectroscopic techniques. One of the representative architecture have also been characterized by single crystal X-ray diffraction analysis (Fig.1). The poster will address a detail comprehensive account of the mentioned workFig1. X-ray crystal structure of one of the representative architecture.





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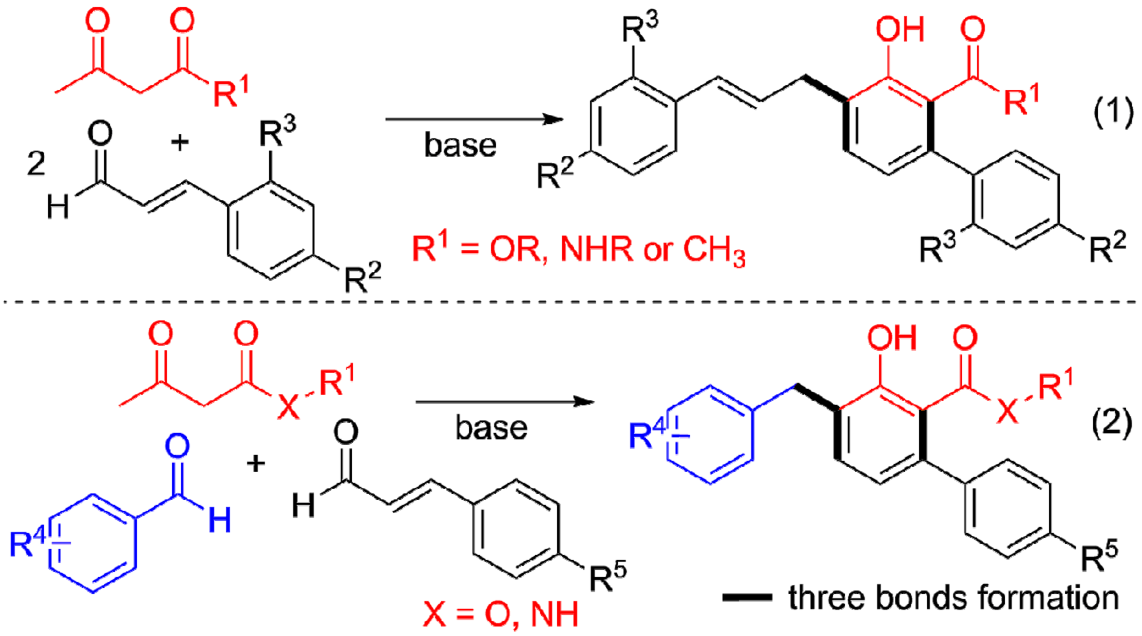
Multicomponent Benzannulation for Construction of Highly Functionalized Biaryls

POUDELTEJNARAYAN 이용록*

영남대학교 화학공학부

Biaryls are used widely as important scaffolds and building blocks for the construction of optical and functional materials. Biaryl units are one of the most important structural motifs found in biologically-active natural products, pharmaceuticals, and agrochemicals. Several methods for aryl-aryl bond formation have been reported. Among these, the transition-metal catalyzed traditional cross-coupling (Suzuki, Stille, Hiyama, etc.) has become one of the useful tools for constructing an Ar-Ar bond by the reaction of aryl halides and aryl metals. Although a number of methods for the direct formation of an Ar-Ar bond by transition metal-catalyzed reactions have been well developed, the loading of catalyst tends to have a high economic cost in industrial processes. Therefore, the development of a facile transition metal-free process is essential and quite significant. Recently, several transition metal-free methods for the formation of aryl-aryl bonds have been developed. These approaches include the arylation of arenes by aryl halides in the presence of strong alkali metal bases and ligand, which proceed via a radical-type mechanism. These reactions provide biaryl molecules by cross-coupling between the two aromatic rings of the aryl metals and aryl halides, arenes and aryl halides, or arenes and arenes. Herein, we present a novel, facile and efficient one-pot biaryl formation through a three-component reaction starting from commercially available β-ketoesters, β-ketoamides, or 1,3-diketones with α,β-unsaturated aldehydes (Scheme 1, eq. 1) or α,β-unsaturated aldehydes and aryl aldehydes (Scheme 1, eq. 2) in presence of mild base.



Scheme 1. Diverse and Polysubstituted Biaryl Formation by Benzannlation Through Three-Component Reactions

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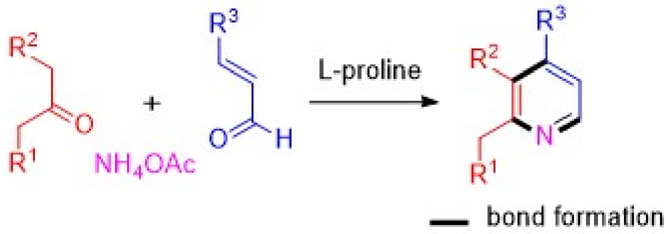
Construction of Various Polyfunctionalized Pyridines via L-Proline Catalyzed Oxidative *N*-Annulation

<u>KHANALHARIDATTA</u> 이용록*

영남대학교 화학공학부

Molecules bearing pyridine moiety are important heterocyclic compounds contained in many natural products and pharmaceuticals. They exhibit a wide range of biological activities, such as anxiolytic, antidiabetic, antiviral, antibacterial, antileishmanial, anti-inflammatory, and anti-chagasic activities. Moreover, pyridine derivatives are widely used as the building blocks for the synthesis of chiral ligands, bioactive natural products, and novel functional materials with photo- or electrochemical properties.Motivated by the importance and usefulness of these privileged motifs, a variety of synthetic approaches have been developed to construct pyridine derivatives based on the condensation of 1,3-dicarbonyl compounds, transition metal catalyzed cycloaddition reactions and organocatalyzed cycloaddition. Despite their merits, many of the reported methods suffer from many drawbacks, including the necessity of transition metal catalysts, harsh reaction conditions and the prerequisite functional groups, such as oximes, imines and azides. Therefore, more environmentally benign and efficient methods are needed to improve these shortcomings for the synthesis of polysubstituted pyridines. In recent days, organocatalysis has emerged as an area of active interest for the construction of functionalized cyclic molecules in organic synthesis. To address this issue, our study evaluated organocatalyzed reactions for the synthesis of diverse and multisubstituted pyridines. Here, we describe a novel, economical, metal-free, and multicomponent reaction strategy for the synthesis of 2,3,4-trisubstituted pyridines via L-proline catalyzed three-component reactions using ketones, α,β-unsaturated aldehydes, and ammonium acetate as the starting materials (Scheme 1). This protocol leads to rapid *N*-annulation through C-C and C-N bond formation in a single operation, thereby avoiding the preparation of essential functional groups, such as oximes, imines, or azides. The synthesized pyridines inhibited bacterial growth resulting in the discovery of new molecules with antibacterial activitiy. Additionally, the synthesized pyridine has been utilized as fluorescence sensors for detection of Cu^{2+} ions in solution.



Scheme 1. L-proline Catalyzed Strategy for Functionalized Pyridines.

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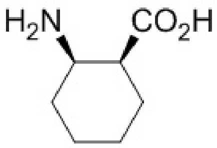
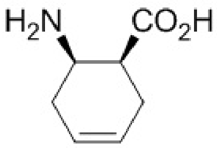
Folding Stability of 11/9-Helix Promoted by Different β-residues

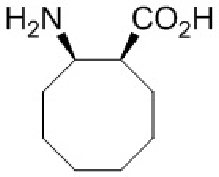
이재연 최수혁*

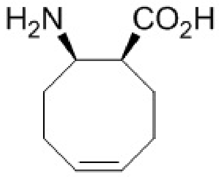
연세대학교 화학과

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. Mixed helices are distinct and most unconventional helical structures, which arise from two types of hydrogen bonds with alternating directions.Here, We will discuss the residue requirements and the modification of building blocks toimprove the mixed-helix stability. We synthesized several peptides units that have different β-residue to test the helix stability









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발표종류: 포스터, 발표일시: 목 11:00~12:30

Co-imaging of Monoamine Oxidase Activity and Amyloid-β Plaques in Alzheimer's Disease

노예진 안교한[1,*]

포항공과대학교 (POSTECH) 화학과 [1]포항공과대학교(POSTECH) 화학과

Alzhemimer's disease (AD) is the most popular senile dementia, leading to progressive memory impairment and change in behavior.[1] Two of the most notable pathological features are neurofibrillary tangles and amyloid-β (Aβ)-laden senile plaques in the brain.[2] Among them, amyloid-β (Aβ) peptide aggregates play a significant role in neuronal cell deaths, neuroinflamation, and enzymatic malfunctions.[1] Size and distribution of Aβ plaques in the brain increase with the time, leading to disturbance of neuronal signaling and regulation of dopamine and serotonin by lowering the level of monoamine oxidase (MAOs).[3] Moreover, Alzheimer's disease patients have a higher level of homovanilic acid, an oxidized product of dopamine with MAOs and a lower level of dopamine.[4] Until now, many imaging probes for Aβ plaques have been developed, such as thioflavin T analogues, Congo red, Pittsburgh compound-B, Curcumin derivatives, molecular motor motif derivatives (DDNP series) and styrylbenzene derivatives (MeO-X04 series). These probes give fluorescence turn-on response toward Aβ-plaques and used for ex vivo imaging.[5] Herein, we report the probe that allows us to imaging both MAOs and Aβ plaques by in vivo two-photon imaging for the first time

References

[1] Tiago S.; Jose T.; Fernando R.; Fernanda B. Angew. Chem. Int. Ed. 2012, 51, 2-14
[2] Shannon R.; Carol F. L. Am. J. Alxheimers Dis. Other Demen. 2002, 17, 11-17
[3] Mark P. M. Nature. 2004, 430, 631-639
[4] Kari J. R.; Leo P.; Toivo H.; Outi M.; Veli-matti K.; Markku L.; Paavo J. R. Neurobiol. Aging. 1988, 9, 245-252
[5] Tamotsu Z.; Mizuo M. Biomater. Sci. 2014, 2, 951-955

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 목 11:00~12:30

A rational approach toward brighter D-A type dipolar dyes in aqueous media

박현진 안교한[1,*]

포항공과대학교 화학과 [1]포항공과대학교(POSTECH) 화학과

The donor-acceptor (D/A) type dipolar dyes are frequently used in molecular probes and biological tags.[1] Fluorescence emission of this type of fluorophores is dependent on the media, strongly emitting in organic solvents but weakly emitting in aqueous media. As they can generate intramolecular charge transfer (ICT) states, their emission is dependent on the donor and acceptor groups. We have investigated the structural factors that affect the emission intensity in aqueous media, in particular, by focusing on the donor amine group. Specifically, we conducted a systematic structure variation of the donor, amino substituent of acedan, which is an important two-photon dye.[2] We have identified several factors that influence the fluorescence of the dipolar dyes in aqueous media: hydrogen bonding with water, rotational freedom, and 1,3-allylic strain. By suppressing those factors, we were able to make acedan emit more strongly in aqueous media. This rational approach can be applied to other dipolar fluorophores, as demonstrated for coumarin, naphthalimide, and (4-nitro-2,1,3-benzoxadiazol-7-yl)amine (NBD) dyes. The new dyes gave much brighter fluorescent images in cells and tissues than conventional forms. A thiol probe was developed based on our study, which demonstrated our approach is applicable to fluorescent probes. The findings hold great promise for the development of efficient dipolar dyes and the corresponding fluorescent probes for biological systems.References1.G. S. Loving,; M. Sainlos,; B. Imperiali, TrendsBiotechnol., 2010, 28, 73?83.2.S. Singha,; D. Kim,; B. Roy,; S. Sambasivan,; H. Moon,; A. S. Rao,; J. Y. Kim,; T. Joo,; J. W. Park,; Y. M. Rhee,; T. Wang,; K. H. Kim,; Y. H. Shin,; J. Jung,; K. H. Ahn.Chem. Sci.,2015, 6, 4335?4342.

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The relationship between LSPR and absorbance behavior of Ag NPs in TiO_2 photoanode of the solid-state perovskite solar cells

양동욱 홍종인*

서울대학교 화학부

Solar energy is expected to be the most renewable alternative energy source. Perovskite solar cells (PSCs), which introduced $CH_3NH_3PbX_3$ (X=Halide) as a sensitizer in solid-state dye-sensitized solar cells, are attracting attention because of their relatively low cost of manufacturing, easy fabrication and comparatively high power conversion efficiency than other kinds of organic solar cells. As a key factor in highly efficient PSCs, the active layer of cells should absorb photons efficiently to obtain a high value of J_{sc} which directly affects the photon-to-current efficiency (PCE). To improve Jsc without increasing resistance of the device, light trapping technique using metallic nanoparticles was introduced. By the effect of localized surface plasmon resonance (LSPR) and/or light scattering of metallic nanoparticles, sensitizers can absorb photons more effectively, which leads to higher J_{sc} and PCE values. By incorporating silver nanoparticles in the photoanode layer of PSCs with optimized concentration, we could obtain increased absorbance of incident light and J_{sc} value without decrease of neither V_{oc} nor FF, thus higher PCE.

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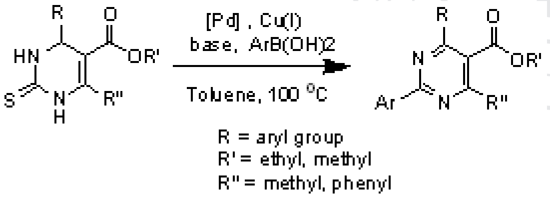
Dehydrosulfurative C-C Cross-Coupling and Concomitant Oxidative Dehydrogenation for the Synthesis of 2-Arylpyrimidine Derivatives

김혜지 손정훈*

충남대학교 화학과

An useful method for carbon-carbon bond formation is described. The procedure make use of the Palladium-catalyzed Copper-mediated Cross-coupling of 3,4-Dihydropyrimidine-2-thiones with Arylboronic acids. The desulfitative Carbon-carbon Cross-coupling usual of the Liebeskind-Srogl type is carried out under neautral conditions. This conditions result in 2-Aryl-pyrimidine in appropriate to high yield. And that can be applied to a series of heterocyclic compound with thioamide fragements.



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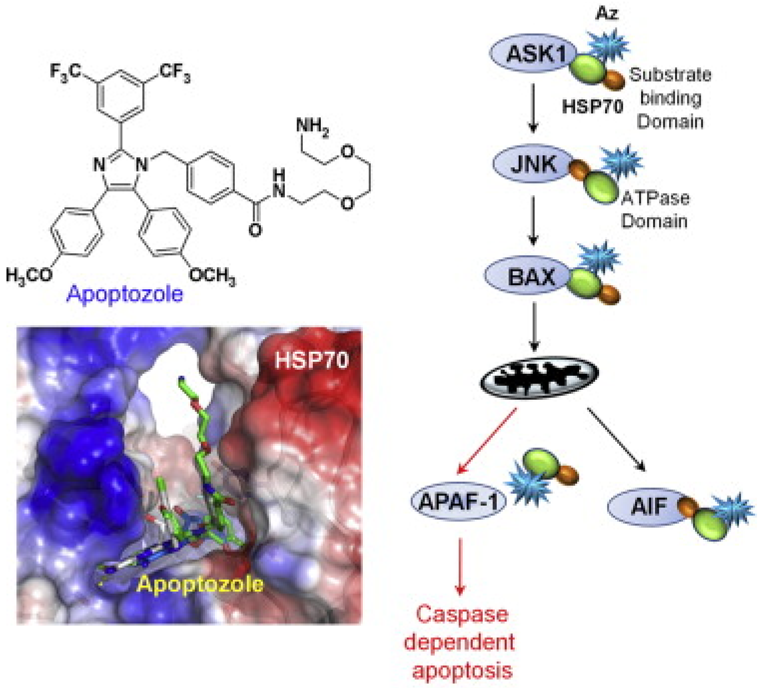
발표종류: 포스터, 발표일시: 목 11:00~12:30

A small molecule induces apoptosis by inhibition of ATPase activity of HSP70 that has antitumor activity

박수길 신인재*

연세대학교 화학과

Small molecules related to cell death have significant potential as therapeutic agents to treat apoptosis or autophagy-related diseases. To select molecules with cell death-inducing activity, cell-based screening with a small molecule library composed by imidazole scaffolds is performed to identify bioactive compounds that induce cell death. We have identified from the cell-based assay a small molecule, apoptozole that interacts with Hsc70 and Hsp70. The heat shock protein HSP70 plays antiapoptotic and oncogenic roles, and thus its inhibition has been recognized as a potential avenue for anticancer therapy. In biochemical studies, apoptozole binds ATP-binding domain of Hsc70 and inhibits the ATPase activity of Hsp70/Hsc70 with dissociation constant of submicromolar concentration. It is likely that this compound induces cell death by inhibiting the function of Hsp70 and/or Hsc70, which antagonize apoptosis by interfering with multiple checkpoints in the cell death pathways. Apoptozole (Az), as a result, induces an array of apoptotic phenotypes in cancer cells. Affinity chromatography provides evidence that Az binds HSP70 but not other types of heat shock proteins including HSP40, HSP60, and HSP90. We also demonstrate that Az induces cancer cell death via caspase-dependent apoptosis by disrupting the interaction of HSP70 with APAF-1. Animal studies indicate that Az treatment retards tumor growth in a xenograft mouse model without affecting mouse viability. These studies suggest that Az will aid the development of new cancer therapies and serve as a chemical probe to gain a better understanding of the diverse functions of HSP70.


Apoptozole
HSP70
Apoptozole
Az
ASK1
HSP70
Substrate binding Domain
JNK
ATPase Domain
BAX
APAF-1
AIF
Caspase dependent apoptosis

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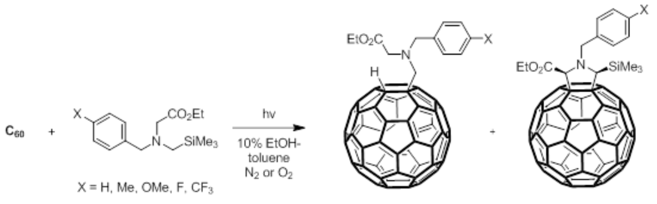
Synthesis of Functionalized Fullerenes by Photoaddition of N-alpha-trimethylsilyl-N-Carboxymethyl-N-Benzylamines to C_{60}

조대원* <u>임숙현</u> **Atar Amol Balu**

영남대학교 화학과

Photoaddition reactions of fullerene C_{60} with N-alpha-trimethylsilyl-N-carboxymethyl-N-benzylamines, which contain various para-substituents, were explored in order to evaluate factors governing efficiencies of this potentially useful method for preparing functionalized fullerene derivatives. Observations made in this study show that two reaction pathways are followed in these photoreactions. The first involves initial formation of alpha-trimethylsilyl-aminium radicals and the C_{60} anion radical by SET from the amines to the triplet excited state of C_{60}. This step is followed by desilylation to produce alpha-amino radicals. Coupling of these radicals with the anion radical of C_{60} followed by protonation or to the hydrofullerene radical generated by protonation of the anion radical of C_{60} then produces aminomethyl-1,2-dihydrofullerenes. When limited amounts of $^3O_2$ are present in the reaction medium, fulleropyrrolidines are generated in low yields by a competitive pathway involving formation of singlet oxygen, which undergoes sequential H-atom abstractions from the N-alpha-trimethylsilyl-N-carboxymethyl-N-benzylamines to produce azomethine ylide intermediates. Dipolar cycloaddition of the ylides to C_{60} then produces fulleropyrrolidines. Photoreactions of the C_{60} and the amines in the presence of high $^3O_2$ concentrations exclusively produce fulleropyrrolidine. In addition, the results show that photoreactions of non-silicon substituted, N-methyl-N-carboxymethyl-N-benzylamines with C_{60} form fulleropyrrolidines independent of the concentration of $^3O_2$ present in the media.



C_{60}
+
X
CO_2Et
N
$SiMe_3$
X = H, Me, OMe, F, CF_3
hv
10% EtOH-
toluene
N_2 or O_2
EtO_2C
N
X
H
+
X
EtO_2C
N
$SiMe_3$

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발표코드: **ORGN.P-348**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Generation of Putative Cationic Pd-Hydride Complex and its' application to Selective Isomerization of a Terminal olefin

임환정* 이진용[1] 손인영[2]

한국화학연구원 의약화학연구센터 [1]충남대학교 신약전문대학원 [2]성균관대학교 화학과

Generation of a stable palladium hydride complex and its' structural identification have been one of the most interesting goals to many organic and organometallic chemists, due to its' exceptional catalytic activities toward diverse organic reactions such as polymerization, hydrofunctionalization, and isomerization of an alkene. For synthesizing a putative "Pd-H" complex, mild reaction conditions were developed. The resulting "Pd-H" complexes were analyzed by NMR and X-ray. The structurally confirmed "Pd-H" complexes were applied for regio-selective isomerization of terminal alkenes. Depending on a ligand and a reaction condition, the developed catalyst isomerized terminal olefins to E-2-alkenes or E-3-alkenes in excellent regio- and stereo-selectivities.

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Synthesis of 1,3,5-trisubstituted-1,3,5-triazines from amines and formaldehyde

강성영 이도훈 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Heterocyclic compounds are abundant in nature and are of great interest because of their biological and industrial significance. N-substituted 1,3,5-triazacyclohexanes are an important class of heterocycles due to their versatile use in the coordination chemistry, catalysis, switchable system with light or redox trigger, crown ether system as well as in recognition, extraction and detection requiring molecular selectivity. Classical Mannich synthesis of 1,3,5-trisubstituted-1,3,5-triazines is accomplished by the condensation reaction between formaldehyde and amine. However, these methods suffer from disadvantages such as harsh conditions, unsatisfactory yields and long reaction time. In this study, we attempted the synthesis of 1,3,5-trisubstituted-1,3,5-triazines in order to obtain novel compounds with biological applications in high yields.

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다공성 금속-유기 골격체(MOF) 내부로의 4차 암모늄 도입과 그 효과

함형우 하현빈 김영조* 김민*

충북대학교 화학과

금속-유기 골격체 (Metal-organic frameworks, MOFs)는 금속 이온과 유기 리간드가 서로 반복적으로 연결되어 합성되는 혼성물질로, 다공성을 갖는 결정 구조체이다.[1] 금속-유기 골격체는 넓은 표면적, 열적 안정성, 그리고 구조적 다양성을 갖기 때문에 기체 흡착 및 기체 분리등 다양한 분야에서 적용이 가능하다.[2-4] 또한, 반복적인 골격 구조를 '분자체'처럼 이용하여 다양한 분자를 분리하는 연구가 다각도로 진행되고 있다.[5] 금속-유기 골격체는 제올라이트나 메조포러스 실리카에 비해 유기 리간드 부분에 여러 종류의 리간드를 상대적으로 쉽게 도입할 수 있고, 도입 된 리간드로부터 기인하는 여러 종류의 효과에 대한 연구가 진행되고 있다. 여러 종류의 유기 리간드는 금속-유기 골격체 합성 전에 리간드에 도입 될 수도 있고, 골격체 합성 후에 합성 후 변환법(PSM)을 이용하여 도입할 수도 있다.[6] 본 발표에서는 선 작용기 도입법을 활용하여 3 차 아민을 포함하는 금속-유기 골격체를 합성하고,[7] 이를 시작물질로 합성 후 변환법을 이용하여 4 차 암모늄 염을 골격 구조내에 도입한 결과를 논의하고자 한다. 또한, 도입 된 4 차 암모늄 작용기를 활용하여 다양한 분자에 대한 선택적인 흡착 결과를 발표할 것이다. 결론적으로, 본 연구를 통해 금속-유기 골격체 구조 내에 4 차 암모늄 기를 효과적으로 도입하였으며, 이를 이용하여 선택적으로 분자를 구별하여 흡착할 수 있는 시스템을 구현할 수 있었다.

Acknowledgement: 본 연구는 교육부와 한국연구재단의 지역혁신인력양성 사업으로 수행된 연구 결과임.(과제번호 2014H1C1A1066874).

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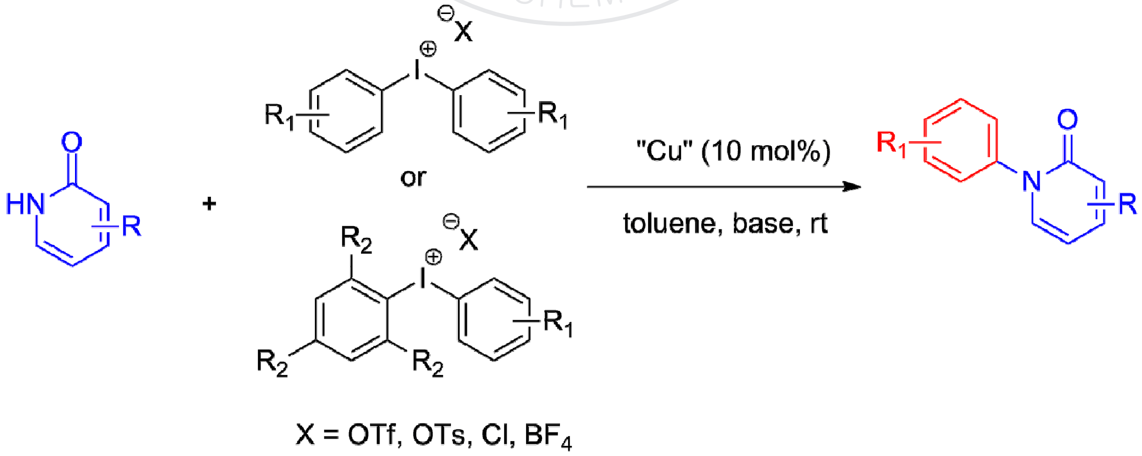
Copper-Catalyzed C-N Bond Formation between 2-Pyridones and Diaryliodonisum Salts at Room Temperature

정서희 김원석*

이화여자대학교 화학 나노과학과

N-aryl heterocycles have attracted synthetic organic chemists due to their intriguing biological activities. In particular, N-aryl pyridine-2(1H)-one is an important moiety present in biological active compounds such as perampanel and 2-(2-oxo-1-phenyl-5-pyridine-2-yl-1,2-dihydropyridin-3-yl)-benzonitrile. Therefore, a number of synthetic methods has been reported to form C-N bond between 2-pyridones and either aryl halides or aryl boronic acids as a coupling partner. Herein, a mild and efficient method for the synthesis of N-aryl pyridine-2(1H)-one is demonstrated by using diaryliodonium salts as an electrophilic coupling partner at room temperature.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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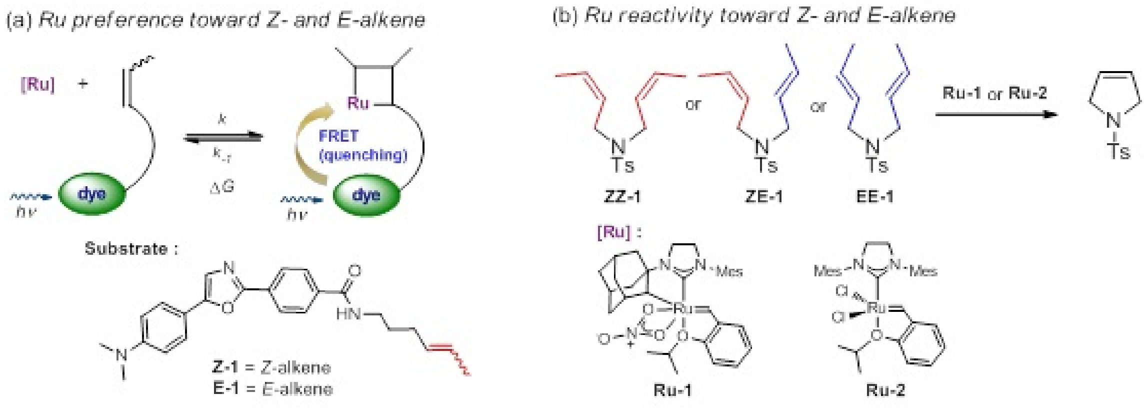
Site-Selectivity in olefin metathesis

이지홍 손정훈*

충남대학교 화학과

The development of z ?selective olefin metathesis catalyst have attracted a lot of attention among the organic chemistry researchers. This situation is based on E-alkene preference of the existing olefin metathesis catalysts. In 2012, the commercially available Ruthenium catalyst (Ru-1) for Z-selective olefin metathesis was developed1. Although this catalyst lead to great advance of methodology throughout the Organic synthesis, the principle of Z-selectivity for Ru-1 have still issues to be identified. In the previous research, Computational calculation based on DFT(density functional Theory) explained the Z-selectivity but exact experimental study currently not exist. So by suggesting thermodynamic and kinetic properties of Ru-1 toward Z- and E-alkenes in formation of the Ru complex (ruthenacyclobutane), we identify the principle of Z-selectivity for Ru-1 in experimental aspect. In addition, we designed intramolecular olefin metathesis of the substrate containing Z,Z-, Z,E-, and E,E-dienes to see whether the preference of Ru-1 to Z-alkene over E-alkene leads to selective reaction for Z-alkene in the reversible reaction. The same experiments with other Ruthenium catalyst (Ru-2: Hoveyda-Grubbs 2nd), which was reported to prefer E-alkene over Z-alkene, were also performed as the comparing experimentsReferences1. Benjamin K. Keitz, Koji Endo, Paresma R. Patel M. B. Herbert, R. H. Grubbs, .J. Am. Chem. Soc. 2012, 134, 693-699;


(a) Ru preference toward Z- and E-alkene
[Ru]
+
k
k-1
ΔG
Ru
FRET
(quenching)
dye
hν
dye
hν
Substrate :
N
O
O
HN
N
Z-1 = Z-alkene
E-1 = E-alkene
(b) Ru reactivity toward Z- and E-alkene
or
or
N
Ts
ZZ-1
N
Ts
ZE-1
N
Ts
EE-1
Ru-1 or Ru-2
N
Ts
[Ru] :
N
N
Mes
O
Ru
O
N
O
O
Ru-1
Mes
N
N
Mes
Cl
Cl
Ru
O
Ru-2

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A study on the synthesis of novel spirohydantoins from ninhydrin

신하윤 송주현 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Hydantoin group can be found in several medicinally important compounds. In pharmaceuticals, hydantoins most often refer to anticonvulsants; phenytoin and fosphenytoin both contain hydantoin moieties and are both used as anticonvulsants in the treatment of seizure disorders. The hydantoin derivative dantrolene is used as a muscle relaxant to treat malignant hyperthermia, neuroleptic malignant syndrome, spasticity, and ecstasy intoxication.In this study, hydantoins are synthesized from ninhydrin and various diamines.Ninhydrin hydrate forms a variety of condensation products with nucleophilic reagents including aromatic amines. A reasonable sequence of events is addition to C=O, substitution of OH and two elimination of water. Of practical important, we report that novel hydantoins are obtained by condensation of KCN and $(NH_4)_2CO_3$ from various ketones.

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코발트 촉매를 이용한 카복실산 유도체의 아마이드 전환 반응

김세은 김수연 김영조* 김민*

충북대학교 화학과

아마이드 결합은 유기합성, 제약, 농화학, 섬유 등에서 중요한 작용기 중 하나인 매우 유용하고 상대적으로 안정한 작용기이다. 아마이드 작용기는 전통적으로 아마이드의 합성은 카복실산 유도체와 아민의 반응, Staudinger 반응, Schmidt 반응, Beckmann 재배열 반응, 알켄 혹은 알카인의 aminocarbonylation 등을 거쳐 합성 된다. 위 반응들은 반응물질을 당량 이상 사용하거나 많은 양의 부산물을 생성하는 단점이 있다. 최근에 루테늄, 알루미늄, 철, 지르코늄, 구리 등의 전이금속을 촉매로 사용하는 다양한 아마이드 합성 조건(예, 환원성 나이트릴의 아민화 반응 [1], 알데히드와 아민의 직접 반응 [2])이 개발되면서 반응 조건이나 합성 가능한 아마이드의 종류가 다양해지고 있다. 본 발표는 상대적으로 다른 전이금속들보다 값이 저렴하고, 공기 및 수분에 안정한 전이금속 촉매인 코발트를 중심 금속으로 사용하는 아마이드 합성 조건을 발표하고자 한다. 최근 본 연구실에서는 코발트/나이트로페놀산 화합물을 촉매로 사용하여 알독심을 1 차 아마이드로 전환하는 반응을 개발하였다. 리간드에 의한 반응 선택성이 주가 된 위 연구에서는 1 차 아마이드는 좋은 수율로 합성할 수 있었지만, 2 차 및 3 차 아마이드는 재배열 반응을 통해 얻을 수 없었다.[3] 이 문제를 해결하기 위하여 아민을 두 번째 반응물로 첨가하여 2 차 및 3 차 아마이드를 코발트 촉매 조건에서 합성하는 조건을 개발할 수 있었다. 여러 종류의 효과적인 아마이드 합성을 위한 반응 조건 최적화 및 결과를 발표하고자 한다.

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Reductive amination of aldehydes by hantzsch ester using N,N'-Diphenyl S-benzyl isothiouronium iodide

이민희 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

To form C-N bond, Reductive amination of carbonyl compounds is one of the most powerful method. Hantzsch ester has proven to be a powerful reductive reagent and solve some of the problems encountered with the traditional reductive reagents. However, this reducing agent was found to be ineffective without catalysis in some cases. Previously, thiourea catalysts were the best in this mechanism. Recently S-benzyl isothiouronium has been reported as more effective catalyst which makes N-H parts more acidic than thioreuas accelerating reaction rate. In this presentation we will discuss the molecular design of isothiouronium compounds and organocatalytic effectiveness.

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Triazole Derivative for OLEDs Red Phosphorescence Host Materials

이다현 장용주 박민주 송동진 강훈민 한진희 **SHAIK BAJI** 이상경*

경상대학교 화학과

Organic light-emitting diodes (OLEDs) have high potential in full-color flat-panel displays and lighting applications. In particular, phosphorescent organic light-emitting diodes (PHOLEDs) are attractive because of their theoretical quantum efficiency can be four times higher than that of the fluorescent based OLEDs. However, high efficiency PHOLEDs are difficult to achieve due to effectively reducing the power consumption and generating emission of different colors. For improving the red host PHOLEDs ability, 1,2,4-triazole derivative was designed. Here in synthesis and physical properties of triazole derivative for OLEDs material was reported. Triazole derivative was synthesized by well known reactions, such as Suzuki reaction, etc. Triazole derivative was confirmed by ESI-Mass, FT-IR, ^{1}H-NMR, ^{13}C-NMR spectroscopy and elemental analysis. The synthesized material has moderate solubility in common organic solvents such as chloroform, methylene chloride and THF. Thermal stability was analyzed by TGA and DSC. Optical and electrochemical properties of the triazole were analyzed by UV-vis absorption spectroscopy and cyclic voltammetry (CV).

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Synthesis and Characterisation of Donor-Acceptor Conjugated Copolymer Contaning Diketopyrrolopyrrole

강훈민 이상경* **SHAIK BAJI** 장용주 송동진 이다현 박민주 한진희

경상대학교 화학과

Recently, diketopyrrolopyrroles have received much attention for their promising application in OTFTs(organic thin-film transistors). Diketopyrrolopyrrole based conjugated copolymers are used as donor and acceptor type materials including a strong electron-accepting and an electron-donating unit. Moreover copolymers showed much higher charge carrier mobility due to strong π-π stacking interaction. Diketopyrrolopyrrole flanked with pyridinyl group as an acceptor was copolymerized with the donor thiophine groups. The synthesized compound was confirmed by FT-IR, ^{1}H-NMR spectroscopy. The molecular weight was determined by gel permeation chromatography. The thermal properties were determined by thermo gravimetric analysis and differential scanning calorimetry (DSC). The optical properties were determined by UV- visible absorption spectroscopy. The electrochemical properties were determined by cyclic voltammeter (CV).

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Synthesis and Characterization Low band gap polymer containing Benzoselenadiazole as Acceptor

한진희 이상경* 장용주 이다현 박민주 송동진 **SHAIK BAJI** 강훈민

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In recent years donor-acceptor based compounds have been most researched for OTFTs. The benzoselenadiazole as an acceptor material was synthesized by the dehydration of 1,2-phenylenediamine in the presence of selenium dioxide. The compound was copolymerized with the donor group 1,2-bis(3-dodecylthiophen-2-yl)ethyne to construct the donor-acceptor material. The synthesized compound was characterized by NMR and the molecular weight was determined by the gel permeation chromatography. The thermal properties were analyzed by TGA and DSC analysis. The electrochemical properties were analyzed by cyclic voltammetry analysis. The optical properties were analyzed by UV-visible absorption spectroscopy. The compound has shown absorption values at 411 nm and 585 nm in solution, while the in the film state the absorption values are red-shifted due to intermolecular interactions and has shown absorption values at 452 nm and 657 nm. The compound has shown less energy band gap at 1.49 ev. The compound has shown the decomposition temperature with 5% weight loss at 352 °C. The HOMO and LUMO values were -5.73 and -4.24 eV, respectively. In the DSC the glass transition temperature was observed at 169 °C. The OTFT characterization is under process.

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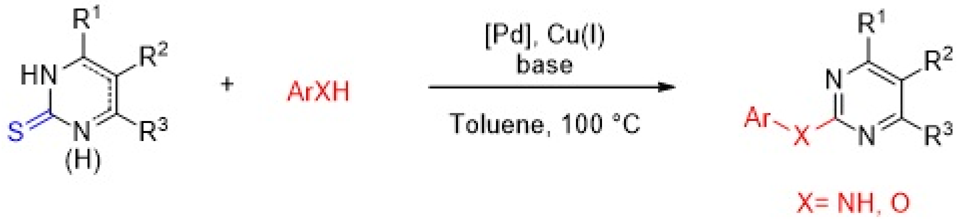
Dehydrosulfurative C-N and C-O Cross Coupling and Concomitant Oxidative Dehydrogenation for General Synthesis of 2-arylaminopyrimidines and 2-aryloxypyrimidines

PHANNGUYENHUUTRONG 이지홍[1] 손정훈[1,*]

충남대학교 화학 생화학과 화학 [1]충남대학교 화학과

Pd-catalyzed carbon-carbon and carbon-heteroatom bond formation methods have contributed to the growing success to organic synthesis in the last two decades. The well-known Liebeskind-Srogl desulfitative carbon-carbon cross coupling protocol, for example, involving the Pd(0)-catalyzed, Cu(I)-mediated coupling of various thioorganics with boronic acids under neutral conditions, has been developed recently. In the context of our interest in the desulfitative reactions, for the first times the novel dehydrosulfurative C-N and C-O cross coupling methods based on the Liebeskind-Srogl and Buchwald-Hartwig reactions have been investigated and successfully applied to a wide range of dihydropyrimidinethione/pyrimidinethione substrates with arylamine derivatives and phenol derivatives from good to excellent yields.



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Selective Phosphorescent Detection of Fluoride by Bis-heteroleptic Ruthenium (II) Complexes

YU SUH YOUNG 홍종인*

서울대학교 화학부

Fluoride (F^-) plays important roles in living bodies including prevention of dental caries (decay) or treatment for osteoporosis. However, a high intake of fluoride can cause fluorosis, which leads to nephrotoxic changes in both humans and animals, and urolithiasis. Therefore, it is needed to develop effective methods that can monitor fluoride ion level.Herein, we designed and synthesized a bis-heteroleptic Ruthenium (II) complex based phosphorescent probe for fluoride by incorporating the reaction site into the luminophor, which exhibits selective phosphorescent responses - decrease of emission intensity and bathochromic shift of emission wavelength - only toward fluoride ion. Furthermore, the phosphorescent probe can be further developed to the ECL(Electrochemiluminescence) probe taking advantage of the electrochemical properties of the ruthenium (II) complexes.

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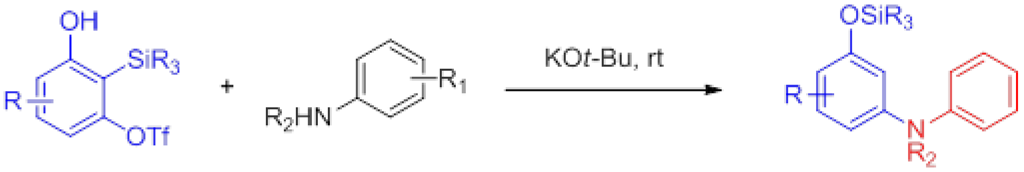
Base-Promoted Benzyne Formation via 1,3-silyl Migration

오인영 박초희 김원석*

이화여자대학교 화학 나노과학과

Benzynes, highly strained and reactive alkynes, are derived form an aromatic ring by removal of two ortho substituents. A number of methods for the preparation of benzyne have been reported and especially, the method using silyaryl triflate in the presence of fluoride source has been employed. Herein, we disclose the design, synthesis and evaluation of just such a new type of benzyne precursor capable of generating highly reactive benzyne intermediate induced via 1,3-silyl group migration on the aryl moiety. This base-pomoted benzyne formation method would be used for the synthesis of 2-aminophenol or acridone derivatives which are the scaffold of some synthetic compounds with various pharmacological activities.



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Synthesis and Characterization of Small molecule Containing Benzoselenadiazole as Acceptor

SHAIK BAJI 이상경* 장용주 이다현 송동진 박민주 강훈민 한진희

경상대학교 화학과

Development of new donor-acceptor based compounds has been one of the major researches in the field of OTFTs and solar cells. The selenium containing benzoselenadiazole as an acceptor has not much studied. The benzoselenadiazole as an acceptor material was synthesized by the dehydration of 1,2-phenylenediamine in the presence of selenium dioxide. Synthesis of small molecules has advantages over polymers in terms of synthesis, purification and reproducibility. Based on this the small molecule was synthesized. The benzoselenadiazole unit was connected to the donor thiophines by Suzuki coupling reaction. In order to lower the LUMO level the electron withdrawing nitrile groups introduced. The synthesized compound was characterized by NMR spectroscopy. The thermal properties were analyzed by TGA analysis. The electrochemical properties were analyzed by cyclic voltammetry analysis. The optical properties were analyzed by UV-visible absorption and PL emission spectroscopy.

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Design and Synthesis of Boron-based Small Molecule Organic Semiconductors

성단비 류가연 김원석*

이화여자대학교 화학 나노과학과

A new A-π-A type small molecules based on thiazole-borane complex (π-spacer) and 2,5-bis(alkyl)-3,6-di(thiophen-2-yl) pyrrolo [3,4-c]pyrrole-1,4(2H,5H)-dione (DPP) derivatives were designed and synthesized employing Pd-catalyzed Stille cross-coupling reaction as a key step. The synthesized thiazole-boron based complex exhibited high electron affinity, which indicates low LUMO level, and chemical stability. Herein, we report the synthetic method for the preparation of thiazole-boron based small molecule organic semiconductors and their application for solar cell.

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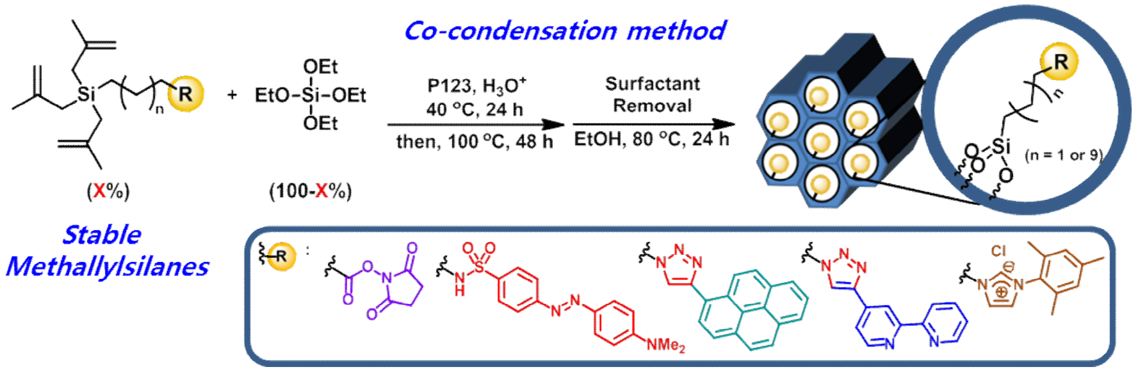
Co-condensation Synthesis of Functionalized Mesoporous SBA-15 Using Trimethallylsilane Derivatives

한예리 전철호*

연세대학교 화학과

The stable trimethallylsilanes are used as a surrogate of alkoxysilanes in this study. Due to their stability, it is convenient to synthesize various functional group-impregnated trimethallylsilanes which are readily purified by column chromatography. In an acidic condition, trimethallylsilane derivatives and TEOS (tetra ethyl ortho silicate) are hydrolyzed to co-condensate to form functionalized SBA-15. As a functional group, fluorophore, chromophore and NHC (N-heterocyclic carbine) ligand for transition metal catalyst are used, and the resulting functionalized SBA-15s are structurally confirmed by TEM, ^{13}C solid state NMR and BET etc. Especially SBA-15 functionalized with amine was utilized as a catalyst for Knoevenagel reaction. In this reaction, different chain length between trimethallylsilane group and amine group was applied for testing the reactivity. For example, undecylamine group-immobilized SBA-15 shows higher reactivity than propylamine-group-immobilized one. In addition, Pd-immobilized SBA-15 through NHC ligand was applied for Suzuki C-C coupling reaction for recycling purpose.



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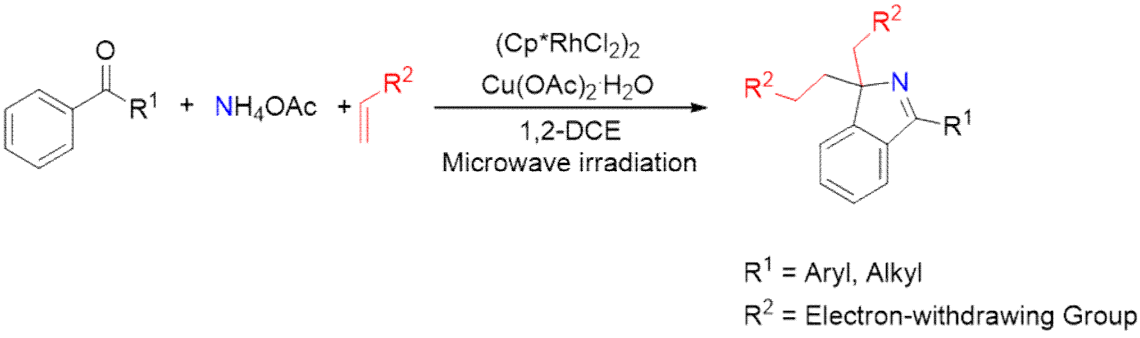
Rh(III)-catalyzed one-pot N-Annulation Reaction of Aryl Ketone with Alkene forming 1*H*-isoindole derivative

이연희 전철호*

연세대학교 화학과

Isoindole derivatives are known to be useful precursor for constructing promising active biological compounds. In this report, we describe Rh(III)-catalyzed one-pot synthesis of 1*H*-isoindole derivatives which have quaternary carbon center from aryl ketones and electron-withdrawing group-substituted alkenes in presence of ammonium acetate as nitrogen source. The reaction takes place at 130 °C for 10 min under microwave irradiation through Rh(III)-catalyzed chelation assisted C-H bond activation and N-annulation to give corresponding 1*H*-isoindole in high yield. This protocol is novel in terms of preparation of N-heterocyclic compounds containing quaternary carbon center, and its advantageous feature includes atom-economy. The proposed reaction mechanism will be discussed.



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Ring constrained beta-hydroxy acid for potent chiral auxiliary resolution

장근혁 최수혁*

연세대학교 화학과

Separation of optically pure compounds is a important process in the production of enentiomerically active drugs.

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Synthesis of Energetic Ring Strained Cyclobutyl Ether Derivatives as Non-Polar Plasticizer

심용균 이창희 김동수 임병욱[1] 임영권[2] 전철호[*]

연세대학교 화학과 [1]국방과학연구소 4본부2부5팀 [2]국방과학연구소 4-2

Recently, development of highly advanced explosive and propellant with plasticizer have been extensively studied. Energetic nitrogen-containing polar organic compounds have been commonly used as a high energetic plasticizer. However, when the explosive performance is enhanced using this polar nitrogen-containing functionality, the explosive becomes unstable and its physical property is changed from native explosive. From this point of view, we have devised cyclobutane-based monoether compounds as new plasticizer candidates since cyclobutane moiety is non-polar and stable organic functional group with high ring-strained energy. In order to find a suitable plasticizer with proper physical property, we determined viscosity, glass transition temperature and thermal decomposition temperature of ether with nonpolar cyclobutyl moieties, and compared them with dioctyladipate(DOA) and isodecyl pelargonate(IDP), widely used non-polar plasticizer.

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A study on the synthsis of 1H-benzo[b][1,4]diazepines with oximes

김건우 이언진 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Benzodiazepines are an interesting class of compounds exhibiting pharmacological properties and in fact, many members of this family are used as tranquilizing or anticonvulsant agents. Traditionally, 1H-benzo[e][1,4]diazepines have been widely used due to their pharmaceutical significance. 1H-benzo[b][1,4]diazepines, however, are not known for any activity even though they are 1H-benzo[b][1,4]diazepine isomers. Therefore in this study, we focus on the synthesis of 1H-benzo[b][1,4]diazepine derivatives and their biological activities. During the course of our study, we have found that dichloramine-T (N,N-dichloro-4-toluenesulfonamide, DCT) can be used as an efficient reagent for the conversion of oxime into the corresponding carbonyl compounds.

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Structure Determination from Powder Diffraction Data of a Hollow Foldecture with Truncated Trigonal Bipyramid Shape

공진택 이희승*

한국과학기술원(KAIST) 화학과

We have reported various 3D shapes of self-assembled structures made with peptide foldamers from the windmill shape and molar tooth shape to rhombic rod shape with anisotropic facet characteristic. Receantly, we found new potential abilities of foldecture in the mechanical properties as well, such as anisotropic shape of micro-sized container by making the hollow cavity inside. At this point, the structure determination of molecular packing structure is essential in order to comprehend its shape and properties of the newly formed foldecture. Additionally, it is expected to play a huge role in designing the original foldecture in future.In this study, the structure of the foldecture made with *N*-Boc-(Aib-ACPC)$_3$-Aib-OBn was successfully solved. At the synchrotron powder diffraction experiment, high-resolution diffracted pattern of caudate trigonal bipyramid foldecture was obtained. The pattern was indexed with a trigonal unit cell in $P3_2$ spacegroup. After the Rietveld refinement, the final molecular packing structure showed good agreement with the obtained pattern, low *R*-factors (R_{wp}=7.99%) values attested the validity of *ab-initio* structure determination from PXRD data. During the procedure, March-Dollase preferred orientation approximation model was applied, considering the Bragg-Brentano geometry of the diffractometer and the particular shape of the foldecture which makes it lies on its side. As refining the March-Dollase preferred orientation parameter (P_{MD}), the direction of the tail was able to designate as [001] direction.

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Synthesis of γ-peptide with Ring-Constrained and Stereochemically Pure Gamma Amino Acid Monomer

정윤식 최수혁*

연세대학교 화학과

Artificial peptides constructed from β- or γ-amino acid residues can adopt protein-like secondary structures. Use of β- and γ-amino acids containing cyclic ring constraints is useful in rigidifying and stabilizing secondary structures.1 However, few studies about γ-amino acid were known compared with that of β-amino acids; difficulty of obtaining stereochemically pure building block and unexpected side reactions during oligomer synthesis.2 Here we describe the preparation of a stereochemically pure γ-amino acid building block and the synthesis of related oligomers. Stereochemically pure γ-amino acid was isolated from racemic mixture by diastereomeric salt formation. Diastereomeric excess was measured by HPLC and proton NMR, relative configuration of racemic mixture monomer and absolute configuration of stereochemically pure monomer were determined by single crystal X-ray crystallography

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Chemosensing and binding of bioactive Fe^{3+} using Vitamin B_6 cofactor derived tripodal receptor in aqueous medium

SAHOO SUBAN KUMAR 최홍진[1,*]

경북대학교 응용화학공학과 [1]경북대학교 응용화학과

AbstractThe recognition of Fe^{3+} ions has attracted significant interest in environmental and biological samples. Deficiency of iron limits oxygen delivery to cells, resulting in fatigue, poor work performance, and decreased immunity and its excessive amounts leads to cellular toxicity with serious diseases such as Alzheimer’s, Huntington’s and Parkinson’s disease. Hence, considerable attention has been focused on the development of selective and sensitive sensors for iron detection. As part of our continuous research on Pyridoxal based chemosensors[1-2] for bioactive ions detection[3], we develop a tripodal Schiff base derived from simple condensation of pyridoxal with TREN for selective detection of the bio-active ion Fe^{3+}. The colour changes from colourless to yellow in aqueous medium along with formation of a new band at ~ 400 nm in the UV-Vis spectra clearly indicates the selective sensing by the developed ligand. Various other analytical tools such as FT-IR and NMR were used to characterise the ligand and to support the mechanistic route of binding interactions. References1.Sahoo et. al., *RSC Adv.*, 2015, 5, 50741-50746.2.Sahoo et. al., *Tetrahedron Lett.* ,2014, 55, 927-930.3.Sahoo et. al., *RSC Adv.* 2014, 4, 1341-1346.

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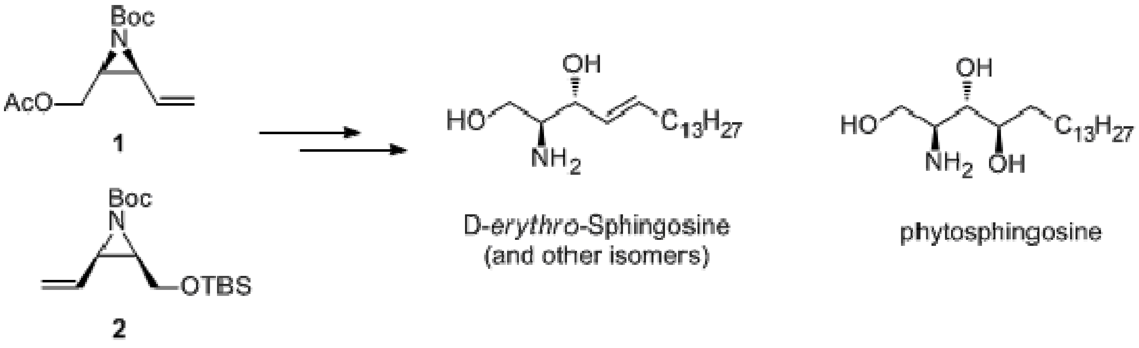
Asymmetric Synthesis of Sphingosines and Phytosphingosine

강한영* 강온유 신미리

충북대학교 화학과

Sphingolipids belong to a large class of natural products which exhibit interesting biological activities in many physiological processes. Sphingosine, the back bone of sphingolipids bears a 2-amino-1,3-diol moiety at the one end. Due the two stereocenters, a total of four isomeric structures become possible although D-erythro-sphingosine is the most abundant form in nature. We have already shown that cis-2,3-bis(hydroxymethyl)aziridine, a meso compound, is easily converted to an enantiomerically pure chiral aziridine by enzymatic desymmetrization. Alkenylaziridines exhibit excellent regio- and stereoselectivity in the ring opening by various heteroatom nucleophiles. An expedient synthetic approach of all diastereomers of sphingosine has been investigated. The selective nucleophilic ring opening of two vinylaziridines (1 and 2) with oxygen nucleophiles led to an expedient synthesis of all possible diastereomeric sphingosines. Furthermore, we have also extended this synthetic route for the synthesis of phytosphingosine.



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Synthesis of 3-Amino-N-substituted-quinazolinone-4(3H)-ones through transamination and ring-formation

김은비 조수경 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Quinazolinone is a well-known heterocyclic compound found in a variety of natural products, synthetic pharmaceuticals and other functional materials. Quinazolinone derivatives have been reported to possess diverse pharmacological properties such as anti-cancer, anti-fungal, anti-bacterial, anti-inflammatory, and antioxidant activities. Recently, the synthesis of 2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids has been described and their catalyst free synthesis in ionic liquids or 2,2,2-trifluoroethanol has also been reported. In this study, we report the reactions of anthraniloyl hydrazine (or salicylamide) and aldehydes with diphenyl phosphate(DPP), cyanuric chloride, tungstosilicic acid and phosphotungstic acid as catalysts. 3-Amino-N-substituted-quinazolinone-4(3H)-ones from anthraniloyl hydrazine was synthesized by the acylation method and imine formation.

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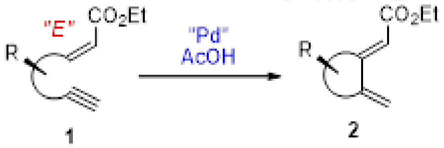
발표코드: **ORGN.P-374**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Palladium-catalyzed Cycloisomerizations of Ethyl (E)-oct-2-en-7-ynoates

고은비 ALKHALAF NORAH SALEH S[1] 오창호[*]

한양대학교 화학과 [1]한양대 대학원 화학

The development of efficient cyclization for 5-membered cycles has been an interesting subject in organic synthesis, because five-membered rings are found in natural products which have a variety of biological activities. In our previous works, palladium-catalyzed cycloreductions or cycloisomerizations have been accomplished by use of various substrates such as 1,6-enynes, 1,6-dienes, and 1,6-diynes. In addition to these, we undertook the reversed substrates in between ene- and yne-group. Herein, we wish to report the palladium-catalyzed cycloisomerizations of ethyl (E)-oct-2-en-7-ynoates.



Scheme1 . Palladium-catalyzed Cycloisomerizations of enynes

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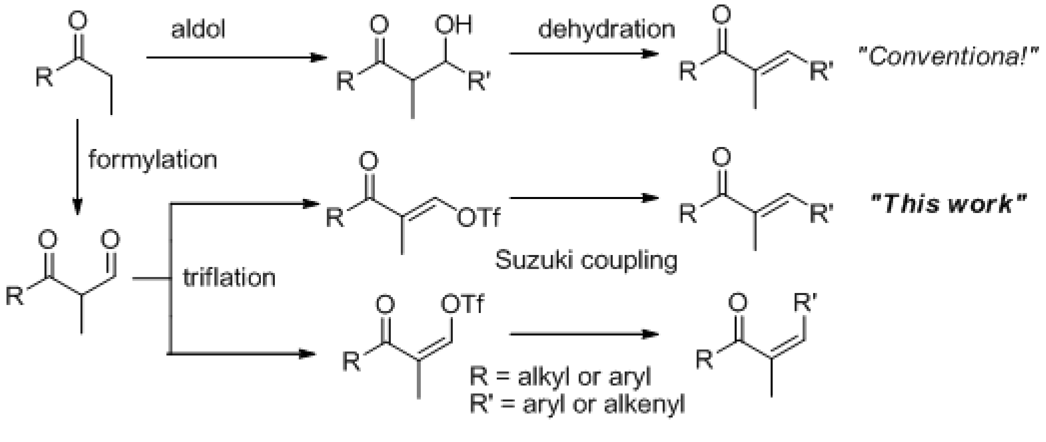
Synthesis of 3-alkyl-2-enones from ketones by formylation, triflation, and Suzuki coupling

이영주 이석창 오창호*

한양대학교 화학과

Synthesis of 3-alkyl-2-enones has long been carried out by means of aldol condensation followed by dehydration. Recently, we developed a stereoselective method leading to various (E)-3-alkyl-2-enones from ketones by three-steps: formylation, triflation, and Suzuki coupling. Compared to conventional aldol/dehydration, this might have an advantage in introducing various alkenyl and aryl groups streoselective manner. And also, the intermediates, β-trifloxyenones might play a key role in various metal-catalyzed couplings. Here we wish to report a preliminary result leading to various (E)-3-alkyl-2-enones from ketones by three-steps: formylation, triflation, and Suzuki coupling.



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Diazotization followed by Intramolecular Cyclization from Pyridinylarylacetates in One-Pot : Synthesis of Pyridoisoindoles

김철의 신서현 이필호*

강원대학교 화학과

Pyridoisoindoles are key priviledged scaffolds in nitrogen-containing heterocyclic compounds, which are widely found in pharmaceuticals, natural products, fluorescent materials, and dyes. Accordingly, development of synthetic methods for preparing pyridoisoindoles having a variety of functional groups represents a considerable task and a significant challenge. Although these functionalizations of pyridoisoindole derivatives have been reported, a limited number of synthetic methods have been described. Thus, a robust synthesis of pyridoisoindole derivatives has been continuously needed. Especially, it is very significant to introduce a wide range of functional groups onto pyridoisoindoles and to prepare 6-ethoxycarbonyl pyridoisoindoles. Moreover, preparation of pyridoisoindole derivatives having other nitrogen heterocycles besides pyridine provides a synthetic challenge.Herein, we have developed a robust synthetic method for a wide range of pyridoisoindoles from pyridinylarylacetates in one-pot through diazotization using TsN_3 and DBU followed by intramolecular cyclization *via* elimination of nitrogen molecule under $Cu(OTf)_2$-catalyzed conditions. Also, the intramolecular cyclization took place efficiently with diazo substrates to furnish pyridoisoindoles in good to excellent yields under metal-free conditions or $Cu(OTf)_2$-catalyzed conditions at room temperature.

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Phosphoryl Alkylindiums and Their Synthetic Application to Arylalkyl Phosphonates *via* Palladium-Cross-Coupling Reactions

김상혁 신서현 이필호*

강원대학교 화학과

Organophosphonate is an essential functional group in synthetic as well as biological chemistry. In synthetic chemistry, it is a starting material for the preparation of alkenes *via* the Horner-Wadsworth-Emmons reaction. In biological chemistry, their distinctive structure and polarity provide them a significant function in pharmaceuticals and agrochemicals. Therefore, a wide range of synthetic intermediates and precursors and biologically active compounds require introduction of a phosphonate group to the molecule. To date, the most conventional approaches for the formation of the P-C (*sp*^{3}) bond are the Michaelis-Arbuzov and Michaelis-Becker reactions. Despite its prevalence, the trivalent phosphorus compounds employed in the Michaelis-Arbuzov reaction have normally low stability and effuse a repulsive odor. The Michaelis-Becker reaction occasionally needs long reaction times and a strong base. Thus, we envisioned that if organometallic reagents having a phosphonate group can be successfully prepared, it will be an efficient synthetic method of functionalized organophosphonates *via* C-C bond-forming reaction. We have developed *in situ* preparation of phosphoryl alkylindiums from the direct insertion of indium with bromoalkyl phosphonates in the presence of CuCl. The Pd-catalyzed cross-coupling reaction of the phosphoryl alkylindium reagents with a number of aryl iodides, bromides, and triflates and vinyl bromide proceeded smoothly to provide the functionalized arylalkyl phosphonates in good to excellent yields. A wide range of functional groups, including ester, ketone, aldehyde, nitrile, nitro, trifluoromethyl, chloride, methoxy, hydroxy, and amino, are tolerable in the cross-coupling reactions. Upon increasing the chain length between the bromide and the phosphoryl group, the directing effect by the phosphoryl group is observed.

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Synthesis of 2-Alkoxyaryl-2-aryl Enamines through Tandem Cu-Catalyzed Cycloaddition and Rh-Catalyzed Alkoxyarylation from *N*-Sulfonyl-1,2,3-triazoles, and Aryl Ethers

신서현 손정유 이필호*

강원대학교 화학과

An efficient synthetic method to a myriad of 2,2-diaryl enamines is developed from Rh-catalyzed arylation of *N*-sulfonyl-4-aryl-1,2,3-triazoles with aryl ethers *via* the elimination of nitrogen molecule. Cu-catalyzed cycloaddition followed by Rh-catalyzed arylation starting from alkynes, *N*-sulfonyl azides, and aryl ethers is also demonstrated for synthesis of 2,2-diaryl enamines in one-pot.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

N-Imidazolylation of Sulfoximines from *N*-Cyano Sulfoximines, 1-Alkynes, and *N*-Sulfonyl Azides

김상혁 최원석 이필호*

강원대학교 화학과

Sulfoximines are significant privileged scaffolds, which are extensively found in bioactive compounds, chiral auxiliaries, and ligands in asymmetric synthesis. In consequence, the development of efficient synthetic approaches for sulfoximines and their functionalizations have been continuously required. In particular, *N*-(hetero)aryl sulfoximines are attractive due to the fact that a multitude of their derivatives exhibited anticancer activity or proved useful as agrochemicals.Recently, a synthetic method using *N*-sulfonyl-1,2,3-triazoles as precursors of α-imino Rh carbenoid has been widely studied. Especially, Fokin and Lee described that Rh-catalyzed reaction of 1,2,3-triazoles with nitriles and bromocyanides afforded imidazoles and 2-bromoimidazoles, respectively. In our continuing studies related to the synthesis of nitrogen heterocyclic compounds using *N*-sulfonyl-1,2,3-triazoles, we envisioned that if *N*-cyano sulfoximines would be used as nucleophile in reacting with *N*-sulfonyl-1,2,3-triazoles, *N*-imidazolyl sulfoximines would be obtained *via* denitrogenative [3 + 2] cycloaddition. Herein, we demonstrate Rh-catalyzed *N*-imidazolylation of *N*-sulfonyl-1,2,3-triazoles with a variety of *N*-cyano sulfoximines for the synthesis of *N*-imidazolyl sulfoximines *via* elimination of molecular nitrogen. Moreover, Cu-catalyzed [3 + 2] cycloaddition followed by Rh-catalyzed *N*-imidazolylation from 1-alkynes, *N*-sulfonyl azides, and *N*-cyano sulfoximines is developed for the synthesis of *N*-imidazolyl sulfoximines in one-pot.

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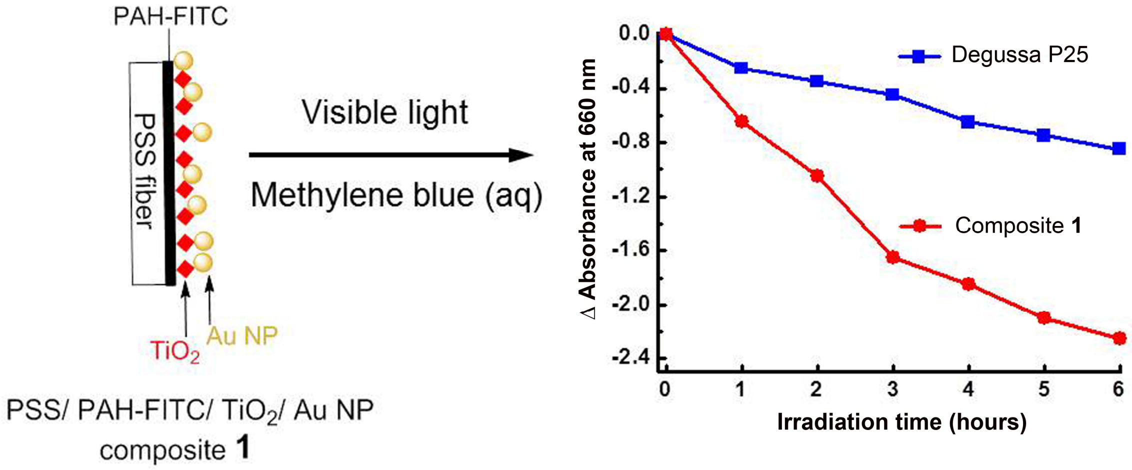
Preparation of Fluorescein-Functionalized Electrospun Fibers Coated with TiO2 and Gold Nanoparticles for Visible-Light-Induced Photocatalysis

하은래 한경엽 최재혁 이정규[1,*] 윤국로[2,*]

경북대학교 화학과 [1]경북대학교 자연대/화학과 [2]한남대학교 화학과

We demonstrated a new type of visible light-induced photocatalyst, comprising fluorescein molecules, TiO2, and gold nanoparticles anchored onto polymer fibers. After the formation of poly(styrene sulfonate) fibers by electrospinning and chemical modification, the active building blocks were coated on the fibers through layer-by-layer deposition processes. The synthesized fiber composite was fully characterized by thermogravimetric analysis, scanning electron microscopy, transmission electron microscopy, FT-IR spectroscopy, contact angle measurement, and fluorescence microscopy. Under sunlight and visible light irradiation, the photocatalytic activity of the fiber composite showed 2-3 times greater photodegradation efficiency for methylene blue than a representative photocatalyst, Degussa P25. Our result shows that the fiber composite, having multiple light-harvesting components, can enhance the photocatalytic efficacy of TiO2-based photocatalysts.


PAH-FITC
PSS fiber
TiO$_2$
Au NP
PSS/ PAH-FITC/ TiO$_2$/ Au NP
composite **1**
Visible light
Methylene blue (aq)
Δ Absorbance at 660 nm
0.0
-0.4
-0.8
-1.2
-1.6
-2.0
-2.4
0
1
2
3
4
5
6
Irradiation time (hours)
Degussa P25
Composite **1**

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Rhodium-Catalyzed Reaction of Azobenzenes with Diazotized Meldrum's Acid

손정유 이은숙 이필호*

강원대학교 화학과

Nitrogen heterocycles are a very significant class of compounds because of their pharmaceutical applications and biological activities. Especially, cinnolin-3(2*H*)-ones are constituents of key privileged azaheterocyclic scaffolds. Thus, the establishment of robust synthetic approaches for affording substituted cinnolin-3(2*H*)-one from easily available compounds has been continuously demanded. Recently, we reported a myriad of C-H activation using phosphoryl group as a directing group and an efficient synthetic method of 2-aryl-2*H*-benzotriazoles from azobenzenes and *N*-sulfonyl azides *via* sequential Rh-catalyzed amidation and oxidation in one pot. In our current program involved with the synthesis of nitrogen heterocycles using azobenzenes, we envisioned that reaction of azobenzenes with diazotized Meldrum's acid would provide a cinnolin-3(2*H*)-one skeleton. Herein, we describe a synthetic method of a wide range of cinnolin-3(2*H*)-one derivatives is developed from the reaction of symmetrical as well as unsymmetrical azobenzenes with diazotized Meldrum's acid *via* Rh-catalyzed C-H alkylation followed by cyclization.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Rhodium-Catalyzed Cyclization of *N*-Sulfonyl-1,2,3-triazoles with Bromocyanides : Synthesis of 2-Bromoimidazoles

이은숙 최원석 이필호*

강원대학교 화학과

Imidazoles are a significant scaffold of azaheterocyclic compounds, which are extensively used in biologically active compounds, in ionic liquids, and as precursors of stable carbene ligands. Consequently, development of synthetic routes of highly functionalized imidazoles from easily accessible starting materials has been a continuing challenge in modern organic synthesis. We developed a synthetic method for 2-bromoimidazoles from Rh-catalyzed cyclization of *N*-sulfonyl-1,2,3-triazoles with bromocyanides. Cu-catalyzed [3+2] cycloaddition followed by Rh-catalyzed cyclization starting from alkynes, *N*-sulfonylazides, and bromocyanides is also demonstrated for *de novo* synthesis of 2-bromoimidazoles in one pot. Moreover, this work was successfully employed to introduce diverse functional groups to the 2-position of imidazoles *via* cross-coupling reaction.

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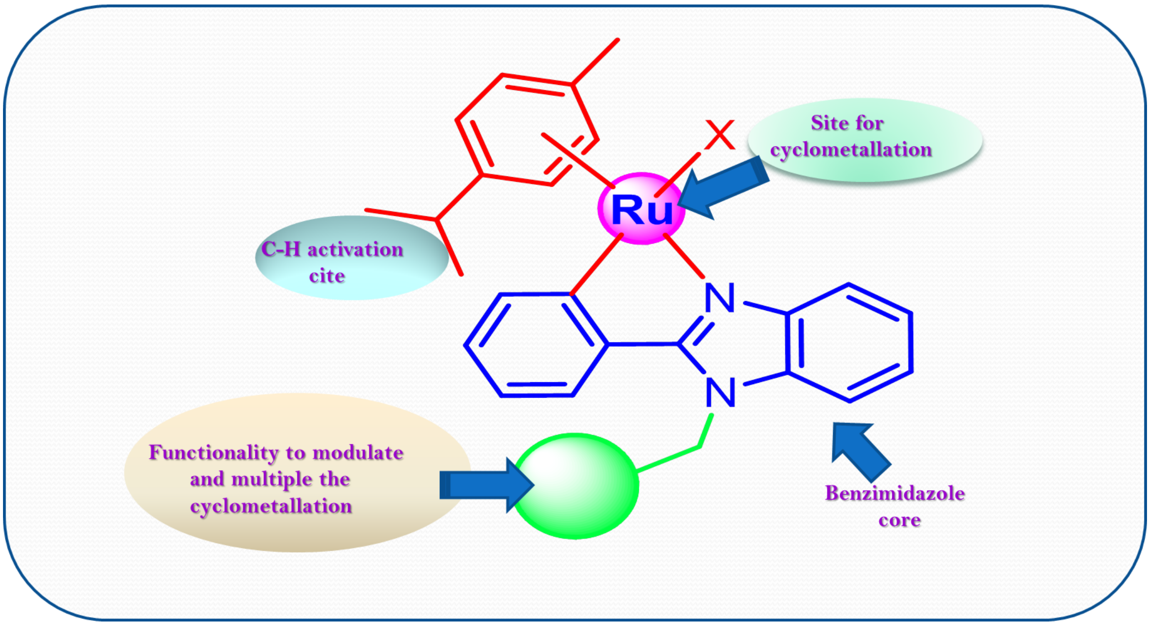
Rational Design and Synthesis of Functionalized Ruthenium(II) Organometallics

PALANIELUMALAI 김동환 지기환*

울산대학교 화학과

Over past few decades the design and synthesis of ruthenacycles got high attention due to their potential in photofunctional materials such as photocatalysts, dye-sensitized solar cells, electroluminescent devices, and sensors. In particular the organometallic based metallacycles are promising candidates for the above mentioned applications. Nevertheless, the biological applications such as cytotoxicity, cellular uptakes, bioimaging studies and anti-tumor properties of the cylometallated organometallic complexes are scare. It is well documented that photophysical properties of metal based supramolecular self-assemblies can be altered by tuning the properties of coordinated ligands. Perpetuation of the research on metal based supramolecular self-assemblies of N-donor ligands, we introduce new flexible di-topic benzimidazolyl core containing ligands, the resent reports are revealed that introducing functionalized benzimidazolyle units in flexible ligand alter the photophysical and antitumor properties of the metallacycles. Herein, we present functionalized phenyl-benzimidazolyl based ditopic ligands and their corresponding ruthenacycles. The ligands and cyclometallated organometallic compounds were characterized by analytical and spectroscopic methods will be presented.


Site for cyclometallation
X
Ru
C-H activation cite
N
N
Functionality to modulate and multiple the cyclometallation
Benzimidazole core

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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Synthesis and Properties 1,2-Bis[N-(N'-alkylimidazolium)]ethane bis(tetrafluoroborate) Salts as a Organic Ionic Plastic Crystal (OIPC) Material

이민재

군산대학교 화학과

1,2-Bis[N-(N'-alkylimidazolium)]ethane bis(tetrafluoroborate) salts were synthesized as organic ionic plastic crystals(OIPCs). The dicationic imidazolium salts show multiple solid-solid phase transitions below their melting temperature. Only the imidazolium salts with ethylene (-CH_2CH_2-) linkage show plastic crystal's properties. The dicationic imidazolium salts with n-undecyl and n-dodecyl termini can be called a "true plastic crystal" by Timmermans' definition. These bisimidazolium salts may be applicable as a solid electrolyte in electrochemical devices such as fuel cells and solar cells.

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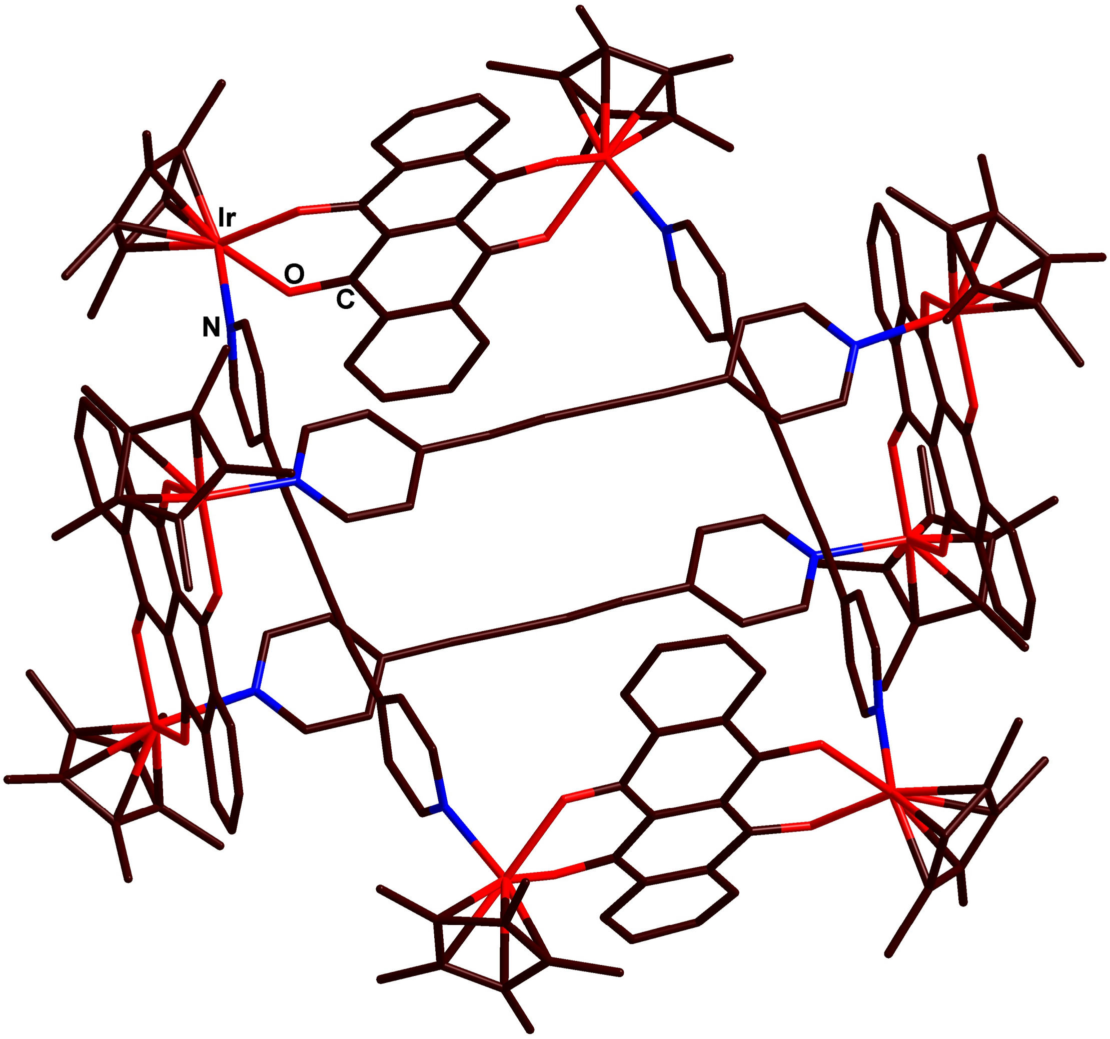
Selective synthesis of iridium based [2]catenane and non-catenanes via coordination driven self-assembly

<u>SINGH NEM</u> 송영호 김태근 지기환*

울산대학교 화학과

Coordination-driven self-assembled container molecules are now well known for guest binding and encapsulation. In last two decades, template effect in the fine-tuning and reorganisation of self-assembly has also been reported. We recently reported the interlocked and non-interlocked molecular dimers self-assembled with tetracene-Ru(II) p-cymene based acceptor and linear dipyridyl donors.1-2 In this poster we will present the self-assembly of similar Ir(III) based catenane and non-catenane rectangles. Template and solvent effect on the catenane and non-catenane structures was compared with known Ru(II) analogues. New self-assembled architectures were fully characterized using various spectroscopic techniques and 2D NMR as well. The structures were confirmed using single crystal X-ray analysis also.ReferencesFig 1. X-ray crystal structures of self-assembled architecture showing “molecule in molecule”1. Vajpayee, V.; Song, Y. H.; Cook, T. R.; Kim, H.; Lee, Y.; Stang, P. J.; Chi, K.-W. J. Am. Chem. Soc. 2011, 133, 19646.2. Lee, H. W.; Elumalai, P.; Singh, N.; Kim, H.; Lee, S. U.; Chi, K.-W. J. Am. Chem. Soc., 2015, 137, 4674.


Ir
O
C
N

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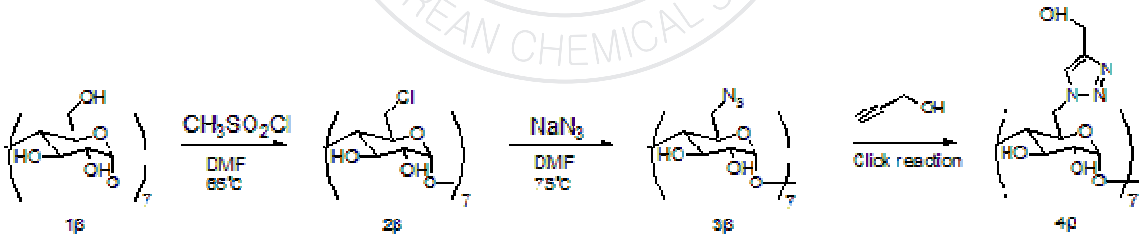
For improving the water-soluble anti-oxidizing material of resveratrol Inclusion Materials Research

이유경 임춘우[*] 남지은 강지혜

한남대학교 화학과

We synthesized Heptakis-(6-chloro-6-deoxy)-β-cyclodextrin and Heptakis-(6-azido-6-deoxy)-β-cyclodextrin, Per-6-(4-hydroxymethyl-1,2,3-triazolmethyl)-6-deoxy-cyclodextrin and characterized through NMR, UV/vis spectroscopy. Then, resveratrol, resveratrol-βCD inclusion compound, resveratrol-HTβCD inclusion compound were measured the absorbance change with time at 254 nm after illumination flashes for 0, 30, 60, 90 miniutes through UV/vis spectroscopy. In addition, resveratrol-βCD complex modeling structure was designed using the gaussian.



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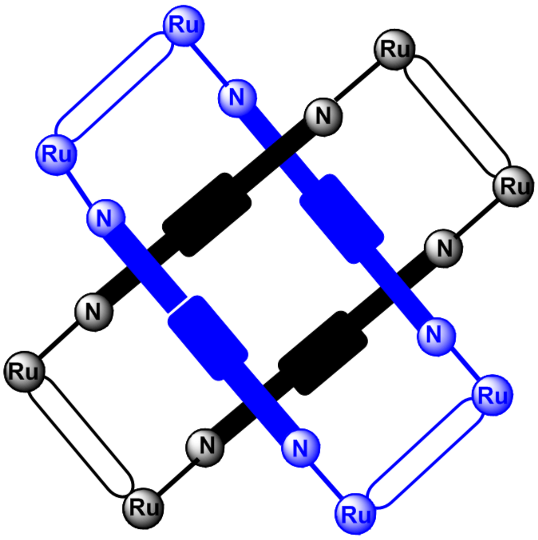
Interlocked and Non-Interlocked Supramolecular Coordination-Driven Self-Assemblies

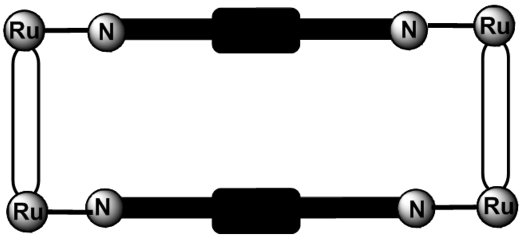
PALANIELUMALAI 송영호 지기환*

울산대학교 화학과

In recent decades, remarkable progress has been made in the synthesis of metal based supramolecular self-assemblies (SCDSs). Curiosity in the interlocked molecular architectures is fast growing not only because of their intriguing structures and topological importance but also because of their potential applications in various fields including biomedical, materials and nano-biotechnological applications. Herein, we reports how interlocked supramolecular self-assembled metalla-[2]catenane and non-catenanes formations varies dependence upon the ligands positional isomers. The organometallic arene-ruthenium based interlocked metalla-[2]catenane and non-catenane architectures were achieved from an arene ruthenium acceptor, respectively based on pyridyl ditopic N-donors.



Metalla-[2]Catenane



Metalla-rectangles

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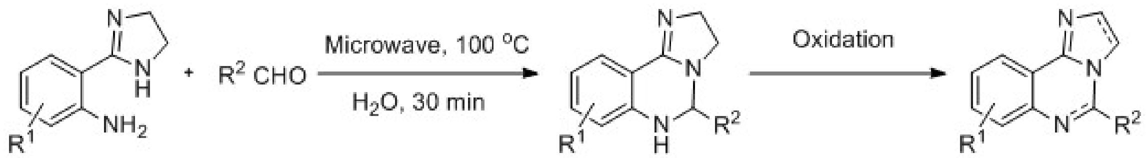
Microwave-assisted Synthesis of 2,3,5,6-Tetrahydroimidazo[1,2-*c*] quinazolines in Water

안수진 염현석[1,*] 류재욱[1,*] 이덕형[*]

서강대학교 화학과 [1]한국화학연구원 친환경신물질 연구센터

Imidazo[1,2-*c*]quinazolines exhibit a tricyclic angularly fused ring system, which combines the biologically valuable imidazole and quinazoline moieties. Variously hydrogenated 5-alkyl- and 5-arylimidazo[1,2-*c*]quinazolines have shown a range of attractive pharmacological activity and insecticidal properties. Cyclometalated late-transitionmetal complexes (Ir or Pt) of imidazo[1,2-*c*]quinazolines have been patented as efficient dopants for organic electroluminescent layers in OLEDs. However, in spite of significant interest in the field, there is still a shortage of mild and reliable synthetic methods for the preparation of selected imidazo[1,2-*c*]quinazoline derivatives. The reported methods are usually indirect, often require the use of drastic conditions, moisture-sensitive poisonous reagents, and/or poorly available precursors, which can limit the overall utility of the process. In this presentation, an efficient synthesis of 5-substituted 2,3,5,6-tetrahydroimidazo[1,2-*c*]quinazolines was elaborated. 2-(2-aminophenyl)-4,5-dihydro-1*H*-imidazole, prepared by phosphorus pentasulfide catalyzed condensation of 2-aminobenzonitrile with ethylenediamine, rapidly reacted with aldehydes to give the corresponding 2,3,5,6-tetrahydroimidazo[1,2-c]quinazolines under microwave irradiation. In addition, we avoid use of toxic organic solvents and lengthy purification steps by water solvent. The precipitates were just filtered, dried, and washed with n-hexane to afford the pure desired products in high yields. An oxidative dehydrogenation with one equivalent of potassium permanganate on silica gel to give 2,3-dihydroimidazo[1,2-c]quinazolines. With two equivalents of potassium permanganate on silica gel, a one-pot exhaustive dehydrogenation to imidazo[1,2-c]quinazolines was accomplished.



R¹
NH₂
N
H
+
R² CHO
Microwave, 100 °C
H₂O, 30 min
R²
Oxidation

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Fluorescent sensor for multi-metals detection using ESIPT

안미란 임치섭 김홍석*

경북대학교 응용화학과

A 2’(2-aminophenyl)thiazole probe 1 was designed to detect transition metal cations in EtOH. Probe 1 detected Zn^{2+} and Cd^{2+} through *“switch-on”* and Co^{2+} and Cu^{2+} through “*Switch-off*” mode of responses. “*On-off*” Fluorescence behavior of probe 1 was modulated through the excited state intramolecular proton transfer (ESIPT) before and after complexation with respective transition metal cations.

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Synthesis of Trisubstituted Pyrazines from Rhodium-Catalyzed Reaction of 2*H*-Azirines with *N*-Sulfonyl-1,2,3-Triazoles

김지은 손정유 이필호*

강원대학교 화학과

Development of a new synthetic method for azaheterocyclic compounds is highly significant in the investigation for new medicines, active pharmaceutical ingredients (API), and fine chemicals. In particular, pyrazine is one of the most representative privileged azaheterocyclic scaffolds, which show cytostatic, antifungal, and antitumor properties and are broadly present in flavorings and alarm pheromones. Accordingly, access to pyrazines from easily available starting materials is highly required. we report herein an efficient synthetic route to a wide range of trisubstituted pyrazines is developed from Rh-catalyzed reaction of 2*H*-azirines with *N*-sulfonyl-1,2,3-triazoles through the elimination of nitrogen molecule and arylsulfinic acid. The present reaction proceeds through formation of *in situ* generated dihydropyrazines.

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Synthesis of *N*-Imidoyl and *N*-Oxoimidoyl Sulfoximines from 1-Alkynes, *N*-Sulfonyl Azides, and Sulfoximines

최원석 서보람 이필호*

강원대학교 화학과

N-Imidoylation of sulfoximines is developed from a Cu-catalyzed three-component reaction from 1-alkynes, *N*-sulfonyl azides, and sulfoximines in THF at room temperature under air. In addition, *N*-oxoimidoylation of sulfoximines is accessed from a Cu-catalyzed three-component reaction from 1-alkynes, *N*-sulfonyl azides, and sulfoximines in THF at room temperature followed by a Cu-catalyzed oxidative reaction at 50 ^{o}C under air, producing *N*-oxoimidoyl sulfoximines.

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Alkenylation of Phosphacoumarins through Aerobic Oxidative Heck Reactions and Their Synthetic Application to Fluorescent Benzophosphacoumarins

김철의 <u>김지은</u> 이필호*

강원대학교 화학과

For several decades, organophosphorus compounds have received attention due to applications in diverse fields such as coordination and materials chemistry, homogeneous catalysis, pharmaceuticals, agrochemicals, additives for polymers, and flame retardants. We were attracted to developing a streamlined method for the synthesis of a myriad of phosphacoumarins and benzophosphacoumarins with the aim of making useful chemical libraries and probes. In addition, the importance of cross-dehydrogenative coupling reactions on Pd-catalyzed direct C-H alkenylation of heteroarenes has been rapidly increased. Herein, we have developed an oxidative alkenylation from the reaction of phosphacoumarins with a wide range of activated as well as non-activated alkenes *via* aerobic oxidative Heck reactions. Moreover, 3-alkenylphosphacoumarins undergo inverse electron demand Diels-Alder reaction with enamines *in situ* generated from ketone and pyrrolidine followed by 1, 2-elimination and a dehydrogenation, affording fluorescent benzophosphacoumarins.

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Synthesis of Acyl Alkenylindium Reagents and Their Application in the Synthesis of (*Z*)-α,β-Unsaturated Ketones *via* Palladium-Catalyzed Cross-Coupling Reaction with Aryl Bromides and Iodides and Alkenyl and Aryl Triflates

최원석 서보람 이필호*

강원대학교 화학과

A synthetic method of acyl alkenylindium reagents was developed from the hydroindation reaction of allenyl ketones with indium and indium chloride in methanol under mild conditions. Their synthetic applications were demonstrated from Pd-catalyzed cross-coupling reactions with aryl bromides and iodides and alkenyl and aryl triflates for the synthesis of (*Z*)-α,β-unsaturated ketones.

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Hemicyanine-based dyes as fluorescent probe for pH changes in vivo and biomarker for mitochondria

이다영 백연주 김현수 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Hemicyanine-based dyes are known for their excellent spectroscopic properties which is high molar extinction coefficient and good fluorescence quantum yield. In this study, we developed a hemicyanine derivatives bearing different substituents. Firstly, we synthesized probe 1 by introducing pyridine moiety onto the hemicyanine skeleton for monitoring pH changes in vivo. Intracellular pH is an important parameter related to cellular behaviors and physiological process. As a consequence, monitoring pH difference is useful for diagnosis of various diseases. The probe 1, ratiometric fluorescence probe, is effective to measure the pH changes in living cells. Secondly, we designed and synthesized probe 2 which is also hemicyanine derivatives bearing aniline moiety for mitochondria imaging. Mitochondria are multifunctional organelles which is associated with energy conversion, apoptosis, and so on. Thus, effective mitochondrial biomarker is essential for study of biological process in mitochondria.

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Copper-Catalyzed Diastereoselective Addition of 1,1-Alkyldiboronates to N-tert-Butanesulfinylaldimines: Synthesis of β-Aminoboronates

박진영 김정훈 조승환*

포항공과대학교(POSTECH) 화학과

The nucleophilic addition of organometallic reagents to imines bearing a chiral auxiliary offers a powerful synthetic strategies with a potential to access to chiral α-branched amines, which are prevalent in natural products, pharmaceuticals, and asymmetric catalysts. Among many strategies available, the diastereoselective addition of organometallic reagents to N-tert-butanesulfinylimines has been considered as one of the most reliable and efficient methods for the synthesis of chiral α-branched amines.] As a result, the development of efficient and selective 1,2-addition to N-tert-butanesulfinylimines procedures has been the focus of intensive research. Despite these significant progress, the development of diastereoselective 1,2-addition using alkylboron reagents remains largely undeveloped.In this poster, we will describe the first chemo- and diastereoselective alkylation reaction of 1,1-alkyldiboronates to N-tert-butanesulfinylaldimines catalyzed by copper salt and achiral bidentate phosphine ligand. The reaction provides β-aminoalkylboronates, which can be further elaborated through oxidation or functionalization to generate synthetically valuable intermediates in organic synthesis.

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Synthesis of terphenyl type unsymmetrical phenylene bis-(1*H*-pyrrole) derivatives from nitroanilines and 1,4-dicarbonyls

배설희 김병효[*] 이병민[1]

광운대학교 화학과 [1]한국화학연구원 계면화학공정연구센터

Pyrroles are useful in many research areas because of its broad applications as conducting polymers, pharmaceutical agents, and building blocks in natural products such as vitamin B12 or hemoglobin. Basic concept of the Paal-Knorr condensation which consists the cyclocondensation of primary amine with 1,4-carconyl compound remains as the most attractive and the easiest method for the synthesis of pyrroles. Also indium metal is widely used for organic synthesis because it has an advantage of low toxicity and good stability in the air or oxygen at room temperature. Herein we report the development of new synthetic strategy to two unsymmetrically substituted phenylene bis-pyrroles using Paal-Knorr condensation reaction followed by reduction-triggered intermolecular heterocyclization starting from nitroanilines with proper 1,4-dicarbonyls. Firstly, Paal-Knorr condensation reaction of nitroanilines with a first 1,4-diketone in the presence of *p*-TsOH was done and it produced nitrophenyl-1*H*-pyrroles in good yield (50-99%). Then, obtained nitrophenyl-1*H*-pyrroles were reacted with the second 1,4-diketones that are different from the first 1,4-diketones of Paal-Knorr reaction in the presence of indium/acetic acid, which resulted in two distinctive bis-pyrrole-containing arenes in reasonable yield (40-92%).

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Regio- and Stereospecific Copper-Catalyzed Allylic Substitution with Readily Accessible 1,1-Alkyldiboronates

김정훈 박진영 조승환*

포항공과대학교(POSTECH) 화학과

Transition metal-catalyzed allylic alkylation represents one of the most powerful tools to form carbon-carbon bonds in organic syn-thesis. Among these reactions, the copper-catalyzed allylic alkyl-ation has become an efficient strategy to provide branched alkyl compounds. While considerable progress has been made in the copper-catalyzed allylic alkylations between allylic electrophiles and organometallics reagents such as dialkylzinc, Grignard, alkyllithium and alkylaluminium, limited functional group compatibility, and air or moisture sensitivity of organometallic reagents often limit their synthetic applications. Moreover, these reactions typically requires cryogenic reaction temperature to achieve a high level of selectivity.In this poster, we will present a copper(NHC)-catalyzed (NHC = N-hetrocyclic carbene) γ-selective allylic alkylation reaction of al-lylic chlorides with 1,1-alkyldiboronates. This methodology represents a rare example of a highly γ-selective allylic alkylation employing readily accessible 1,1-alkyldiboronates and the reaction opens the door for the future development of enantio and diastereoselective variants.

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First total synthesis and evaluation of novel aminophenyl pyridinium-5-(hydroxybenzoyl)-hydrazonomethyl-2-oxothiazol-3-ide(PBHT) derivatives for anticancer activities

민동국 김민규[1] 이가영 정만길*

연세대학교 화학과 [1]연세대학교 화학과

The novel aminophenylpyridinium-5-(hydroxybenzoyl)-hydrazonomethyl-2-oxothiazol-3-ide (PBHT) (1) and its derivatives were totally synthesized for the first time to large scale. The anticancer activity against human colon adenocarcinoma (HCT15) cells of PBHT was approximately four-fold greater than that of 5-fluorouracil, with IC_{50} values ranging from 10.1 to 14.2 *u*M.

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Synthetic approaches to 1-substituted 5-aminotetrazoles

이세진* 배세원[1] 임영권[2]

국방과학연구소 제4기술연구본부 2부 [1]국방과학연구소 4본부 2부 [2]국방과학연구소 4-2

Tetrazoles are attractive core structure for high energy density materials (HEDMs) because of their high nitrogen content and thermal stability despite large positive enthalpies of formation. Also tetrazole derivatives could be utilized for the replacement of carboxylic acids in biologically active compounds. They have been widely applied in research areas of medicinal chemistry because more stable metabolically. Although alkylation reactions between 5-aminotetrazole and halo-alkanes in basic condition are the simplest way for preparation of 1-substituted 5-aminotetrazoles, most of these reactions gave 2-substituted 5-aminotetrazoles as major product. Various reactions are reported to prepare 1-substituted 5-aminotetrazoles by substitutions of 5-halotetrazoles, C-H activation reactions of 5-H tetrazoles, and cyclization reactions of nitriles with azide. However hazardous reagents are used in these reactions. For environment, our goal is that preparation of 1-substituted 5-aminotetrazoles are achieved using less harmful reagents. Herein, we will present some approaches to prepare 1-substituted 5-aminotetrazoles by simple alkylation reaction using amino group of 5-aminotetrazole as a tether.

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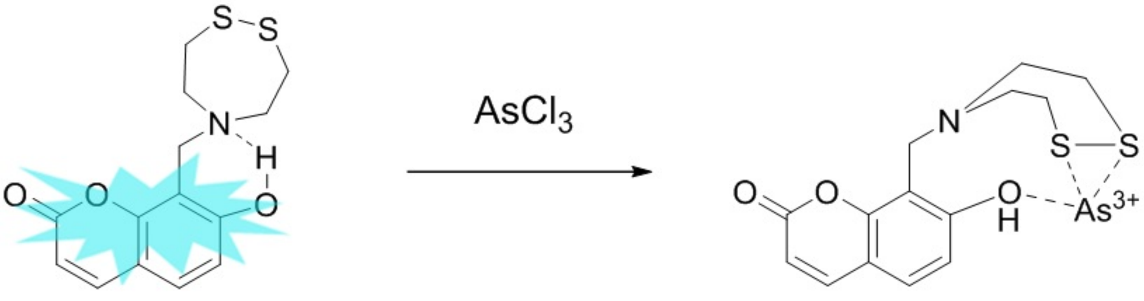
A fluorescent probe for Lewisite simulant

이두희 이동남[1] 홍종인[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Chemical warfare agents (CWAs) are dangerous due to their potential of causing indiscriminate damage with severe chronic effects. So, growing international concern over terrorist attacks using CWA call for affordable, quick, and specific methods of detecting CWA. CWAs are divided into two categories, nerve agents and blister agents. There have been various methods for detection of nerve agents but sensing methods for arsenic-based blistering warfare agents have not yet been reported. Lewisite, an organoarsenic compound, is a blister agent which causes severe skin, eye and mucosal pain and irritation upon exposure. Herein, we report a fluorescence-based sensing of a lewisite simulant, arsenic trichloride (AsCl3), using a 7-hydroxycoumarin containing a dithiazepane moiety. Fluorescence emission of 7-hydroxycoumarin is nearly quenched after the addition of AsCl3 due to heavy atomic effect induced from the arsenic metalloid chelate near the coumarin fluorophore.



1 **1-AsCl$_3$**

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Asymmetric Formal C-H Insertion of Aryldiazoalkanes into the C-H Bond of Aldehydes: Synthesis of α-Tertiary Aryl Ketones

강병철 남동국 신성호 강기태 **JINHUI** 류도현*

성균관대학교 화학과

α-Aryl ketones are useful building blocks for the synthesis of natural products and pharmaceuticals. Due to their ubiquity and utility, the development of transition metal catalyzed α-arylation reactions has attracted considerable attention in past decades. Despite successful pioneering studies on enantioselective α-arylation to generate chiral quaternary carbon centers, catalytic enantioselective construction of α-tertiary aryl ketones has only recently been realized, presumably due to racemization of the product in related transition metal catalyzed α-arylation methods. In this presentation, a novel, catalytic enantioselective route to synthesize a variety of α-tertiary aryl ketones will be discussed. In the presence of chiral (S)-oxazaborolidinium catalyst 1d, the reaction proceeded in good yields (up to 94%) with excellent enantioselectivities (up to 99% ee).

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Synthesis of Fluorenes through Tandem Cu-Catalyzed [3 + 2] Cycloaddition and Rh-Catalyzed Denitrogenative Cyclization in a 5-*exo* Mode from 2-Ethynylbiaryls and *N*-Sulfonyl Azides

서보람 김철의 이필호*

강원대학교 화학과

Fluorenes have attracted a great deal of attention due to their optical and electronic properties and their function as π-conjugated materials. They have been widely used as significant privileged structure in a myriad of areas such as optical agents, dyes, organic transistors, and light-emitting devices. Hence, an efficient synthesis of fluorene and its derivatives from easily available compounds has been continuously required. Especially, it is very important to prepare selectively unsymmetrically substituted fluorene derivatives and to introduce substituents at the C-9 methylene bridge of the fluorene moiety without use of base.We report an efficient synthetic method of a wide range of unsymmetric fluorenes having enamine moiety at C-9 methylene bridge from *N*-sulfonyl-4-biaryl-1,2,3-triazole derivatives *via* Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode. Rh-catalyzed denitrogenative cyclization followed by catalytic hydrogenation produces the aminomethyl-substituted fluorenes in a one-pot. Moreover, this protocol can be applied the synthesis of fluorenes *via* tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode starting from 2-ethynylbiaryls and *N*-sulfonyl azides in a one-pot.

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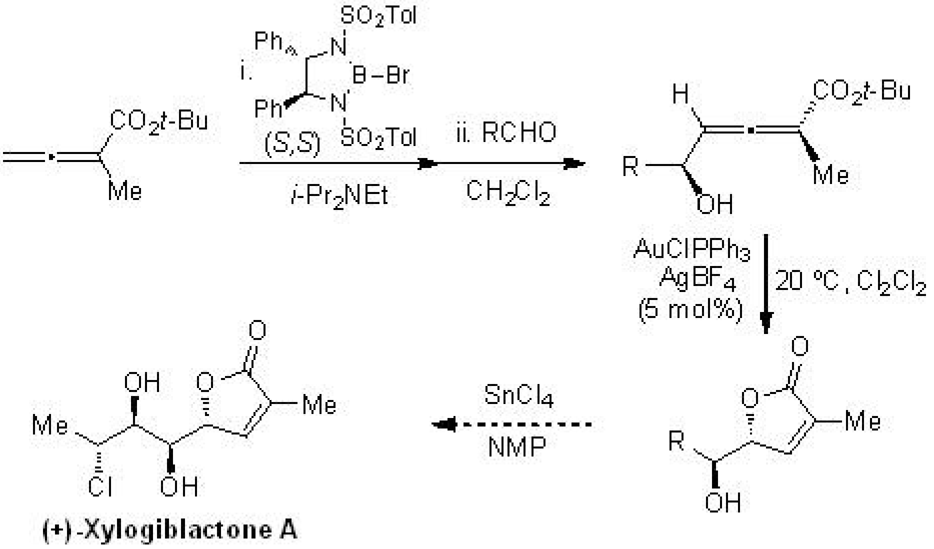
Governing Factors for Gamma-Selective Route for Asymmetric Aldol Reaction of Allenoates and Their Synthetic Applications

이은혜 유찬모*

성균관대학교 화학과

As part of our investigations utilizing allenoates as versatile substrates for asymmetric carbonyl additions, we present herein our discovery of control elements to regulate selective formation of gamma-addition adduct from allenoates to establish axial and center chiralities during the reaction, which allows in good yields with high levels of stereoselectivity as shown following Scheme. We will present regulation factor for reactions and synthetic applications including gold catalyzed cyclization and synthetic studies to (+)-xylogiblactone A will also be discussed.



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Asymmetric Catalytic C-H Insertion Reaction of Diazoamides Using Chiral Lewis Acid Catalyst

신성호 백은희 심수용 김태형 정현실 김재연 김승태 류도현*

성균관대학교 화학과

C-H insertion reaction, a Lewis acid catalyzed reaction of alkyl diazoesters with aldehydes, is a powerful synthetic method to construct β-keto carbonyl compounds, which have been utilized in the synthesis of natural products. An asymmetric variant of this transformation was previously effected using the chiral-auxiliary-based approach. Also catalytic C-H insertion reaction was developed using chiral N,N’-dioxide?scandium(III) complexes., A successful example of catalytic asymmetric C-H insertion reaction of α-alkyl diazoesters with both aromatic and aliphatic aldehydes was recently reported by our group. As an application of this synthetic method, chiral α-aryl-β-hydroxy amides were prepared by the following sequential reactions; selective C-H bond insertion reaction and carbonyl reduction. Using this methodology, optically active aldol-type compounds were obtained in good yield, high enantioselectivity and excellent diastereoselectivity.

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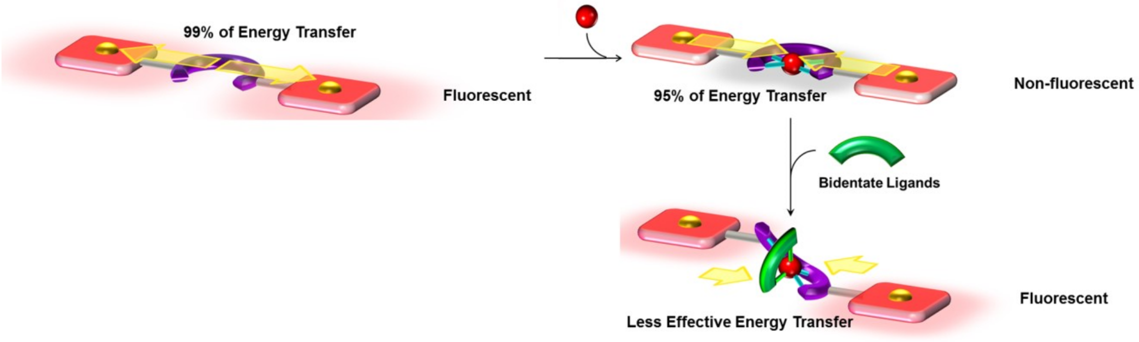
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Porphyrin Molecular Tweezer Having Forward and Backward Energy Transfer

윤홍식 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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발표분야: 유기화학

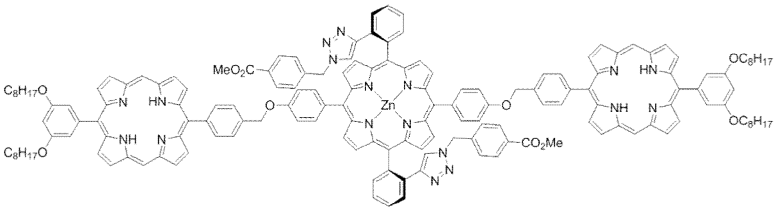
발표종류: 포스터, 발표일시: 목 11:00~12:30

Guest-induced Switching of Energy Transfer in a Porphyrin Triad

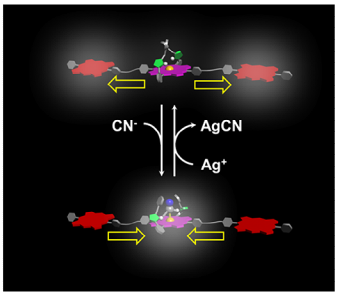
임다정 윤홍식 장우동*

연세대학교 화학과

Natural photosynthetic light-harvesting systems have not only high efficient in energy transfer but also continuous conversion of light energy to other forms. Natural light-energy conversion is initiated by photon absorption of complex molecular assemblies called light-harvesting antenna complexes (LHC). Well-ordered three-dimensional multiporphyrin arrays in LHC facilitate effective photon capture and energy migration to the reaction center, which is composed of a non-covalently associated pair of chromophore units. Based on the process of natural photosynthetic systems, many chemists have reported highly efficient energy transfer. However, few studies have been conducted to control energy transfer pathway by guest binding.In this study, triazole-bearing porphyrin triad ($P_{Zn}Tz$-$2P_{FB}$) consists of central zinc porphyrin ($P_{Zn}Tz$) and two freebase porphyrin wings (P_{FB}). $P_{Zn}Tz$-$2P_{FB}$ exhibited unique photoluminescence switching phenomena by guest binding. As a result of fluorescence spectroscopy, $P_{Zn}Tz$-$2P_{FB}$ exhibited the emission of freebase porphyrin regardless of excitation wavelength, and this result suggests that effective energy transfer takes place from P_{Zn} to P_{FB}. After the addition of cyanide, emission spectrum of $P_{Zn}Tz$-$2P_{FB}$ was consistent with the emission of CN^- complex of P_{Zn} whether P_{FB} or P_{Zn} excitation.



$P_{Zn}Tz$-$2P_{FB}$



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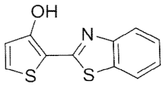
Fluorescent emission according to solvent polarity of oligothiophene functionalized with benzothiazole

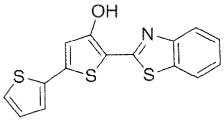
홍경임 장우동*

연세대학교 화학과

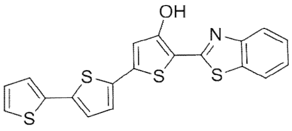
Excited State Intramolecular Proton Transfer (ESIPT) has attracted much attention due to applications for molecular probes, luminescent materials, molecular logic gate, bioimaging etc. ESIPT molecules exhibit different fluorescent emissions via tautomerization depended on solvent polarity. The most remarkable property of ESIPT is large stoke shift, which avoids self-absorption. We have synthesized a series of ESIPT molecules, which have mono-, bis-, tri-oligothiophene with benzothiazole (1T-HBT, 2T-HBT, and 3T-HBT respectively). As the number of thiophene moieties increasing, the fluorescent emission bands were shifted to longer wavelength. 2T-HBT exhibited remarkable solvatochromism; green emission in non-polar solvent and blue emission in aprotic solvent. 2T-HBT-OMe didn`t show fluorescent emissions change in neither non-polar nor polar solvent. These results demonstrated that ESIPT affected emission change of 2T-HBT. Detailed aspect of this system will be reported in the symposium.



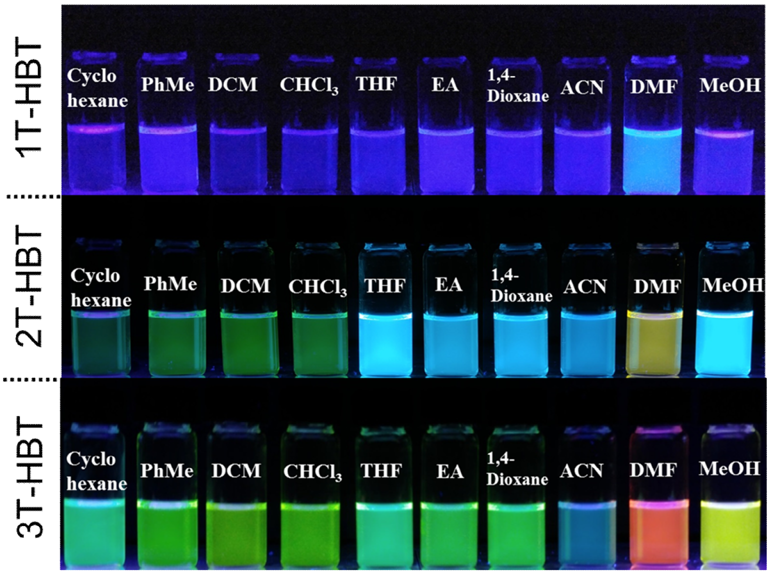
1T-HBT



2T-HBT



3T-HBT



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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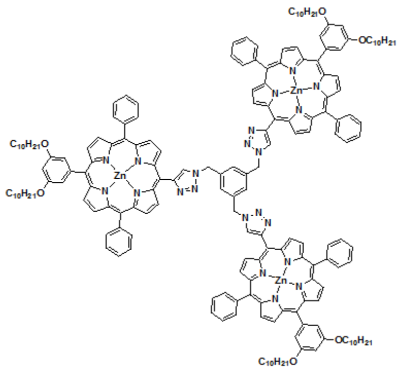
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

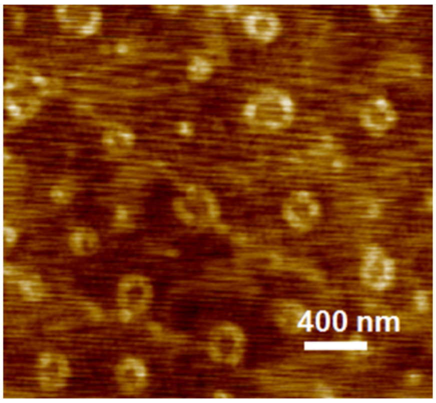
Supramolecular Assembly of Triazole-containing Tripodal Porphyrins

이다정 김주호 장우동*

연세대학교 화학과

Supramolecular polymer has been received much attention due to remarkable structural properties and functions as materials. We synthesized a new type of zinc porphyrin tripod prepared by Cu(I)-catalyzed click reaction and characterized by ^{1}H NMR, and MALDI-TOF-MS analysis. We investigated reversible Soret and Q band shift behaviors in toluene upon heating and cooling processes. On the other hand, tripod porphyrin in THF or demetallized tripod compound did not exhibit any notable phenomenon upon thermal stimulus. The tripod compound showed toroidal structures on HOPG substrate. Finally, we applied this system to isodesmic aggregation model driven by metal coordination with triazole moieties.The tripod formed 2:3 host-guest complex with 4,4'-bipyridyl, and it was confirmed by spectroscopic titration. The detailed aspect of the metal-coordination system of porphyrin tripod will be reported in the conference.





AFM images of toroidal structures obtained by the evaporation of zinc porphyrin tripod (4 μM) in toluene.

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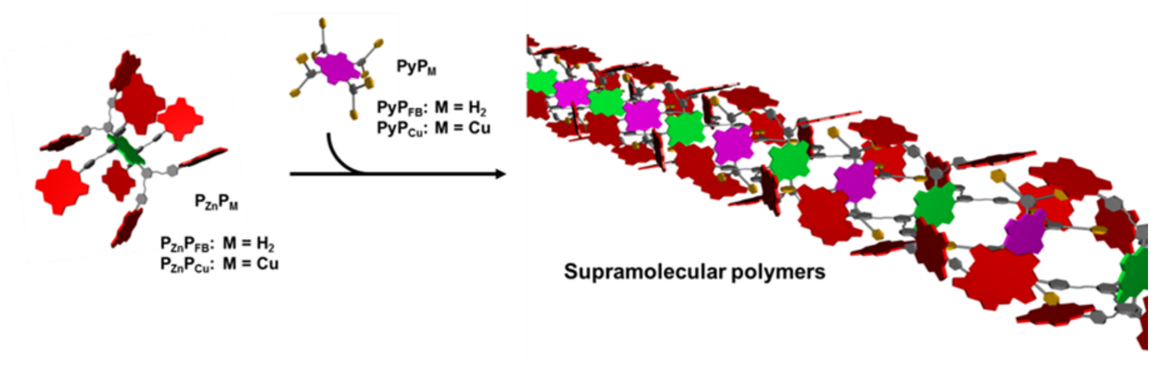
Fibrous Supramolecular Polymer Formed from Artificial Light-Harvesting Multiporphyrin Dendrimer and Multipyridyl Porphyrin

이호수위 김주호 장우동*

연세대학교 화학과

We report the formation of supramolecular coordination polymers formed from multiporphyrin dendrimers $P_{Zn}P_{M}$ ($M=H_2$, Cu) composed of the focal freebase porphyrin or cupper porphyrin with eight zinc porphyrin wings, and multipyridyl porphyrins PyP_{M} ($M=H_2$, Cu) with eight pyridyl groups, through multiple axial coordination interactions of pyridyl groups to zinc porphyrins. UV/Vis absorption spectra were recorded upon titration of PyP_{FB} to $P_{Zn}P_{FB}$. Differential spectra, obtained by subtracting the absorption of $P_{Zn}P_{FB}$ without guest addition as well as the absorption of $P_{Zn}P_{FB}$, exhibited clear isosbestic points with saturation binding at 1 equivalent addition of PyP_{FB} to $P_{Zn}P_{FB}$. Job's plot analysis also indicated 1:1 stoichiometry for the saturation binding. The apparent association constant between $P_{Zn}P_{FB}$, and PyP_{FB}, estimated by isothermal titration calorimetry (ITC), was high enough for fibrous assemblies to form at micromolar concentrations. The formation of a fibrous assembly from $P_{Zn}P_{FB}$, and PyP_{FB} was visualized by atomic force microscopy (AFM) and transmission electron microscopy (TEM). When a 1:1 mixture solution of $P_{Zn}P_{FB}$, and PyP_{FB} in toluene was cast onto mica, fibrous assemblies with regular height (ca. 2 nm) were observed. TEM images obtained from 1:1 mixture solution of $P_{Zn}P_{FB}$ and PyP_{FB} in toluene clearly showed the formation of nanofibers with a regular diameter of ca. 6 nm. Fluorescence emission measurement of $P_{Zn}P_{M}$, indicated efficient intramolecular energy transfer from P_{Zn} to the focal P_{FB} or P_{Cu}.


$P_{Zn}P_M$
$P_{Zn}P_{FB}$: M = H_2
$P_{Zn}P_{Cu}$: M = Cu
PyP_M
PyP_{FB}: M = H_2
PyP_{Cu}: M = Cu
Supramolecular polymers

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Suzuki reaction using volatile bis(β-ketoiminate) Pd(II) complexes

정명진 박찬필*

충남대학교 분석과학기술대학원

Volatile Pd(β-ketoiminate)2 catalysts, with palladium(II) strongly chelated by two bidentate ligands, demonstrated excellent stability and catalytic activity for prolonged use in Suzuki-Miyaura reactions (up to 99% yield with 0.0005 mol% catalyst). They tolerated a wide range of temperatures (rt~170 oC) and various solvents inclusive of water.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of relatively long PNA oligomer using fully protected PNA oligo-blocks

윤창수 김은택 홍인석*

공주대학교 화학과

Traditionally, peptide nucleic acid (PNA) oligomers have been synthesized using Fmoc-PNA monomers by the solid phase peptide synthesis (SPPS). However, in case of relatively long PNA oligomer, the total synthetic yields of oligomer are not good, so it requires a lot of time and money for further purification. In order to overcome these problems, the long target PNA oligomer was divided into the several blocks. After each fully protected PNA block was synthesized separately, those fully protected PNA blocks were assembled by SPPS for target PNA oligomer. As a result, 15-17mer PNA oligomer has been synthesized in good yields by 3 to 4 times coupling reactions by using these PNA blocks.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Photocatalytic Trifluoromethylation/1,2-Rearrangement Sequences for the Synthesis of CF_3-Substituted Cyclic Ketones

서창원 김대영*

순천향대학교 화학과

A visible-light-mediated photocatalytic ethoxycarbonyldifluoromethylation/1,2-carbonmigration of alkenols is described. This approach provides a mild and operationally simpleaccess to the synthesis of difluoralkyl-substituted cyclic ketones via difluoralkylation and 1,2-carbon migration of 1-(1-arylvinyl)cyclobutanol derivatives.

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Catalytic Asymmetric Conjugate Addition of α-Fluoro β-ketophosphonates to Nitroalkenes

정현정 김대영*

순천향대학교 화학과

The catalytic enantioselective conjugated addition reaction of α-Fluoro β-ketophosphonates to nitroalkenes promoted by chiral catalysts is described. Tratment of α-Fluoro β-ketophosphonates with nitroalkenes under mild reaction conditions afforded the corresponding Michael adducts containing fluorinated quaternary stereogenic center with excellent enantioselectivity (up to >99% ee).

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Cross-dehydrogenative coupling reactions of tetrahydroisoquinolines with β-keto acids

권수진 김대영*

순천향대학교 화학과

An efficient methodology for the functionalization of sp^3 C-H bond adjacent to nitrogen has been developed utilizing visible light-induced photoredox catalysis. Through optimization ofsolvent and light source, the reaction can be rapidly achieved to provide the desired product under mild reaction conditions.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Catalytic asymmetric cross-dehydrogenative coupling of β-ketoesters and xanthene

김문용 김대영*

순천향대학교 화학과

Catalytic asymmetric cross-dehydrogenative coupling reaction (CDC reaction) has attracted great attention because it provides efficient methods to construct versatile and useful building blocks. We wish to develop a catalytic asymmetric CDC reaction of α-substituted β-etoesters with xanthene in the presence of air- and moisture-stable chiral palladium complex. By using a chiral palladium complex, good yields and excellent enantioselectivities were achieved for various optically pure xanthene derivatives bearing a quaternary stereogenic carbon center.

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Asymmetric Conjugate Addition of α-Substituted Cyanoacetates to Maleimides Catalyzed by Binaphthyl-Based Thiourea

장희승 김대영*

순천향대학교 화학과

Substituted succinimides are valuable synthetic targets and important structural scaffolds and precursors of biologically interesting substances. We wish to report the asymmetric Michael addition of α-substituted cyanoacetate to maleimides catalyzed by chiral binaphthyl-based thiourea. In the presence of bifunctional tertiary amine-thiourea catalysts, succinimides bearing vicinal quaternary-tertiary stereocenters adducts were obtained in good yields, enantioselectivities, and diastereoselectivities

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은을 이용한 브로모아렌의 선택적 카복실화 및 수산화 반응 연구

유광호 김민*

충북대학교 화학과

전이금속을 이용한 유기 화합물의 작용기 변환은 유기 합성 및 유기 합성 방법론 연구에서 중요한 과제이다. 특히 새로운 탄소-탄소 골격을 형성하거나 새로운 탄소-질소, 탄소-산소 결합 등을 원하는 위치에 선택적으로 형성하기 위한 연구가 다각도로 진행 되고 있다. 본 발표에서는 다른 후전이금속 촉매들에 비하여 상대적으로 손쉽게 구할 수 있는 은을 매개로 하여 브모로아렌 화합물을 새로운 작용기를 가지는 화합물로 전환한 연구를 논의하고자 한다. 우선, 당량 수준의 은을 이용한 카복실화 반응을 통해 브로모 그룹의 위치에 에스터 그룹을 효과적으로 도입할 수 있다. 여러 위치에 다양한 종류의 치환체를 가진 에스터를 도입할 수 있었으며, 반응 조건의 변화를 통해 카복실화 반응과는 별도로 브로모 그룹을 수산화기로 선택적으로 전환할 수 있다. 반응 조건의 조절에 따른 생성물의 조절과 다양한 기질 선택성에 대한 연구 결과를 발표하고, 본 반응을 수행하기 위해 필수적인 배위기의 효과도 다룰 것이다. Acknowledgement: 본 연구는 교육부와 한국연구재단의 지역혁신인력양성 사업으로 수행된 연구 결과임.(과제번호 2014H1C1A1066874).

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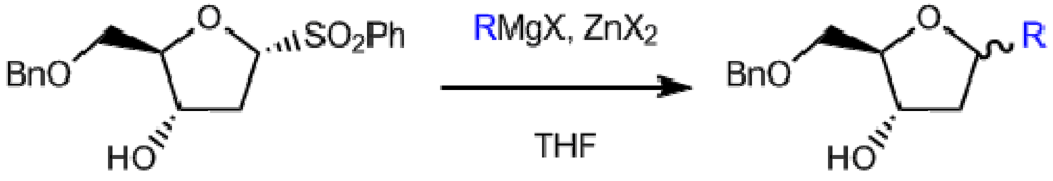
O-glycosylation & C- glycosylation of 2-phenylsulfonyl cyclic ethers

김윤정 이희윤*

한국과학기술원(KAIST) 화학과

Nucleosides are important building blocks in nature and thus frequently served as synthetic target. In addition to nuclesides, 4-membered ring to 6-membered ring system are found at the core of many pharmaceutically active compounds and that significant research effort has been expanded to gain synthetic access to natural products and non-natural analogs. Since we have developed a selective synthesis of cyclic ethers from intramolecular cyclization of epoxy sulfone, functionalization of the sulfones of the products for preparation of natural products and non-natural products also studied. The scope and limitation of the stereoselective reaction and the functionalization of the sulphones using Grignard reagents or alkoxides with/without zinc salts will be presented.



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발표종류: 포스터, 발표일시: 목 11:00~12:30

Hybrid DFT B3LYP Study of Fifteen C20Br3 Regioisomers

이기학* 안영지[1]

원광대학교 화학과 [1]원광대학교 바이오나노화학부

The hybrid density-functional (B3LYP/6-31G(d,p)) method was used to analyze the addition effect on the C20 cage based on calculation of fifteen C20Br3 regioisomers. All were geometrically optimized without constraints. The results suggest that the cis-1 cis-1 cis-2 regioisomer is the most stable isomer, which implies that a bonding exerts a stronger effect on the relative energies of them than long-range interactions. Here, we suggest how to comprise the bonding, by using the orbital interaction.

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Combinatorial dansyl library and its applications to pH-responsive probes

홍성철 Murale Dhiraj[1] 이준석[2,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 분자인식연구센터 [2]한국과학기술연구원(KIST) 분자인지연구센터

1-Dimethylaminonaphthalene-5-sulfonyl chloride, called “dansyl chloride”, is a non-fluorescent reagent that can react with primary amines to produce sulfonamide fluorescent adducts with a large Stokes shift. Since its development by Weber in 1951, dansyl chloride has been widely applied as a chromatographic derivatization reagent to determine N- terminal amino acids, proteins, neurotransmitters and tissues. Despite these applications, studies on combinatorial chemistry, which is a powerful tool to find novel hit compounds for library of dansyl derivatives, are still scarce in literature. Herein, we report the first 48-membered, dansyl-based, combinatorial fluorescent library. From the electronic and structural properties of the probes, we analyzed their optical properties and chemical yields, with an average of 49 %. The molecules were examined for their pH responses, and DS-2 and DS-45 showed blue-shifts, whereas DS-7 and DS-40 showed red-shifts in wavelength with increasing pH. Finally, cell permeability was investigated by treating SNU-2292 cells. Our results demonstrate the potential application of this library in biosensors, bio-imaging and pH indicators.

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Cage volumes and relative stabilities of C20Cl3 regioisomers by the hybrid density-functional B3LYP method

이기학* 권희영[1]

원광대학교 화학과, 나노과학기술연구소 [1]원광대학교 바이오나노화학부

We performed full-geometry optimizations of 15 C20Cl3 regioissomers which are geometric isomers, by using the hybrid density functional (B3LYP/6-31G(d, p) method. We obtained the total energies and volume changes of them. Our results suggest that the order of thermal stability for regioisomers is the same to the order of the HOMO-LUMO gap for them, which implys the kinetical stability.

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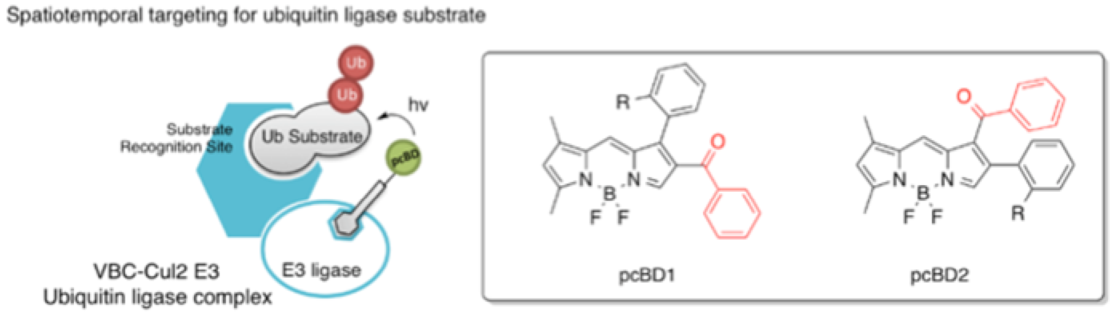
Rational design of a photo-crosslinking BODIPY for *in situ* protein labeling

Murale Dhiraj 홍성철[1] 이준석[2,*]

한국과학기술연구원(KIST) 분자인식연구센터 [1]과학기술연합대학원대학교(UST) 생물화학 [2]한국과학기술연구원(KIST) 분자인지연구센터

Photo-crosslinking agents have emerged as critical tools to investigate protein-protein interactions in complex proteome, but there are few photocrosslinkers available at the moment. Here, we report the first rational design of a photo-crosslinking BODIPY fluorophore (pcBD) and its biological application for biomolecule labeling in a spatiotemporally controlled manner. As a photosensitizing functional motif, the aryl ketone group was incorporated into BODIPY fluorophore, and series of proteins were labeled by pcBD compounds upon UV irradiations. Particularly, these probes could crosslink proteins under both 254 nm and 365 nm UV lights, though they generally exhibited high crosslinking efficiency under 254 nm light conditions. The chief advantage of this BODIPY-benzophenone conjugate system for photo-activated protein labeling is the capability to attach BODIPY fluorophore at any kinds of target proteins depending on the spatial vicinity. Here we chose ubiquitin ligase complex as a model system since several enzymes tightly cooperate to tag substrate proteins with ubiquitin during the ubiquitination process. We have synthesized a photo-affinity probe, pcBD-E3binder, by conjugating E3 ligase binding peptide and BODIPY-benzophenone conjugate. As a result of this experiment we proved the utility of photo-crosslinking fluorophore for spatiotemporal protein labeling in complex mixtures. In our future work we want to use this BODIPY-benzophenone conjugate probe to tag and identify the substrates for ubiquitin ligases along with their binding partners.



Spatiotemporal targeting for ubiquitin ligase substrate

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Catalytic recycle of rGO/AuNP for 4-NP reduction reaction using continuous flow system

송주하 박찬필*

충남대학교 분석과학기술대학원

AuNPs are the most stable metal nanoparticles, and can be applied to catalysis. In this reasearch, rGO/AuNP was assembled by using phase transfer method. The rGO/AuNP exhibited a good catalytic activity for reduction of 4-nitrophenol(4-NP). Reaction was confirmed using microreactor can be continuolusly progressed. rGO/AuNP can reusable, we introduced catalyst recycle system and successfully implemented.

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Chemo-Enzymatic Approach for the Synthesis of 1,11-Dicarboxylic Acid from Ricinoleic Acid

박현정 권용억*

이화여자대학교 화학.나노과학과

A practical chemo-enzymatic synthetic method for 11-hydroxyundecanoic acid and 1,11-undecanedioic acid from ricinoleic acid (12-hydroxyoleic acid) was investigated. Biotransformation of ricinoleic acid into the corresponding ester via 12-ketooleic acid was driven by recombinant *Escherichia coli* cells expressing an alcohol dehydrogenase from *Micrococcus luteus* and the Baeyer?Villiger monooxygenase from *Pseudomonas putida* KT2440. The carbon-carbon double bond of the ester was chemically reduced, and the ester bond was hydrolyzed to afford n-heptanoic acid and 11-hydroxyundecanoic acid, which were converted into other related derivatives. For example, 11-hydroxyundecanoic acid was transformed into 1,11-undecanedioic acid under fairly mild reaction conditions. Whole-cell biotransformation at high cell density (i.e., 20 g dry cells/L) allowed the final ester product concentration and volumetric productivity to reach 53 mM and 6.6 mM/h, respectively. Overall molar yield of 1,11-undecanedioic acid from ricinoleic acid was 55% based on the biotransformation and chemical transformation conversion yields of 84% and 65%, respectively.

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Syntheses of Naphthalene Diimides for the Investigation of the Electron Transfer Processes

김성식* T. Majima[1] M. Fujitsuka[1]

전북대학교 화학과 [1]Osaka University

Naphthale monoanhydride moniimide was used to synthesize several diimides which is useful to investigate the electron transfer processes. The diimide contains naphthalenediimide as a common structure. They also contain other types of diimides, such as phthalimide, naphthalimide, pyromellitic diimide, and perylenemonoimide. The two types of diimides were linked by aromatic spacer groups. The synthetic procedure of the diimides is as follows. Monoanhydrides contanining naphthalenemonoimide and pyromellitic monoimides were prepared first, according to the previously reported procedure, then one anhydride was connected with aromatic diamine, and finally connected with the other monoanhydride to get the final compounds as diimides.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural Sensitivity and Gel Properties of Peptoid-Based Low Molecular Mass Organogelator

김정윤 권용억*

이화여자대학교 화학.나노과학과

Peptoid-based low molecular mass organogelators were prepared by the aza-Michael addition reaction. The gelation was observed only for *tert*-butyl group substituted peptoid in chlorinated solvents including chloroform, 1,2-dichloroethane, and 1,2-dichlorobenzene. Interestingly, the peptoids with methyl, ethyl, n-propyl, n-butyl, and isobutyl groups did not exhibit gelation, indicating unique structural sensitivity of organogelation. The compound reported here is one of the simplest and lowest molecular mass organogelators prepared so far. The physical properties, and spectral and ab initio calculation data suggest that nanofibrous morphology developed through the intermolecular hydrogen bonding of peptoid molecules plays a crucial role in organogelation. This study provides insights in designing various peptoid-based small molecule organogelators, and suggests that a minute structural difference should not be neglected in developing organogels.

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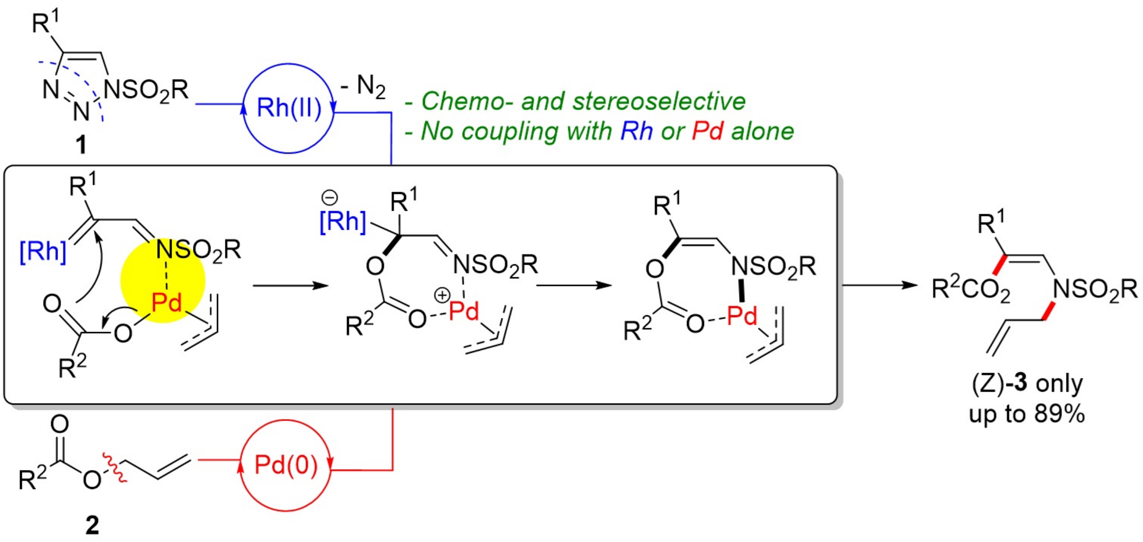
Synergistic Rh/Pd Dual Catalysis: Chemo- and Stereoselective Coupling between Rh(II)-Carbenes and ?-Allyl Pd(II) Complexes

Chen zisheng 이상기[1,*]

이화여자대학교 [1]이화여자대학교 화학/나노과학과

Synergistic dual catalysis has emerged as a new and powerful strategy in chemical synthesis.1 In this dual catalytic process, each catalyst could selectively activate the substrates to enable the chemical transformations that are not possible with either one of the catalysts.1 The main challenge for the development of synergistic catalysis is ensuring catalyst cross-compatibility, balancing kinetics for substrate activation and avoiding catalyst deactivation. Here we present a novel synergistic Rh(II)/Pd(0) dual catalysis strategy that promotes the denitrogenative cross-coupling of 1-sulfonyl-1,2,3-triazoles 1 with allyl carboxylates, which does not occur when using a Rh(II) or Pd(0) catalyst alone. In this dual catalysis process, Rh(II) and Pd(0) catalysts activate 1-sulfonyl-1,2,3-triazoles and allyl carboxylates in a substrate-selective manner with balanced-kinetics to generate an ?-imino Rh(II)-carbene and a ?-allyl Pd(II)-complex. Coordination of the pendant ?-imine of the Rh(II)-carbene with the Lewis acidic Pd-complex plays a key role in not only placing the activated species in proximity but also in reversing electronic nature of the Pd-complex, which may facilitate the nucleophilic transfer of the carboxylate onto the electrophilic carbenic carbon. This effectively accomplishes the formal 1,3-insertion of ?-imino Rh(II)-carbenes into the sp3 C?O bond of allyl carboxylates to yield N-allylated (Z)-amino vinyl carboxylates (Scheme 1).2(1)Allen, A. EMacMillan, .; D. W. C. Chem. Sci. 2012, 3, 633-658. (2)Chen, Z.-S.; Jeon, H. J.; Chen, S.-W.; Xuan, Z.; Lee, S.-g. 2015, manuscript submitted.



R1
NSO2R
1
Rh(II)
- N2
- Chemo- and stereoselective
- No coupling with Rh or Pd alone
[Rh]
Pd
R2
[Rh]
R1
NSO2R
Pd
R2CO2
(Z)-3 only
up to 89%
2
Pd(0)

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Development of imidazo[1,5-a]pyridine-derived *N*-heterocyclic carbene Cu(I) complexes for direct C-H carboxylation using CO_2

박다애 이준승[1] 홍석원[*]

광주과학기술원(GIST) 신소재공학부 [1]전남대학교 화학과

N-Heterocyclic carbenes (NHCs) are often used as strong σ-donor ligands and numerous structural variation have been made to the prototypical imidazolylidene skeleton. Imidazo[1,5-a]pyridin-3-ylidenes (ImPy) have been developed as a rigid bicyclic variant of NHC to show unique electronic and steric properties. The substituents on the bicyclic ImPy can be projected deeply into the metal coordination sphere. Furthermore, the extended π-system in ImPy structure could increase the electron density at the carbene center. Herein we wish to report the synthesis of a series of bulky imidazo[1,5-a]pyridin-3-ylidenes copper(I) complexes and their application in direct C-H carboxylation of benzoxazole with CO_2. The direct C-H carboxylation with CO_2 would be highly attractive and atom-economical routes to carboxylic acids. The molecular structure of a novel ImPy-Cu(I) complex was determined by X-ray crystallography and the ImPy-Cu(I) complex efficiently catalyzed the direct C-H carboxylation of benzoxazole derivatives with CO_2 in good yields. It is interesting to note that ImPy-Cu(I) complex with a 2,6-diisopropyl phenyl unit exhibited a better catalytic activity than the similarly substituted imidazol-2-ylidene copper(I) complex [(IPr)CuCl] (95% vs 80% isolated yields after 14 h).

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Using "bottom-up" Route Synthesis of Carbon Quantum Dot that emits a long wavelength

김민욱 박찬필*

충남대학교 분석과학기술대학원

CQD(Carbon Qauntum Dot) is new type material different with graphene fullerene which is made of nano-crystalline structure has the size under the 10nm. CQD has many property such as low toxicity, bio-compatibility, chemical inertness, Photoluminescence. Most importanat thing about CQD's property is photoluminescence. It has depending on the size represents a different light CQD synthesis is used by Bottom-up route and this is the method of heating the carbohydrate such as glucose and organic acid for synthesis setting the carbonization.Commonly, Microwave irradiation, Hot-injection, Hydrothermal, These methods have been widely used. Through this method, We experiment the synthesis of CQD which show a long wavelength

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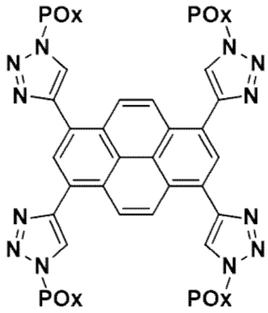
Fluorescence-tunable thermo-responsive polymers

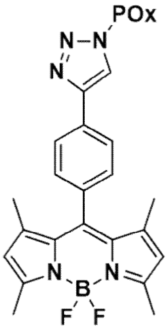
김주호 정용석 장우동*

연세대학교 화학과

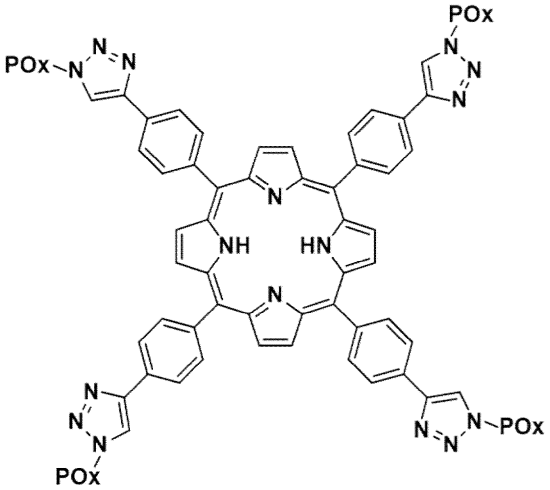
Fluorescent dyes with various colors have been received much attention during the past decades in diverse area such as sensors and display devices. We synthesized several dyes conjugated with poly(2-isopropyl-2-oxazoline)s (POx) having lowest critical solution temperature (LCST) behaviors through click reactions. Pyrene, BODIPY, and porphyrin moieties were used for B, G, and R color emitting dyes, respectively. All synthesized dyes showed thermo-responsiveness behaviors such as fluorescence quenching or color changing in water, because of LCST behavior of POx. Using these properties of prepared dyes, we could make G → B → R color shifting system and white-emitting system with just mixing three dyes with various proportions. The detailed aspect of these systems will be reported in the conference.



Pyrene-POx

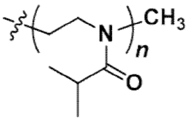


BODIPY-POx



Porphyrin-POx

POx =



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Treating Grignard reagents on enamides facilitates tandem acyl group migration and nucleophilic addition

AcharyRaghavendra **황종연[1] 윤창수[2] 김필호[3,*]**

한국화학연구원 의약바이오본부 [1]한국화학연구원 신약연구본부 [2]한국화학연구원 신약연구본부 의약화학연구센터 [3]한국화학연구원 난치성질환치료제연구그룹

Enamides have been extensively used in natural product synthesis as well as functional group transformation due to its stability along with the reactivity. Enamide plays an important role as an electrophile, also as a nucleophile due to its unique character. Considering the instability of enamines, enamides can be used as an alternative to enamines for further synthetic transformation. To date enamides have been extensively used for the chemical transformations, such as heterocyclic ring formation, transition metal catalyzed reactions, Diels-Alder reactions, and photochemical oxidations. Recently, we discovered an unusual migration of acyl group on dihydroisoquinoline-enamides in the presence of Grignard reagents, which led to produce beta-hydroxyimines. Herein, the scope and reactivity of this unique reaction will be discussed.

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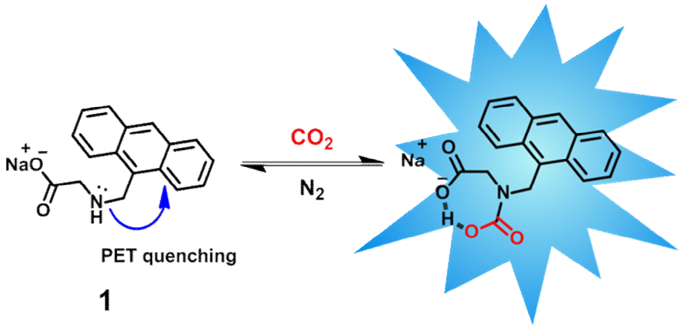
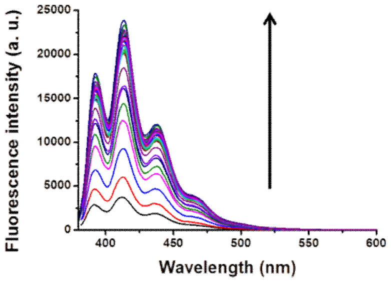
Intra-molecular hydrogen bonding stabilization based-fluorescent chemosensor for CO_2: Application to screen relative activities of CO_2 absorbents

강승윤 한민수*

광주과학기술원(GIST) 화학과

A fluorescent turn-on chemosensor for CO_2 was developed using intra-molecular hydrogen bonding stabilization. The chemosensor (sodium (anthracen-9-ylmethyl)glycinate (1)) reacts with CO_2 and forms chemosensor-CO_2 adduct stabilized by strong intra-molecular hydrogen bonds. The stabilization consequently allows sensing CO_2 with high sensitivity and the detection limit of this chemosensor for CO_2 was estimated to be ~2 ppm. In addition, the chemosensor was applied to develop an easy screening protocol to evaluate the efficiency of CO_2 absorbents. The protocols discriminate the relative ability of CO_2 absorbents as strong, intermediate, and weak using easily measured fluorescence changes.





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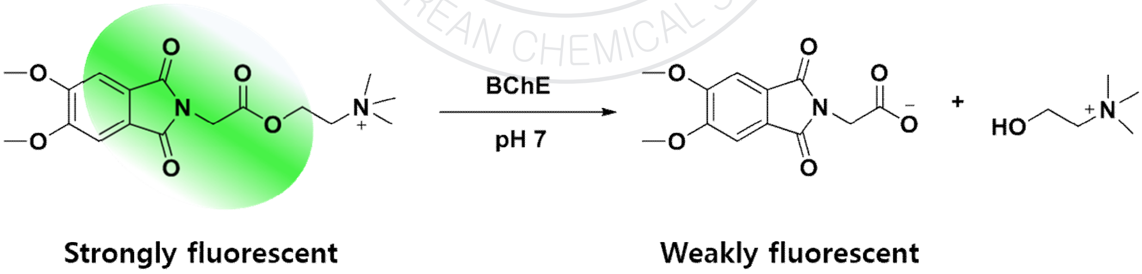
A simple assay for butyrylcholinesterase using a fluorescent substrate

이수지 강승윤 한민수*

광주과학기술원(GIST) 화학과

Butyrylcholinesterase (BChE) catalyzes the hydrolysis of butyrylcholine and other esters to choline, it plays a key role in the central nervous system and the peripheral nervous system. Inhibitor of cholinesterase has been used as the drug for Alzheimer disease and other neurological disorders. Thus, assay of cholinesterase is very important to develop a better medicine and treat Alzheimer disease. Fluorometric analysis using fluorescent substrate is much discussed because fluorometry has higher sensitivity than other methods. In this research, we synthesized fluorescent substrate containing choline moiety and confirmed the possibility of fluorometric BChE assay using synthesized fluorescent substrate.



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Synthesis of N-sulfenylimines from amines and thiols via aerobic cross-coupling

이찬 장혜영[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

N-sulfenylimines are used in various field as precursors of N-sulfinylimines, N-sulfonylimines, β-lactams, vinyl formamides, and H2S-releasing reagents. But, for the past hours the efficient way to synthesis N-sulfenylimines are rare in literature. For example, N-(phenylthio)phthalimine which is synthesized from thiol was used to prepare sulfenylimines from oximes. Recently, we proposed one pot synthesis of N-sulfenylimines from amines and thiols using copper catalyst and oxygen as oxidant. Furthermore, established method formed over-oxidation product; N-sulfinylimines or N-sulfonylimines. But, in this method, N-sulfenylimines are selectively formed in a good yield.

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Metal-Free Carboxylation of acetylene using Carbone dioxide

임유나 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Carbon dioxide is becoming the most attractive carbon source as it is abundant, renewable, and cheap. In addition, the use of carbon dioxide as a chemical feed stock would contribute to the reduction of carbon dioxide and global warming solution. As a CO_2 adsorption reagent, 1,5,7-triazabicyclo[4,4,0]dec-5-ene(TBD) has been utilized. In this study, the reactivity of TBD toward CO_2 was introduced to the reaction of acetylene and CO_2, resulting in acetylene carboxylation. In particular, dicarboxylation of acetylene followed by reduction affords commercially useful succinic acid, which has been produced from crude oil. By this organic base-mediated carboxylation, CO_2 fixation to acetylene occurs under environmentally benign and free of metal species conditions.

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Synthetic method of vinylic alkoxyamines using TEMPO and alkynes

최윤정 강예원[1] 장혜영[2,*]

아주대학교 에너지시스템학과 [1]아주대학교 에너지시스템학부 응용화학과 [2]아주대학교 화학과

Alkoxyamines are well known initiator of radical polymerization and radical mediated addition/cyclization of alkenes. unlike previous carbon-centered radicals and enamines needed synthetic methods for alkoxyamines, we propose an improved method for the synthesis of vinylic alkoxyamines. In this work, vinylic alkoxyamines synthesized via allenic radical intermediates which formed by induced single-electron oxidation through copper and TEMPO complex. Regardless of any substituted alkynyl alcohols, variety vinylic alkoxyamines obtained in good yields.

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Carbon-Carbon Bond Cleavage of Primary Propargyl Alcohols Through The Hemiaminal Intermediates

조유진 강예원[1] 장혜영[2,*]

아주대학교 에너지시스템학과 [1]아주대학교 에너지시스템학부 응용화학과 [2]아주대학교 화학과

Carbon-Carbon single bond cleavage is attractive issue due to relatively its strong bond strength. So, transition metal catalysts are needed to make the reaction more easy generally such as ruthenium and palladium catalysts. However it proceeds using copper catalyst. Also the hemiaminal intermediates occurs β-carbon elimination but not β-hydride elimination. Based on this study, we present carbon-carbon bond cleavage of primary propargylic alcohols under mild aerobic oxidative condition through hemiaminal intermediitate

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Preparation of 4-nitrosoaniline by reaction of nitrobenzene with thermally stable salts of urea

박재범 김형진[1,*]

휴켐스(주) 신사업개발팀 [1]전남대학교 응용화학공학부

Preparation of 4-nitrosoaniline by reaction of nitrobenzene with thermally stable salts of urea was investigated. Effect of precursors for the preparation of 4-nitrosoaniline, thermal stability test of the salt, and purification and hydrogenation of produced 4-nitrosoaniline have been performed. In preparing 4-nitrosoaniline, alkali metal ureate shows better performance than the mixture of alkali metal hydroxide and urea for thermal stability. Ureates from hydroxide precursor showed similar yield to that of hydride precursor. Sodium showed better result than potassium for preparing 4-nitrosoaniline. Produced 4-nitroaniline can be purified over 99.0%, and hydrogenation of the purified product can produce polymer grade 1,4-benzenediamine.

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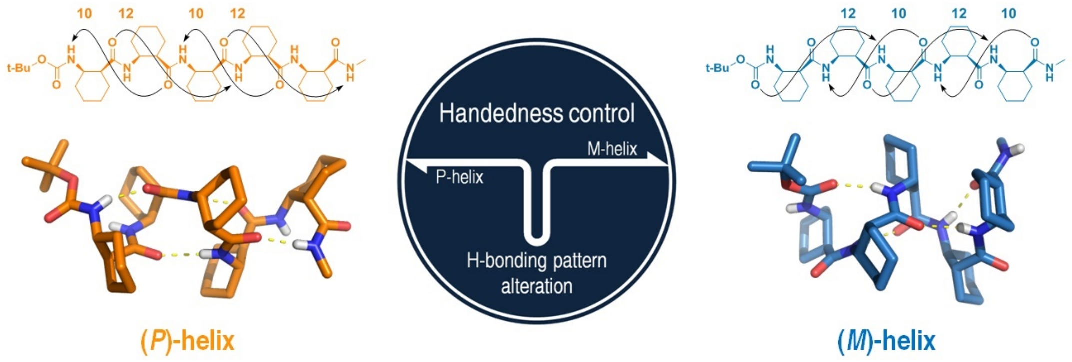
Controllable Handedness of β-peptides adopting 12/10-helical conformation

신선호 최수혁*

연세대학교 화학과

We synthesized β-peptides with alternating (1*S*,2*R*)-aminocyclohexanecarboxylic acid ((1*S*,2*R*)-ACHC) and (1*R*,2*S*)-ACHC. We were interested in controllable handedness of the β-peptides which adopt 12/10-helical conformation. First of all, we tried to control chair conformation by using *cis*-4-methyl-2-ACHC (*cis*-*m*ACHC). Chiral methyl group determines orientation of NH and C=O. Since their orientation changes θ value of torsion angle, chiral *cis*-*m*ACHC is quite important. If the pattern of hydrogen bond is altered by *cis*-*m*ACHC, handedness can be switched. We confirmed switched handedness by using circular dichroism, NMR spectra and single-crystal X-ray crystallography. Especially no crystal structures have been reported to date.



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Microreactor-Mediated Benzylic Bromination in Concentrated Solar Radiation

김영준 정명진 김지은 박찬필*

충남대학교 분석과학기술대학원

Sunlight-induced bromination of benzylic compounds was conducted in a capillary microreactor, resulting in mono-brominated compounds with yields of up to 94%. These reactions can be considered to be eco-friendly since they were carried out without an artificial light source or additional temperature control. In addition, up to 257.9 mmol could be produced daily using cost-effective molecular bromine, which leads to potential improvement of industrial processes.

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Synthesis of epoxy alcohols using metal-catalyst

김지은 박찬필*

충남대학교 분석과학기술대학원

The enormous potential of epoxy alcohols as key building blocks in production of valuable materials especially in the synthesis of highly functionalized natural products has led to intensive research for their preparation, metal-catalyzedepoxidation of allylic alcohols with hydroperoxides was the most practical route.Microreactor with discontinuous contact between alternating gas bubbles and liquid slugs has a larger gas-liquid contact area and light receiving area than a conventional batch system, controlling of the gas-liquid flow and absorbed light is very simple and efficient in the microreactor.Also, reaction parameters like pressure, temperature, residence time and flow rate are much easier to control in reactions with small volumes than in conventional reactors and the hazard potential of highly exothermal or explosive reactions is clearly decreased.The goal of this study find the optimal conditions, and to provide an efficient synthetic method which can produce the epoxy alcohol.

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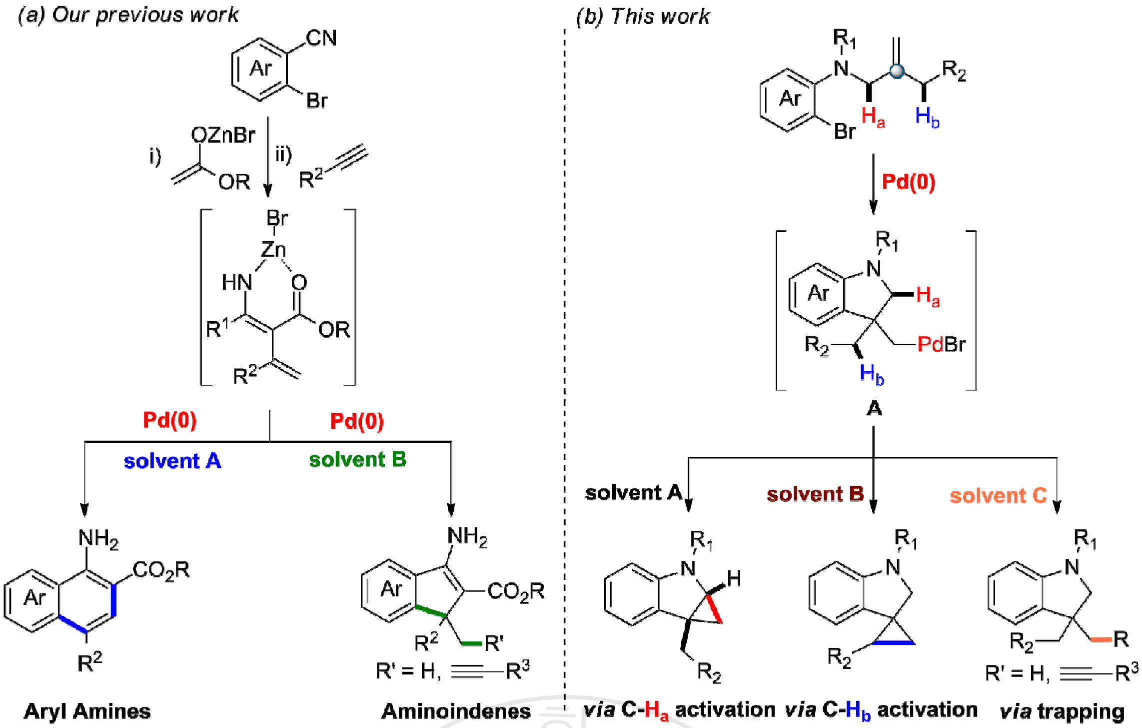
Tandem Divergent Catalysis *via* Transient Palladium(II) Complexes

이재성 이원구 이상기[1,*]

서강대학교 화학과 [1]이화여자대학교 화학/나노과학과

The divergent catalytic reaction provides quick access to structurally diversified compounds from a common precursor *via* controlled reaction pathway, and is highly attractive tool in discovery of drugs and functional materials.[1] In light of our interest in the use of transient palladium intermediates for divergent palladium catalysis, we recently reported a novel tandem divergent catalytic method that allow formation of four different aromatic scaffolds from nitriles (Eq. a).[2] Along this line, we have investigated a tandem divergent $C(sp^3)$-H activation of the common transient σ-alkylPd(II)-intermediate, formed by carbopalladation of N-allylated 2-bromoarylamines. Here we present our finding that the amine α-$C(sp^3)$-H or 1° and 2° alkyl $C(sp^3)$-H could selectively activated simply by choice of palladium/lignad and solvent to deliver the fused- or spiro-cyclopropanated indolines, or protonative and alkynylative trapping products (Eq. b).[3]1) A Review on the catalyst-controlled reactions, see: J. Mahatthananchai, Dumas, A. M.; Bode, J. W. Angew. Chem. Int. Ed. 2012, 51, 10954.2) Kim, J. H.; Bouffard, J.; Lee, S.-g. Angew. Chem. Int. Ed. 2014, 53, 6435-6438 (Highlighted in SYNFACT)3) Lee, J.-s.; Lee, W. K.; Lee, S.-g. manuscript in preparation.


(a) Our previous work
CN
Ar
Br
i)
OZnBr
OR
ii)
R2
Br
Zn
HN
O
R1
OR
R2
Pd(0)
solvent A
Pd(0)
solvent B
NH2
CO2R
Ar
R2
NH2
Ar
CO2R
R2
R'
R' = H, ≡—R3
Aryl Amines
Aminoindenes
(b) This work
R1
N
Ar
Br
Ha
Hb
R2
Pd(0)
R1
N
Ar
Ha
R2
Hb
PdBr
A
solvent A
solvent B
solvent C
R1
N
H
R2
R1
N
R2
R1
N
R2
R
R' = H, ≡—R3
via C-Ha activation
via C-Hb activation
via trapping

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Stereoselective Epoxidation of Aziridine-2-yl-Acrylaldehyde

양지은 하현준* 양정운[1,*]

한국외국어대학교 화학과 [1]성균관대학교 에너지과학과

The stereoselective epoxidation of aziridin-2-yl-acrylaldehydes and 30% aqueous hydrogen peroxide utilizing chiral 2-[diphenyl[(trimethylsilyl)oxy]methyl]pyrrolidine as an organocatalyst was successfully conducted to furnish 3-(aziridin-2-yl)epoxyaldehyde bearing both aziridine and epxoide moieties in a single molecule. In the presence of a catalytic amounts of 3-benzyl-4,5-dimethylthiazol-3-ium chloride with *N*,*N*-diisopropylethylamine in methanol, a series of 3-(aziridin-2-yl)epoxyaldehyde was readily converted to methyl 3-(aziridin-2-yl)-3-hydroxypropanoate in high yield, and then determined their stereochemistry of the products at this stage. Especially, these 3-(aziridin-2-yl)oxirane-2-carbaldehydes serve as valuable synthetic intermediates for the synthesis of poly-functionalized molecules by selective ring-opening reactions. These studies are currently ongoing in our laboratory.

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Synthesis and Anion Recognition Properties of Calix[4]pyrrole Carrying 5,6-Dichlorobenzimidazolium moiety at the Diametrical meso-Positions

이창희* **<u>bezaendalemulugeta</u>**

강원대학교 화학과

New calix[4]pyrroles bearing a 5,6-dichlorobenzimidazolium dicationic units at diametrically crossing meso-positions have been synthesized and characterized by standard spectroscopic means. The binding properties of this receptor at 250C were investigated first by proton NMR spectroscopy in CD3CN and DMSO-d6, as well as by UV-Vis spectroscopy and isothermal titration calorimetry (ITC) in CH3CN. The synthesized receptors display strong colorimetric response when exposed to the fluoride, chloride, benzoate and acetate anions (as their tetrabutylammonium salts) and exhibit an enhanced affinity as compared to the calix[4]pyrrole dicationic benzimidazolium without chloride substitution. The detailed guest binding studies including 1H NMR titration, UV-Vis spectroscopic changes and ITC measurement will be presented.

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Conformation of a Nile red/BODIPY-based bimodal probe on Lyposome

강철훈

경희대학교 동서의학대학원

We synthesized a Nile Red/BODIPY hybrid probe 1 composed of BODIPY and Nile Red coupled with PEG linker, capable of selectively recognizing fluidity changes in the ER membrane as a result of its preferential localization to the ER and the emission of fluorescence by Nile Red exclusively in non-aqueous environments. It was found that an efficient energy transfer to the Nile Red moiety from its BODIPY moiety occurs and that both of BODIPY and Nile Red locate in the membrane, anchored on the membrane by its PEG linker.

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Endoplasmic reticulum tracker with photostable multi-colour imaging capability

강철훈

경희대학교 동서의학대학원

An ideal fluorescent Endoplasmic Reticulum (ER) selective dye would have ER-selectivity, photo- or bio-stability for long term ER tracing, and a narrow spectral width for multicolour imaging. An ER tracker with all of the characters is rare. In this study, an ideal ER tracker (ER-RK1) is introduced and compared the commercially available ER trackers. It shows good solubility in aqueous solution, insensitivity to the environmental factors such as pH change, polarity, the types of the charges on micelles, photo-stability and a narrow emission band width at far red-region. A triple colour imaging with two other organelle trackers is also demonstrated.

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Paper based colorimetric sensor for C-H borylation screening

엄민식 김한성[1] 이선우[1,*] 한민수[*]

광주과학기술원(GIST) 화학과 [1]전남대학교 화학과

The direct conversion of C-H bonds to C-B bonds is a recently developed class of metal-catalyzed C-H bond functionalization. The conversion of C-H bonds to C-B bonds is both thermodynamically and kinetically favorable. Furthermore, C-B bond is easy to convert to other formations. Hence, significant progress has been made toward the development of systems that catalyze such borylation reactions of C-H bonds in alkanes, alkenes, and arenes in high yields and with high selectivity. For these studies, powerful analysis method is essential for development of efficient reaction conditions: catalyst, ligand, base, solvent, time and temperature. Traditional methods required expensive instruments or specific materials, such as nuclear magnetic resonance spectroscopy (NMR), infrared spectroscopy (IR), mass spectrometry (MS), gas chromatography (GC), and high-performance liquid chromatography (HPLC). To address this problem, we developed paper-based colorimetric sensor for C-H borylation using Bis(pinacolato)diboron (B_2Pin_2). Iodine resulted from B_2Pin_2, the residue of brylation and I_2O_5 in paper makes complex with starch. Then the complex turn up violet color. We can determine yield of the reaction by analyzing color using scanner. This paper based colorimetric sensor for C-H borylation is easily and economically accessible in any general laboratory(analysis using scanner).

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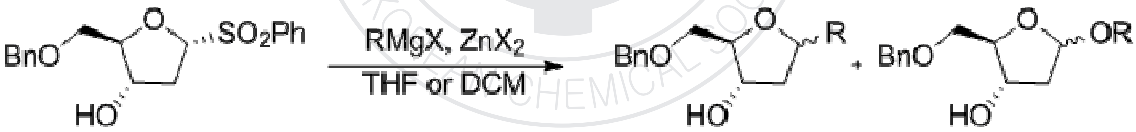
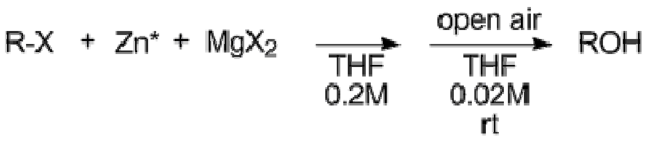
Oxidative conversion of alkyl halides to alcohols

김윤정 이희윤*

한국과학기술원(KAIST) 화학과

During our synthetic studies of sulfone displacement with Grignard reagents using in presence of zinc salts, alkoxy substituted products were obtained as byproducts. Though the exact mechanism of oxygen insertion by zinc salts was not known, zinc salts clearly accelerate oxygen insertion into Grignard reagents. Based on this observation, we have developed direct conversion of alkyl halides to alcohol using activated zinc and magnesium salts. This mild and practical strategy shows wide substrate scope. This methodology was also applied to produce phenols from aryl halide as well.





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Synthesis of Amino-Substituted Polycyclic Aromatic Hydrocarbons from Propiolic Acids and Amines

최진섭 이선우*

전남대학교 화학과

Amino-substituted polycyclic aromatic hydrocarbons were obtained by the reaction between aryl alkynyl carboxylic acids and amines in the presence of a copper catalyst. The hydrocarbons were obtained in good yield without the need to isolate the 1,4-diaryl-1,3-butadiyne intermediate. The best result was obtained using a combination of CuCl and $Cu(OTf)_2$, and the reactions of cyclic and acyclic secondary amines afforded the desired products.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Asymmetric Synthesis of Chiral *N*-Substituted Pyrazoles by Phase-Transfer-Catalyzed Aza-Michael Reaction

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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발표분야: 유기화학

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Synthesis and fluorescence properties of Phenothiazine derivatives

한재익 Ai Qi[1] 홍승주 류지경 안광현[1,*]

경희대학교 일반대학원 화학과 [1]경희대학교 응용화학과

유기발광다이오드(Organic Light-Emitting Diode, OLED)의 풀컬러화 방법은 삼색분열도포법, 색변환 방법, 컬러필터법이 있다. 삼색분열도포법은 광 손실이 적으면서 낮은 소비전력으로 고휘도를 낼 수 있는 것이 장점이나 RGB 화소의 열화정도가 다른 것이 문제점이다. 특히 청색발광체의 장기수명을 개선하고 발광수명이 짧으면서도 색 순도 및 발광효율의 장기적 열 안정성이 우수한 발광체 개발은 매우 중요하다. 본 연구에서는 Phenotiazine 을 기반으로 한 녹색발광체인 BBMP 와 MPPO 를 합성하고 oxidation 하여 새로운 청색발광체를 합성하였다. H1-NMR, C13-NMR, FT-IR 과 HR-MS 를 이용하여 분자 구조를 확인하고 이 물질의 광학적 특성과 전기적 특성을 분석하고 평가해 보았다.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Blue fluorescence materials based on Diphenylamino-dibenzo[*g,p*]crysene for organic light emitting diode

정수진 김세현 김동영 윤승수*

성균관대학교 화학과

In this study, we have synthesized three blue materials based on diphenylamino-dibenzo[*g*,*p*]crysene. To explore electroluminescence properties of these materials, following device was fabricated: ITO / NPB (50 nm) / 3 % blue emitting materials in mADN (20 nm) / Alq3 (30 nm) / Liq (1 nm) /Al. All devices showed blue emission with good electroluminescent efficiencies. Therefore, these results suggest that diphenylamino-dibenzo[*g*,*p*]crysene derivatives have the good potentials as the efficient blue emitters for OLEDs .

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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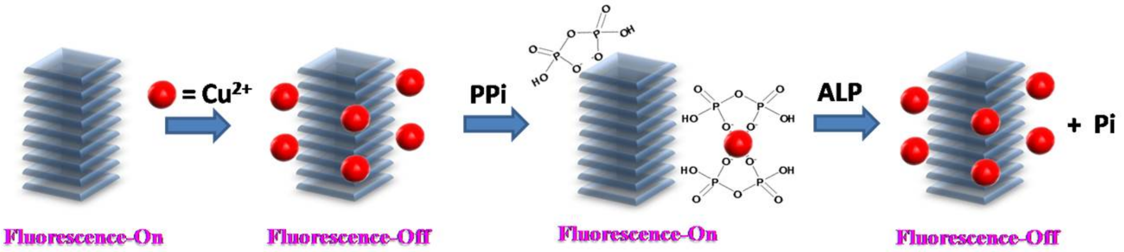
Photophysical Properties of PyA4 Aggregate and Its Application to Pyrophosphate Sensor Based on Turn-On System

김보연 이성호*

대구대학교 화학응용화학과

A new water soluble fluorescence chemosensor bearing four sodium carboxylates linked to tetra-phenylacetylene substituted pyrene, PyA4, has been designed and developed. PyA4 displays self-assembly behavior with strong intermolecular excimer emission in aqueous buffer solution. Fluorescence changes upon the addition of various metal ions show that PyA4 has high selectivity for the Cu^{2+} ion over other metal ions tested via fluorescence suppression, i.e. 98.5% fluorescence quenching. This system, the Cu^{2+} ion complexed to the PyA4, acts as a highly selective and sensitive fluorescent sensor for pyrophosphate, showing fluorescence enhancement which leads to 98% fluorescence recovery. For the bioanalytical applications, the activity of alkaline phosphatase (ALP) was successfully monitored by the real-time turn-off assay.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **ORGN.P-454**
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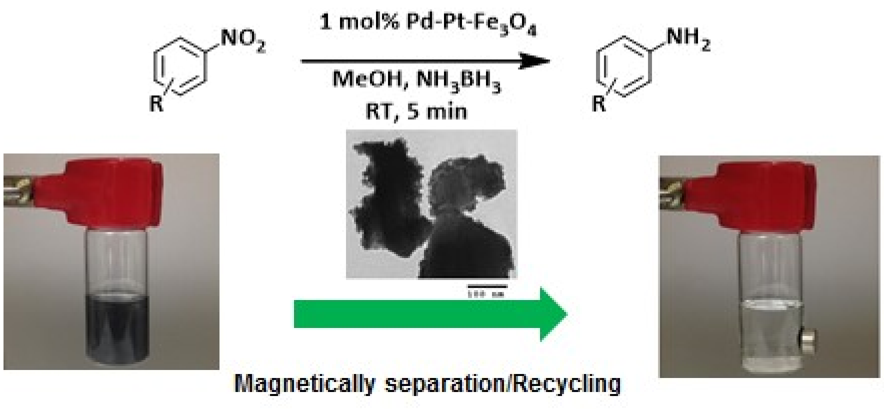
발표종류: 포스터, 발표일시: 목 11:00~12:30

Magnetically recyclable bimetallic Pd-Pt-Fe_3O_4 as catalysts for reduction of nitrocompounds

송예미 변상문 김병문*

서울대학교 화학부

We report the synthesis of bimetallic nanoflake-shaped Pd-Pt-Fe_3O_4 nanoparticles (NPs) and their application to the reduction of nitro- compounds. Using simple hydrothermal procedure, we decorated nano sized crystals of platinum and palladium on the Fe_3O_4 NPs' surface. The nanoflake-shaped Pd-Pt-Fe_3O_4 NPs were very efficient in effecting the one-pot cascade catalysis of dehydrogenation of ammonia borane and reduction of nitro compounds to anilines in methanol at room temperature. Development of efficient methods for the reduction of nitro compounds becomes one of the important synthetic methods in relation with the advent of various medicinal and display materials. A series of aromatic nitro compounds were reduced with excellent conversions and yields to desired products in a very short time (5min). The reactions using the Pd-Pt-Fe_3O_4 catalyst proceeded faster than those using either Pd-Fe_3O_4, Pt-Fe_3O_4 or the combination of both Pt-Fe_3O_4 and Pd-Fe_3O_4 catalysts, confirming a unique "synergistic effect" of the bimetallic nano-catalyst system. The catalyst could be recycled through the use of an external magnet in a very straightforward manner and was reusable for over 250 times without loss of its catalytic activity. Thus, this new catalyst could offer a very sustainable, useful and environment-friendly tool for potential industrial applications in the reduction of nitro compounds.


NO$_2$
R
1 mol% Pd-Pt-Fe$_3$O$_4$
MeOH, NH$_3$BH$_3$
RT, 5 min
NH$_2$
R
100 nm
Magnetically separation/Recycling

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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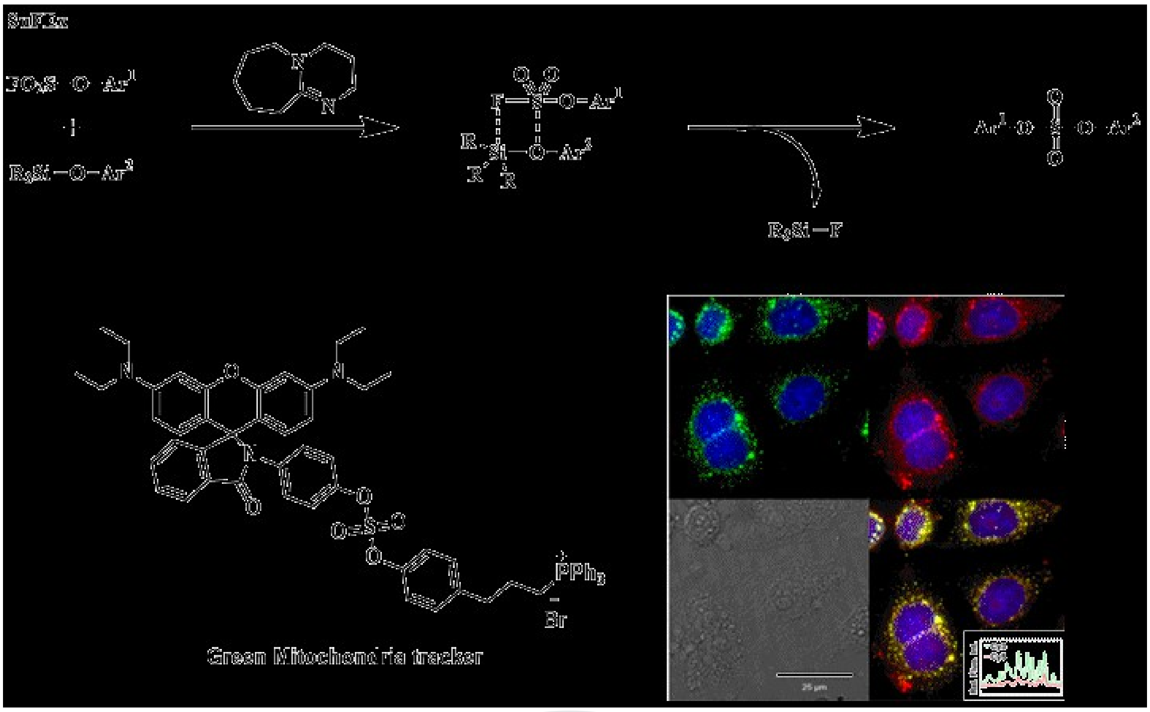
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel fluorosulfate based fluorophores (FS-Fluor) for “Click chemistry” by sulfur fluoride exchange (SuFEx)

박지수 김병문*

서울대학교 화학부

Chemical biology is essential for the investigation of biological processes in the living system. Especially, site-specific biomolecule tagging with functional groups such as fluorescent probe, spin probes, and affinity tags has been greatly utilized for understanding biological system. However, some possible drawbacks including side reactions and non-site-specific tagging have been reported. Therefore bioorthogonal chemical tools have been devised to tag biological targets within complex living systems. Among those, one of the most powerful reaction is click chemistry such as Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC), Strain-promoted alkyne-azide cycloaddition (SPAAC) and Tetrazine-trans-Cyclooctene Ligation. On the other hand, these reactions still have problems related with residue of metal, slow reaction rate and chemical instability. Recently, sharpless et al. discovered the valuable new click reaction for biological chemistry: Sulfur(VI) Fluoride Exchange (SuFEx). Herein, we report the effectiveness of the fluorosulfate based fluorophores (FS-Fluor) applying the SuFEx in chemical biology, introducing two applications of biological chemistry; biorthogonal modification of the side chain of tyrosine derivatives and specific mitochondrial staining in cancer cells using green fluorescent tracker.


SuFEx
FO2S–O–Ar1
+
R3Si–O–Ar2
R3Si–F
Ar1–O–S(O2)–O–Ar2
Green Mitochondria tracker
25 μm

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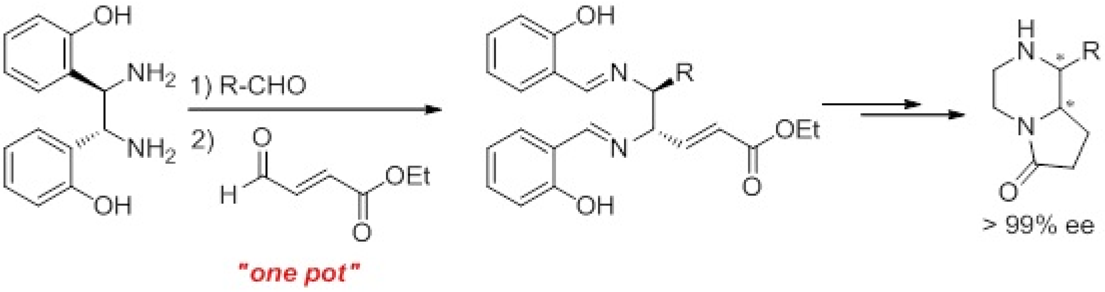
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Asymmetric Synthesis of Chiral Pyrrolopiperazine Derivatives via Diaza-Cope Rearrangement

송명종 김병문*

서울대학교 화학부

An efficient synthetic method was developed for the construction of enantiomerically pure pyrrolopiperazine derivatives using diaza-Cope rearrangement (DCR) as a key step starting from (R,R)/(S,S)-1,2-bis(2-hydroxyphenyl)-1,2-diaminoethane (HPEN). A complete transfer of stereochemical integrity was observed for the transformation. Pyrrolopiperazine is a useful building block often employed in the design of biological active molecules.1 This functionality is found in nootropic drugs like unifiram that is used as memory enhancers.2 Additionally, these types of chiral diamines were used as chiral ligands in the reduction of prochiral ketones by treatment of a mixture of stannous chloride and a diamine with diisobutylaluminium hydride.3We previously showed that diaza-Cope rearrangement reactions can be used to make a wide variety of alkyl- and aryl-substituted diamines as well as non-symmetrically substituted diamines.4 Herein, we report stereospecific synthesis of chiral pyrrolopiperazine derivatives by using the rearrangement reaction.



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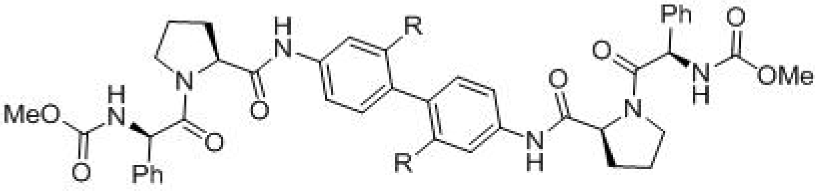
발표종류: 포스터, 발표일시: 목 11:00~12:30

A new series of benzidine and fluorene prolinamide derivatives as potent hepatitis C virus NS5A inhibitors

유영수 김병문*

서울대학교 화학부

Hepatitis C virus (HCV) is a blood-borne, positive-sense RNA virus, which belongs to the Hepacivirus genus in the Flaviviridae family. A majority of people infected with HCV develop chronic HCV infection, which leads to serious disorders such as liver cirrhosis, followed eventually by hepatocellular carcinoma. For treatment of HCV infection, a widely used combination includes pegylated interferon-? and ribavirin. A new treatment has also been introduced based on HCV protease inhibitors. However, the current treatment protocols are riddled with substantial adverse effects like fatigue, depression together with partial efficacy, and sustained virologic response (SVR) for genotype 1 is about 60~80%. Therefore it is necessary to develop new anti-HCV drug candidates exhibiting less side effects and more effective cure rate. Recently, novel treatments through the use of direct acting agents (DAA) are in the limelight of many pharmaceutical companies and research laboratories.Herein we report the discovery of a series of extremely potent HCV NS5A inhibitors based on the benzidine prolinamide skeleton. Taking a simple synthetic route, we developed a novel inhibitor flatform, which allows easy modification, and through optimization of the benzidine core structure, we identified BMK-20313, BMK-20613, and BMK-20713 possessing highly potent anti-HCV activities. Especially, BMK-20313 is nontoxic and anticipated to be an effective HCV drug candidate.



Type 2a: EC_{50} = 0.01 nM, G-1b: EC_{50} = 0.007 nM

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

[발표취소] Efficient synthesis of fullerene-based materials for organic solar cells

임태현 김병문*

서울대학교 화학부

발 표 취 소

본 논문은 발표취소된 논문입니다.

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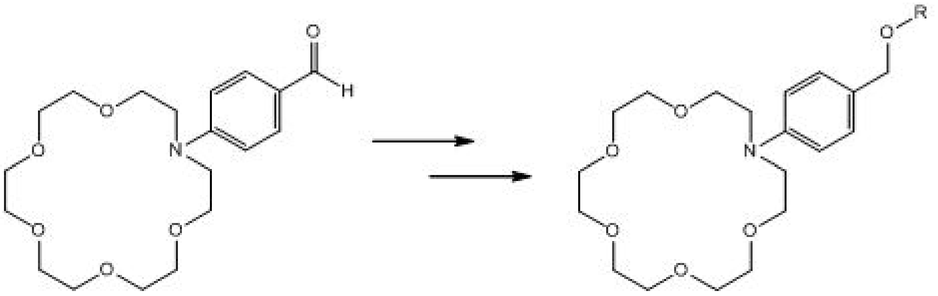
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of new CO2-soluble aza-18-crown-6-ether derivatives and its evaluation as a metal chelating agent in scCO2

송희 yan xinhao 오유리 양병도[1] 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

In present study, new CO2-soluble aza-18-crown-6-ether derivatives have been designed and synthesized from N-(4-formylphenyl)aza-18-crown-6-ether by simple chemical modifications for the CO2-philic chelating agent. Their solubilities and metal ion extraction ability in supercritical carbon dioxide (sc CO2) have been tested and the relationship between structure and CO2-solubility has been proposed.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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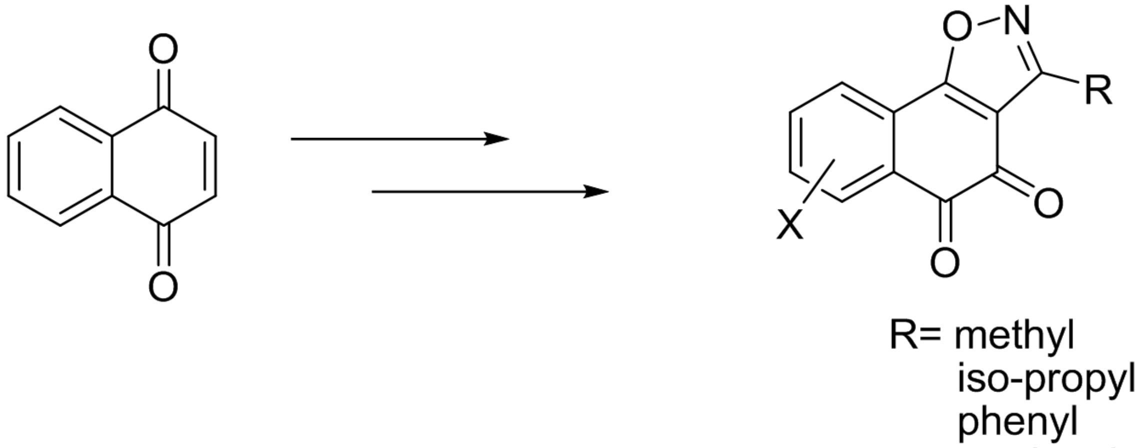
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 3,4-isoxazolo-1,2-naphthoquinone derivatives and their biological evaluation

김학원* 이현진 박슬찬[1]

경희대학교 응용화학과 [1]경희대학교 화학과

β-Lapachone (β-LAPA), is a chemotherapeutic agent derived from the bark of the South American *Lapacho* tree. It has recently emerged as a potent antitumor, anti-virus, anti-parasitic, and anti-inflammatory agent *in vitro*, and *in vivo*. Especially, β-lapachone has been reported to kill human cancer cells selectively not normal cells through rapid reactive oxygen species (ROS) occurrence mediated by NAD(P)H:quinone oxidoreductase-1 (NQO1) enzyme. In our research, several isoxazole analogs of β-LAPA, 3,4-isooxazolo-1,2-naphthoquinones, for the new drug development have been synthesized and tested for the NQO1 activation and Lactate variation in the cell.



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발표코드: **ORGN.P-461**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

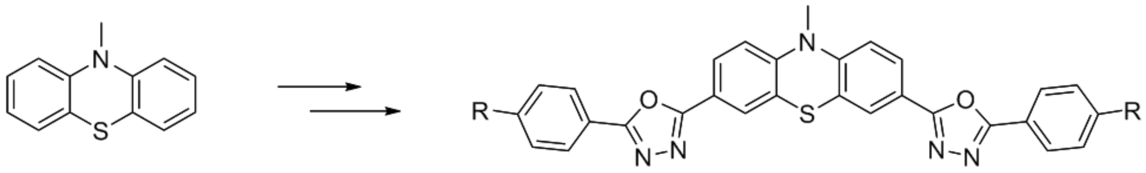
Synthesis of Di-phenyl-phenothiazyl-1,3,4-Oxadiazoles and Its Electroluminescence Characteristics

이고은 박수진 김학원[*]

경희대학교 응용화학과

1,3,4-Oxadiazole derivatives are considered as important compounds due to their pharmaceutical, biological, corrosion inhibition and electron transporting properties. Especially, they can be used in electronic and optoelectronic applications consisting π-conjugated organic materials.

In this work, we prepared di-phenyl-phenothiazyl-oxadiazole derivatives (DPPO), a new green-emitting material with donor-acceptor architecture containing phenothiazine core using previous synthetic method with simple modifications. The modified synthetic method allows a concise, highly efficient, solvent-free synthesis of DPPO derivatives from hydrazide through an *N*-acylhydrazone intermediate. Newly synthesized several DPPO derivatives have been tested for their thermal, optical and electroluminescent characteristics using organic light-emitting diodes (OLEDs).



Scheme 1. Synthesis of Di-phenyl-phenothiazyl-oxadiazole(DPPO) derivatives

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, solubility and metal extraction of novel 18-crown-6 ether derivatives into supercritical CO_2

오유리 yan xinhao 안소연 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Supercritical carbon dioxide (sc-CO_2) has been suggested as an environmentally benign, green solvent for heavy metal ions extraction. Sc-CO_2 has a variety of advantages such as nontoxic, inexpensive and moderate critical constants (Tc = 31.1℃, Pc = 73.8bar). But, the solvation characteristics of sc-CO_2 are similar to hexanes. It acts as a non-polar solvent. Due to weak solute (polar metal ions) ? solvent (non-polar CO_2) interactions, the direct extraction of metal ions with sc-CO_2 is inefficient. Therefore, we have introduced several CO_2-philic groups such as carbonyl, ether, perfluorinated ester and siloxane. For more effective metal extraction in sc-CO_2, we have designed and synthesized novel CO_2-soluble chelating ligands containing both metal binding segments (18-crown-6 ether moiety) and CO_2-soluble segments. Solubilities of synthesized 18-crown-6 ether derivatives have been tested and the relationship between structure and solubility has been suggested. With these CO_2-soluble 18-crown-6 ether derivatives the sc-CO_2 metal extraction (Cs^+ and Sr^{2+} etc) have been studied.

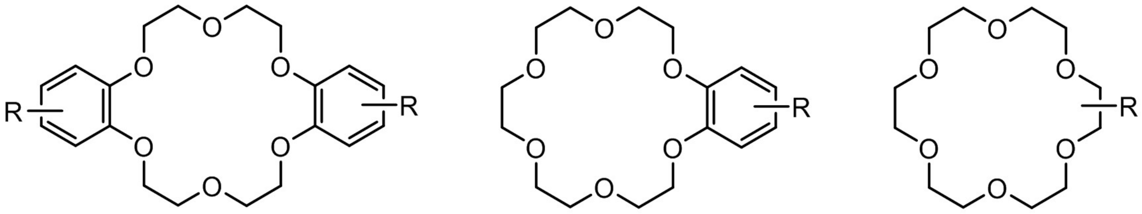

Figure 1. Various 18-crown-6 ethers
R = H, alcohol, carbonyl, perfluorinated ester, siloxane etc

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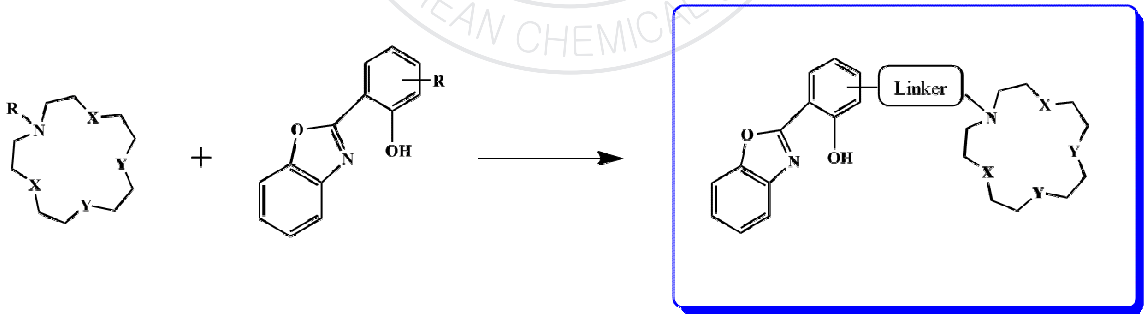
Synthesis of 2-(2-hydroxyphenyl)-1,3-benzoxazoles containing an azacrown-ether as a potent metal sensor

안소연 yan xinhao 유영민[1,*] 김학원[2,*]

경희대학교 화학과 [1]이화여자대학교 화학신소재공학부 [2]경희대학교 응용화학과

2-(2-Hydroxyphenyl)-1,3-benzoxazole (HBO) derivatives are known for an important class of fluorophores, because they show fluorescence emission with large Stokes' shifts through excited-state intramolecular proton transfer (ESIPT). Taking advantage of the ESIPT fluorescence, we designed fluorescence probes for metal ions. The design principle here is to combine the HBO fluorophore and azacrown ether, where the latter serves as a metal receptor. A series of fluorescence probes have been successfully synthesized and examined their capability for metal sensing.



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발표분야: 유기화학
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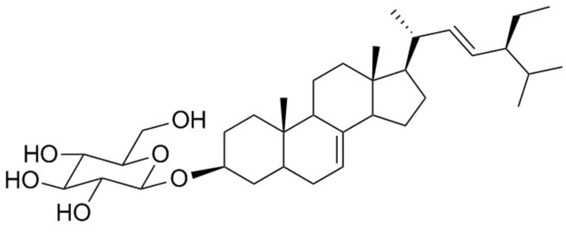
Synthesis and its biological activity of α- and β-glycosyl 5,6-dihydroergosterol

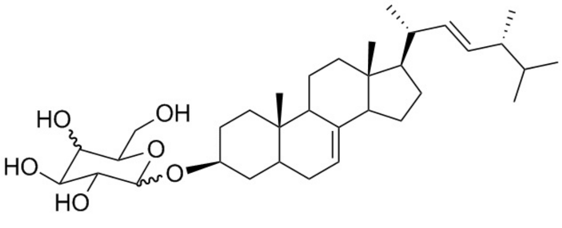
오현정 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Natural spinasterol-glucose (3-O-β-D-glucopyanosylspinasterol) has been identified as a compound not only to promote procollagen production but also to exhibit strong anti-inflammatory activity. However, spinasterol-glucose is difficult to isolate from natural plants or synthesize. To overcome these difficulties, we have already synthesized the β-glucosyl-ergosterol and β-glucosyl-5,6-dihydroergosterol (DHE), structurally similar to spinasterol, by the relatively easy synthetic method. The key intermediate 5,6-dihydroergosterol can be obtained through a selective reduction of the double bond of commercially available ergosterol. Then, we synthesize target molecules through Lewis acid-catalyzed glycosylation of trichloacetimidates with a sterol. Those molecules have been tested for biological activities on iNOS inhibition and cell viability in LPS-stimulated macrophage cells. In this report, we will describe the highly efficient synthesis of several α- and β- glycosyl-5,6-dihydroergosterol and their biological activities against skin inflammatory disease like atopic dermatitis.



Spinasterol glucose



Glycosyl-5,6-Dihydroergosterol

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ORGN.P-465**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Morpholino dinucleotide의 합성 및 자가 정렬 특성 조사

김태연 전근호[1,*]

승실대학교 화학과 [1]승실대학교 화학

PNA 이합체(dimer)는 특정 완충용액에서 자가 정렬(self-assembly)에 의해 매우 규칙적인 나노 구조체를 형성함이 보고되었다. 이러한 현상은 PNA 의 염기들 간의 쌓임(st0.king) 현상과 Watson-Crick 형태의 수소결합에 의하여 일어나게 된다고 보고되었다. 생성된 결정은 voltage-dependent electroluminescence 과 광범위한 가시광선 영역에서 excitation-dependent fluorescence 특성을 나타내는 것이 관찰되었다. 이 결과에 의거하여 PNA 과 함께 최근 인공 유전자의 재료로 사용되는 morpholino nucleotide 의 올리고머 역시 유사한 광학특성을 나타내는 나노 구조체를 형성 하는 가를 알아보기 위하여 C 와 G 를 염기로 갖는 morpholino nucleotide 단량체를 개선된 방법으로 합성하고 이를 이용하여 morpholino dinucleotide, G-C, C-G, C-C, G-G 를 합성 하고 이들의 자가 정렬 가능성에 대하여 조사 하였다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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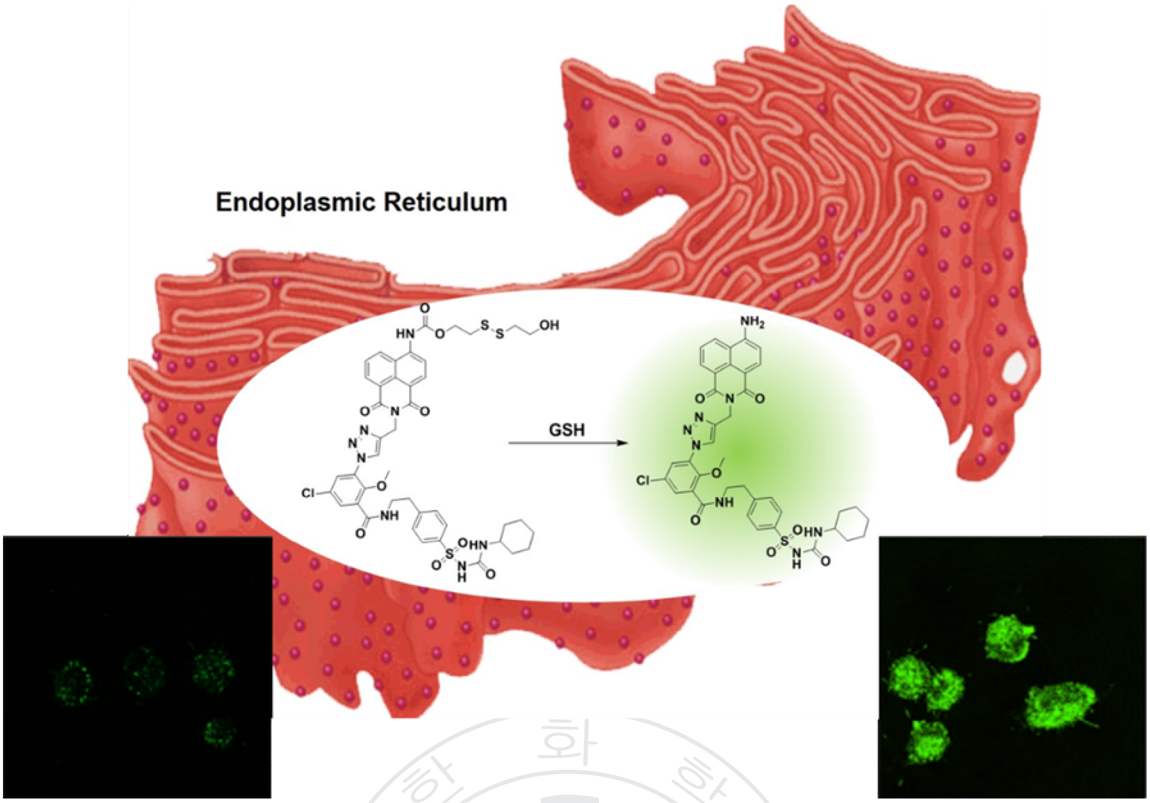
발표종류: 포스터, 발표일시: 목 11:00~12:30

Glibenclamide-mediated Endoplasmic Reticulum Glutathione Sensing

이재홍 위영진 강철훈* 김태우*

경희대학교 동서의학대학원

A naphthalimide-based fluorescent probe 9 containing a disulfide bond group (?S?S?). The disulfide bond groups are a versatile tool to trigger reactions by Glutathione. Herein, we designed and synthesized, which could detect physiological level of Glutathione in aqueous and biological environments. Upon addition of thiols, the fluorescence intensity of probe 9 increases by about 14-fold. Moreover, probe 9 shows good water solubility, is inactive towards other biologically relevant analytes such as various thiols, thiol-free amino acids, and metal ions is easy-to-visualize. From confocal microscopic experimental studies, the fluorescence image of probe 9 was mainly overlapped with ER markers. Therefore, our probe, described above, could afford a. powerful new approach for the specific thiol sensor and bio imaging. In addition this system may have a role in opening new possibilities for the screening of new diagnosis and bioimaging applications in vitro and in vivo.


Endoplasmic Reticulum
GSH

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장소: 대구 EXCO
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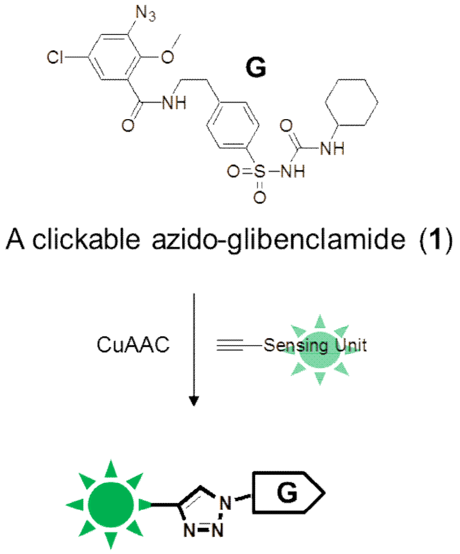
발표종류: 포스터, 발표일시: 목 11:00~12:30

A CuAAC-based ER Targeting Module: Azido-glibenclamide

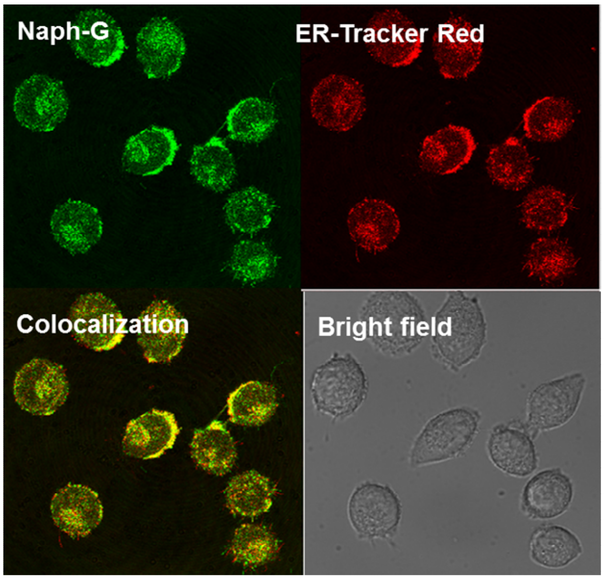
이용재 김태우*

경희대학교 동서의학대학원

Endoplasmic reticulum (ER) is primarily responsible for the protein folding and the proper sorting of lipids and proteins. The ER specific biosensor is important to understand ER response under oxidative stress on sub-cellular level. Glibenclamide in ER-TrackerTM has been known as an ER targeting compound. Using glibenclamide moiety azido-glibenclamide (1) was synthesized. Compound 1 would be easily functionalized by CuAAC (copper azide-alkyne cycloaddition) reaction with a variety of sensing units. The synthesis of 1 was characterized by 1H, 13C NMR, HH COSY (correlation spectroscopy) and CH HSQC (heteronuclear single quantum coherence) spectroscopy, and HR MS. In addition the colocalization experiment of naphthalimide-glibenclamide conjugate (Naph-G) and ER-TrackerTM Red suggests that compound 1 keep ER targeting ability after CuAAC modification.



CLFM colocalization experiment



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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Novel Aminopyrrolo[2,3-d]pyrimidine Derivatives and Their FAK Inhibition and Antitumor Activities

정은임 최성은 김종승 유경호[1,*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

Focal adhesion kinase (FAK) is a non-receptor tyrosine kinase that transduces signaling from a diverse group of stimuli to control a variety of cellular pathways and processes, including cell proliferation, migration, morphology, and cell survival. FAK is overexpressed in many tumors, including those derived from the head and neck, colon, breast, prostate, liver, and thyroid. Therefore, FAK has been proposed as a potential target in cancer therapy and small molecule inhibitors for use as potential cancer therapies have been developed.The purpose of this study is to develop the potent compounds with FAK inhibition and antitumor activities. Based on the structural combination of TAE226 and PF-562,271 as FAK inhibitors, a series of aminopyrrolo[2,3-d]pyrimidine derivatives were designed. And in vitro FAK inhibition assay and cell-based assay against seven cancer cell lines for the synthesized compounds were carried out. Further biological evaluation for the selected compounds is in progress.

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Identification and Elucidation of degradation through the stress testing for Fimasartan potassium trihydrate

이지혜 한남석 김재민 이종혁[1] 유병욱[2] 이준광[3,*]

보령제약(주) 중앙연구소 [1]보령제약(주) 분석연구팀 [2]보령제약(주) 중앙연구소 합성연구팀 [3]충북대학교 약학대학

The impurity profile has implication for drug product. In order to identify the impurity profile, we have conducted stress tests for Kanarb's API (Fimasartan potassium trihydrate) in which acid, base, oxidation, thermal, photolysis, humidity. The significant degradation is observed in oxidative condition. Two degradation products (Impurity B and unknown impurity) obtained by prep. were detected by High performance liquid chromatography (HPLC) and mass spectroscopy (MS). Based on spectral data, unknown impurity is identified S-oxide. Additionally, We could confirm that S-oxide increases depending on the sonication time when we prepare the sample solution by HPLC.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mode of Inhibition of PIM Kinases by Indole Derivatives

이성호 이진호 **HONG VICTOR SUKBONG***

계명대학교 화학과

PIM serine/threonine kinases composed of PIM-1, 2, and 3 play a key role in cellular responses such as cell growth and apoptosis. PIM kinases have been widely studied as potential therapeutic targets in cancer treatment. In this study, we report on the optimization of an immobilized metal ion affinity-based fluorescence polarization (IMAP) method for high-throughput screening and structure-activity relationship (SAR) study of potential PIM inhibitors. Furthermore, inhibition modality of two indole derivatives (KMU010486 and KMU010517) as a novel class of potent PIM inhibitors was assessed using a fluorescence polarization method under optimized assay condition. Kinetic analysis demonstrated that these compounds were competitive inhibitors with respect to ATP. The sensitive fluorescence polarization method reported here will facilitate discovery of anticancer compounds that target all PIM kinases.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Identification of Potent Serum and Glucocorticoid-Inducible Kinase (SGK) Inhibitors Using a Kinase-Focused Library Screening Approach

김정은 이진호 **HONG VICTOR SUKBONG**[*]

계명대학교 화학과

Serum and glucocorticoid-inducible kinase (SGK) belongs to a AGC family of serine-threonine kinases that consists of three members SGK-1, SGK-2 and SGK-3. All three isoforms appear to play a crucial role in controlling cell growth, survival, proliferation, migration and hormone release. Thus, SGKs have recently generated substantial interest as therapeutic targets in cancer and diabetes. In this report, we describe the adaptation of an immobilized metal ion affinity-based fluorescence polarization (IMAP) kinase assay to screen 160 compounds from a kinase-focused small molecule library. We identified a group of compounds containing thiazolidinedione and pyrazine scaffolds that inhibit SGKs with IC50s in the low micromolar or submicromolar range. We further determined the inhibitory mechanism of 2 hit compounds which are KMU010402 based on thiazolidinedione scaffold and KMU010515 based on pyrazine scaffold. Kinetic analysis revealed that both compounds are competitive inhibitors against ATP.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Fasudil Analogue as MELK Kinase Inhibitors through High Throughput Screening (HTS)

최현정 이주연[1] 홍승우[*] 이광호[2,*]

한국과학기술원(KAIST) 화학과 [1]한국화학연구원 한국화합물은행 [2]한국화학연구원 신물질본부/난치성

MELK (Maternal embryonic leucine zipper kinase) is a snf1/AMPK family of serine/threonine kinases. It is associated with various cellular and biological processes including cell cycle progression, stem cell renewal, pre-mRNA splicing, apoptosis and embryonic development. Overexpression of MELK is often found in several human cancers such as prostate cancer, rectal cancer, gastric cancer, breast cancer, brain tumor, glioblastoma. High level of MELK overexpression is found in a basal-like breast cancer (BBC), suggesting MELK has critical role in BBC. MELK can be a novel target for treatment of BBC. To identify MELK inhibitors, We have conducted High Throughput Screening (HTS) against 13,472 compounds of KRICT library. We have get 81 compounds which inhibition activity over 44% on MELK under 5 μM treatment. Among them, we have selected novel Fasudil and performed enzyme assay, which is shown IC50=0.49 μM on MELK. This fasudil will be worth doing research further to treat BBC. Additional derivatization of fasudil is currently underway.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

The synthesis of chalcone derivatives and their protective effect against cisplatin-induced cyotoxicity in kidney cells

문성원 이재욱[1,*]

한국과학기술연구원(KIST) 천연물융합연구센터 [1]한국과학기술연구원(KIST) 천연의약센터

A series of chalcone analogues were prepared with various aryl aldehyde and acetophenone by treatment of aq. NaOH solution. These synthesized chalcone analogues were evaluated for any renoprotective effects on cisplatin-treated cultured kidney cells (LLC-PK1). Among these analogues, two chalcone analogues exhibited a potent renoprotective effect. In an additional study, we demonstrated that the blocking of MAPKs-p53-caspase-3 signaling cascade plays an important role in mediating the protective effect of these compounds against oxidative cytotoxicity in cultured LLC-PK1 cells.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Indirubin Derivatives as a New Class of DRAK2 Inhibitors

이나리 이주연[1] 이광호[2,*]

과학기술연합대학원대학교(UST) 의약화학 및 약리생물학 [1]한국화학연구원 한국화합물은행 [2]한국화학연구원 신물질본부/난치성

DRAK2(DAP Kinase-related apoptosis-inducing protein kinase 2), a serine/threonine kinase belonging to the death-associated protein kinase family acts as a negative regulator of TGF-β mediated signal transduction. DRAK2 is believed to promote tumorigenesis by limiting the TGF-β1 tumor suppressor activity. Besides cancer, it has also been found to play vital role in a variety of autoimmune diseases. In our efforts towards the discovery of small molecule inhibitor for DRAK2, we carried out high performance throughput screening compaign which resulted in the identification of indirubine-3'-monoximes as a novel class of DRAK2 inhibitors.

HTS Conditions

- **Assay format: 384 well plate**
- **Assay volume: 7.5 µl**
- **Compound number: 11,564**
- **[DRAK2] = 12.5 ng/well**
- **[MRCL3]= 1 µM**
- **[ATP] = 1 µM**
- **[compound] = 10 µM**

11,564 compounds

↓ **HTS, 10 µM**
% inhibition > 70%

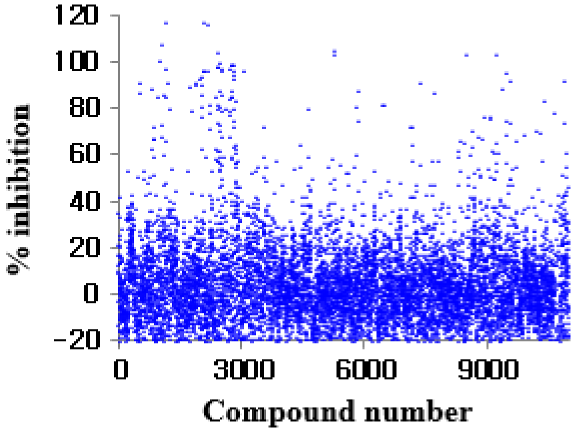
99 compounds

↓ **Hit confirmation, 10 µM**
% inhibition > 60%

56 compounds

↓ **IC_{50} (6 conc.)**

41 compounds



Potency IC_{50}(µM)	**N. of compounds**
$IC_{50} < 0.1$	7
$0.1 < IC_{50} < 0.5$	13
$0.5 < IC_{50} < 1.0$	5
$1.0 < IC_{50} < 5.0$	16

Fig.3. **High throughput screening.**

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발표분야: 의약화학
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Core-Shell 구조의 PLGA-PEG 이중블록공중합체를 이용한 방사성 의약품 개발

이상윤 이준영 김상욱* 김건균

동국대학교 신소재화학과

약물들의 부작용을 최소화하고 효과를 높이기 위한 새로운 고분자합성 및 고분자제제들이 각광을 받고 있다. 낮은 용해도로 인하여 제형화가 어렵고 낮은 생체흡수율을 보이는 소수성 약물들이 수용액상에서 잘 분산될 수 있는 가용화 시스템이 계속해서 개발되고 있는 가운데, 최근 고분자 Micelle 시스템이 난용성 약물 및 방사성의약품 치료 및 진단용으로도 많은 연구 및 개발이 되고 있다. Micelle 은 수용액 상에서 양친성 고분자의 자기집합으로 형성되며 이들의 독특한 Core-Shell 구조는 고분자 마이셀을 이용하는데 있어 많은 장점이 있다. 본 연구에서는 고분자 Micelle 의 제조를 위해 생분해성 고분자 원료인 PLGA [Poly(Lactide-Glycolide)]와 생체적합성 고분자인 PEG [Poly(ethylene glycol)]을 이용해여 양친성 이중블록공중합체를 합성 하였으며, 분광학적 분석장비(1H-NMR, FT-IR, UV-Vis)를 통해 합성여부를 확인 하였다.이중블록공중합체(Di-block-copolymer)에 약물 표적화 전달체계를 높여주기 위해 엽산을 도입하였으며, 암 진단 장비인 PET 영상 시약으로써 진단용 방사성동위원소인 124I 을 표지한 후 수용액 상에서의 자기 조립을 통하여 Micelle 구조의 나노입자를 합성하였다.사람 혈청에 대한 화합물 안정성평가는 나노입자 42 MBq 도입하여 15, 30, 60, 120 분 동안 진행한 결과 시간이 지남에 따라 Micelle 형태의 나노입자가 분해 되는것을 확인 할 수 있었다. 세포섭취도 평가는 KB, CT-26, A549 암 세포주를 대상으로 15, 30, 60, 120 분 그리고 12, 24 시간 까지 측정을 한 결과, 시간이 지남에 따라 Micelle 형태의 나노입자가 분해되면서 섭취도가 낮아지는것을 확인 할 수 있었다. PLGA-PEG-Folate&124I 이중공중합체 생분해성 고분자는 암 진단을 위한 양전자 방출 단층 촬영기(Positron Emission Tomography)의 이미징 시약으로 사용가능 할 것으로 전망된다.

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Biorelevant Temperature Effect on Physicochemical Properties of Drugs Comparing to a Prediction Method

<u>백규원</u> 한미정[1] 윤혜리[1] 강남숙[1,*]

Sirius Analytical Asia Support Chemist [1]충남대학교 신약전문대학원

The measurement of physicochemical properties of active pharmaceutical ingredients (API) such as ionization, lipophilicity, and solubility are very important to pharmaceutical development. In fact, the majority of published values for these properties are mostly determined under standard conditions, which mean a room temperature at 25 °C and a background electrolyte with 0.15M KCl. Famous softwares to predict these values from drug structures are supportive only for a room temperature. However, since drugs for oral delivery are theoretically considered at the physiological relevant temperature, it is necessary to verify if the biorelevant temperature of 37 °C has an effect for ionizable drugs to understand physicochemical behaviors. Therefore, this study aims to compare the values of physicochemical properties between a prediction software (ACD Labs/Percepta) and the actual measurement (SiriusT3, Sirius Analytical Ltd.) under the standard condition. Furthermore, the measurements at the biorelevant temperature (37 °C) were conducted and compared with the results of room temperature (25 °C) to figure out the temperature effect, so hopefully that it can provide accurate information and contribute to better in vitro-in vivo correlations (IVIVC) in future.

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Chemiverse: Search and Share Medicinal Chemistry

서영주 김한조 강경태 서용일 장병하 윤정혁[1,*]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

Though medicinal chemists have used random screening or high-throughput screening (HTS) in drug discovery research for the purpose of hit identification, they use more cheminformatics and molecular modeling techniques nowadays. The most straightforward example of these techniques is the virtual screening including molecular descriptor based filtering, QSAR model based filtering and docking simulation, which can be used for hit-to-lead and lead optimization process also. Virtual screening can reduce the time and money for tedious cycle of compound synthesis-activity(property) screening-structure modification and this is why virtual screening is widely adopted in pharmaceutical industry.Even though there are so many cheminformatics and molecular modeling tools available (many of them are free and open sourced even), molecular descriptor based filtering, QSAR based filtering or docking simulation is not readily usable for bench scientists. The tools should be easy for bench scientists. In the era of ‘Big Data’, chemical database should be updated fast enough for embracing the most up-to-date research information. Here we present ‘Chemiverse’, an integrated chemical database service combined with pharmacophore-based docking simulation tool called ‘PharosDre@ms3’. In chemiverse website, users can search desired chemicals from available chemical database (22 millions of unique structures) with several filters including molecular descriptors and QSAR models. The results of different search jobs can be saved in subsets which can contain any number of compounds. Pharmacophore based docking simulation can be launched by PharosDre@ms3 software for find-tuning of virtual screening results. Once getting the result of virtual screening, users can order compounds in any subset for biological assay campaign.

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Assessment of Kinase Selectivity Using Electronic Property Analysis of Water Network in Protein Binding Sites

장우대 이명휘 강남숙*

충남대학교 신약전문대학원

Protein kinases are a huge group of evolutionary and structurally conserved enzymes, which is the transfer of a phosphate group from ATP to other proteins. Several human kinases are involved in a large variety of diseases such as cancer and inflammation, so that they are of important drug target within the pharmaceutical industry. However, the design of selective inhibitors can be challenging due to showing a highly conserved binding site for ATP. Here we show that a novel method for classifying protein kinases predicts the selectivity based on the water-ring network in protein binding sites. To quantify the water-ring network in the binding site, we came up with a way to calculate the dipole moments of water-ring network at specific position in the ATP binding pocket. We found that the orientation of dipole moments is a critical role in protein-ligand binding mechanism. This solvent-centric approach can complement current theoretical methods that only consider steric and electrostatic properties of the protein surfaces.

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A Novel 2-Arylethynyl-substituted Pyrrolo pyrazine Derivatives as a Human Trasnglutaminase 2 inhibitor

Puttavva meti 김나연 이은실[1] 공영대[*]

동국대학교 화학과 [1]동국대학교 의약화학연구실

A transglutaminase is an enzyme that catalyzes the formation of an isopeptide bond between a free amine group. TGase 2 is associated with various diseases in particular it influences drug resistance in cancer cells. we have focused on the exploration of small novel molecules as a TGase 2 inhibitor as these kind of molecules have become good candidates to replace peptide based inhibitor drugs. After an initial screening of skeletal representative , ethynyl substituted pyrazine derivatives showed strong inhibition properties against TGase 2 activity. In order to discover better drug like compounds we have designed new core skeletons based on the bioisostere concept. We have tried to develop core skeleton by changing the quinoxaline ring. An unprecedented core skeleton that could improve the physiological properties and cell proliferation compared with quinoxaline compound in renal cancer cells.

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Efficient construction of 2-aminothiazolopyrazine derivatives via tandem reaction on the solid-phase synthesis

ABDILDINOVA AIZHAN 양승주 공영대*

동국대학교 화학과

Combinatorial chemistry is a strategy for quick access to molecule libraries with an emphasis on diversity. Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Especially various bicyclic nitrogen-containing heterocyclic compounds can serve as the core components of many substances that possess a wide range of interesting biological activities. In this family, N-substituted-2-aminothiazolopyrazine derivatives can be used as privileged scaffolds to produce substances of interest in numerous therapeutic areas, such as anti-inflammatory, anti-microbial, anti-cancer, etc. In this reason, we used tandem reaction of 2-aminohalopyrazines with benzyl isothiocyanate for the cyclization reaction of thiazolopyrazine intermediate to synthesis N-substituted-2-aminothiazolopyrazine analogues. The resulting N-substituted-2-aminothiazolopyrazine core skeleton was functionalized with various electrophiles, such as alkyl halides, acid halides.

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Novel 3-arylethynyl-substituted furo[2,3-b]-pyrazine derivatives as human transglutaminase 2 inhibitors

전희구 김은미 이은실[1] 공영대*

동국대학교 화학과 [1]동국대학교 의약화학연구실

Transglutaminase 2, known as calcium-dependent enzyme, plays a variety of roles in the biological process. For instance, Transglutaminase 2 performs transamidating function via forming isopeptide bonds. Up-regulated transglutaminase 2 is also associated with many diseases like fibrosis, certain types of cancer, Alzheimer's, Huntington's and Parkinson's diseases. During oncogenesis, transglutaminase 2 leads to NF-κB activation which is involved in the drug resistance and metastasis. As a result, we established a target to transglutaminase 2 and synthesized new 3-arylethynyl-substituted furo[2,3-b]-pyrazine derivatives as transglutaminase 2 inhibitors through core skeleton optimization precess.

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Synthesis of a Novel N-five-membered-heterocycle-N',N"-disubstituted guanidine derivatives as S-nitrosoglutathione reductase inhibitor

임수정 유현정 공영대*

동국대학교 화학과

S-Nitrosoglutathione reductase (GSNOR) regulates a level of S-nitrosoglutatione (GSNO) in human lungs. GSNO is an endogenous bronchodilator that elicits many biological functions of NO, increases of which are associated with dilation of bronchi and bronchioles and the bronchial smooth muscle relaxant effects. In human asthma, via the GSNO reductase overexpression, the GSNO and NO concentrations are lower and then bronchoconstriction and airway allergens occurs. Therefore GSNOR has emerged as a potentially important target for the treatment of asthma. These results implicate GSNO metabolism as a target for therapeutic intervention of asthma. In previous study, we focused our effort to construct benzopyran derivatives, which showed goal biological activity to inhibit S-nitroglutathione reductase. Now we are turn our interest to a synthesis of five-membered heterocycle derivatives equipped with N',N"-disubstituted guanidine as a novel small organic drug-like lead compound without side-effect of existing Asthma drugs.

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토착 외래종 천연물의 지표성분 변화에 관한 연구

김영석 황병수[1] 김규선[2] 함정엽[1,*]

강릉원주대학교 화학신소재학과 [1]한국과학기술연구원(KIST) 천연물연구소 [2]강릉원주대학교 해양자원육성학과

최근 지구 온난화로 인한 기후 변화와 글로벌화로 인한 나라간의 교류가 활발해지며 국내에는 300 여종의 외래종 식물들이 자생하고 있다. 많은 외래종 식물들이 국내에 토착되면서 이를 유용자원을 활용하기 위한 연구가 진행되고 있고 다양한 결과들이 발표되고 있으며, 대표적인 예로 가시박을 들 수 있다. 북아메리카가 원산지인 가시박(Sicyos angulatus)은 국내산 가시박과 일본 가시박을 비교하였을 때 분리된 flavonoid 성분에 차이가 있는 것으로 보고되었다. 이처럼 외래종 식물들이 국내에 유입되고 이 천연물들의 연구가 진행되면서 유용지표성분에 차이가 있는 것들이 발견되고 있다. 본 연구에 사용된 쥐꼬리망초는 문헌검색 결과 중국, 일본, 타이완 등에서 lignan 계열 화합물인 Justicidin 의 다양한 생리활성이 보고되었고, 지역에 따라 유용성분에 차이가 있음을 확인할 수 있었다. 하지만 국내에서는 쥐꼬리망초에 대한 연구가 미비하여 자원으로써의 활용도를 조사한바 없다.따라서 본 연구진은 국내에서 채집한 쥐꼬리망초가 다른나라와 비교하여 어떠한 유용지표성분을 함유하고 있는지 연구하였고 이에 대한 결과를 발표하고자 한다.

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Efficient Photosensitization of Chlorin-Polyoxometalate and Chlorin-Gold Nanorod Complexes

윤일* 심영기[1]

인제대학교 PDT 연구소 [1]인제대학교 나노융합공학부

We prepared 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.In addition, GNR?PS complex was prepared using anionic PS (sodium salt of purpurin-18) and cationic poly(allylamine hydrochloride) by layer-by-layer method, and was characterized by transmission electron microscopy, UV-vis spectroscopy, and zeta potential. The GNR?PS complex is a promising agent for synergistic (photothermal and photodynamic) therapy (PTT/PDT), in which PTT generates heat as well as operates the PS release which maximize the following PDT activity. The combined dual therapy, PTT followed by PDT, exhibits a significantly higher photocytotoxicity result based on synergistic effect of hyperthermia from PTT as well as singlet oxygen photogeneration from PDT.

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Design, Synthesis, and Biological Evaluation of Small Molecule as Hsp90 inhibitor

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계명대학교 약학과 [1]계명대학교 약학대학

Most single-target drug encounters the emergence of drug-resistance in long-term use. The tumor cells outsmart single-target 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 a ubiquitous and abundant ATP-dependent molecular chaperone, which plays a key role in the conformational maturation, activation, stability and function of numerous intracellular signaling pathways, utilized by cancer cells for proliferation and survival. Hsp90 is documented to interact with more than 200 different “client” proteins involved in signal transduction, receptor maturation and protein trafficking. Most of Hsp90 clients are oncoproteins, including MET, Akt, Raf-1 MMP-2 and HIF-1α, all of which exist in various signaling pathways for the survival, proliferation, invasion, metastasis, and angiogenesis of cells. Accordingly, the inhibition of Hsp90 function promotes degradation of its client proteins, which can eventually lead to cell death. Besides, Hsp90 would also seem to have higher affinity toward small-molecule inhibitors in tumor cells than in normal cells. For this reason, Hsp90 has emerged as an interesting molecular target for developing new anticancer agents against several malignancies and some of them are currently tested clinical trials. 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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Design and Synthesis of Heat Shock Protein 90 inhibitors to impair the growth of Non-small cell lung cancer (NSCLC)

최명아 서영호[1,*]

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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 EGER 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. Considering both EGFR and Met are client proteins of Hsp90, blocking Hsp90 folding machinery may be best suited to overcome the resistance form EGFR mutation and Met amplification. Heat shock protein (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 ten essential hallmarks of cancer. Its client proteins include EGFR, Her2, Met, Akt, Raf, HIF-1, and MMP2. Hsp90 is overexpressed in tumor cell more than normal cell. Hsp90 inhibitor can lead to the degradation of a large collection of oncogenic proteins. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways. In this study, we designed and synthesized a number of inhibitors and they disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer (H1975). The result suggested that these compounds could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

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Structure-based drug design of Hsp90 inhibitors and their anti-proliferative effects against cancerous diseases

정주희 서영호[1,*]

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Heat shock proteins 90 (Hsp90) is a ATP-dependent chaperone that is required 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-a. 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. In this study, we had performed a structure-based drug design (SBDD) of small molecule inhibitors against Hsp90. Designed inhibitors were synthesized and their antitumor activities were evaluated. Consequently we discovered potent compounds with nanomolar efficacy. Our data indicates that the compound can serve as a novel clinical against Hsp90 in cancer.

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Pim kinase inhibitors: a novel series of 3,5-disubstituted Indole derivatives

MORE KUNAL HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

Pim kinases are first identified as a proviral integration site in Moloney murine Leukemia virus (MuLV) induced in T-cell lymphomas. Pim kinases are a small family of kinases comprising of highly homologues members as Pim-1, 2 and 3. They are proto-oncogenes with serine/threonine kinase activity. Over-expressed Pim kinases may lead to progress of solid tumors such as colon, prostate and hematologic malignancies including lymphomas, chronic lymphocytic leukemia and acute leukemias. Thus inhibition of Pim kinase activity might be a promising strategy for the treatment of cancers. 3,5-Disubstituted indole scaffold is known to possess kinase inhibitory activity. Previous reports also suggested that 3,5-disubstituted indoles are potent inhibitors of Pim kinases. In this study, a novel series of 3,5-disubstitued indole have been synthesized and evaluated against Pim kinases. Structure activity relationship at 3- and 5-positions of indole was also performed to understand effect of substituent variation on Pim kinase inhibition activity. Synthesized compound showed very potent activity as low as single digit nanomolar IC50.

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Synthesis and biological evaluation of 1,3-disubstituted benzene derivatives as Pim kinases inhibitors

이아연 **HONG VICTOR SUKBONG[1]** 이진호[1,*]

계명대학교 유기화학전공/화학과 [1]계명대학교 화학과

Pim kinases are serine/threonine kinases and are mainly involved in signal transduction such as survival, proliferation, cell cycle, and cellular metabolism. Overexpression of Pim kinases has been reported to cause leukemia, lymphoma and solid tumors such as prostate cancer. Thus, based on the role of Pim kinases in normal and tumor tissues, it is clear that this kinases are an interesting target for the development of anti-cancer agents. The present report describes the discovery of a new class of Pim inhibitors. A novel series of 1,3-disubstituted benzene derivatives were designed and synthesized. Introduction of the functionalities, one interact with ammonium group of lysine and the other interact with carboxylate group of aspartate and glutamate of Pim kinases, in optimal positions provided the compound with Pim kinases inhibitory activities. The synthesized compound showed potent inhibitory activities against Pim kinases. The most potent compound exhibited IC_50s of 0.029μM for Pim-1 and 0.065μM for Pim-3.

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1,2,3,4-Tetrasubstituted benzene as Pim kinase inhibitors: Synthesis and Biological evaluation

강지희 HONG VICTOR SUKBONG[1] 이진호[1,*]

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Pim kinases, proviral integration site for moloney murine leukemia virus kinases, are consisting of three isoforms Pim-1, Pim-2, and Pim-3. Pim kinases are constitutively active enzymes whose activity is mainly regulated by their gene transcription and protein translation. Pim kinases regulate several signaling pathways that ultimately control the balance between cell survival and apoptosis. Pim kinases are proto-oncogenic serine/threonine kinases that have been shown to be overexpressed in a number of human malignant tumors such as myeloid leukemia and lymphomas. Pim kinases are one of the attractive target for the development of cancer therapy. The present work describes the discovery of Pim kinases inhibitors with high potency. Novel series of 1,2,3,4-tetrasubstituted benzene derivatives were designed and synthesized. Synthesized compounds showed potent inhibitory activities against Pim kinsase. The most potent compound exhibited IC50s of 0.033μM for Pim-1, 0.120μM for Pim-2 and 0.027μM for Pim-3.

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Design and Synthesis of New Potent Anti-Hepatitis C Virus (HCV) Agents

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The virus-encoded non-structural protein 5A (NS5A) has attracted the attention of contemporary medicinal chemists. NS5A is a multifunctional protein which is essential for HCV replication and has been implicated in Interferon (IFN) resistance in vivo. Targeting NS5A, some symmetric and asymmetric heterocyclic compounds were synthesized and evaluated for their activity compared to BMS-790052 (Daclatasvir) as a reference compound. As revealed from the bioassay results over HCV cell line, most of the investigated compounds displayed promising anti-HCV activities (EC50 in picomolar ranges). As an example, KK6147 showed EC50 value of 1.85pM in Genotype 1b Replicon Assay. In addition, several other compounds showed efficacies on HCV resistant mutants. Taken together, these series of compounds could be good candidates for new potent Anti-HCV agents.

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Quantitative 18F-Labeling at room temperature via Al18F Chelation

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18F is the most commonly used radionuclide for PET imaging. Its half-life of approximately 110 min is suited for same-day imaging of many compounds that clear quickly from the body to allow visualization of uptake in the intended target. Recently, 18F-labeling method using Al?F complex in aqueous solution was devised and offered a straightforward 18F-labeling procedure. The radiolabeling of various chelates with Al-18F at high temperature (~100-110oC) is very well documented in literature1. The major drawback of implementation of higher temperature is unsuitable for radiolabeling of heat sensitive biomolecules. So facile method for radiolabeling at lower temperature is highly needed. We developed a procedure in which the Al18F complex could be quantitatively labeled at room temperature. Furthermore, the in vitro and in vivo stability studies are under process.

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Synthesis and biological property of 7,9-dideaza-7-oxa-adenosine derivatives

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For the synthesis of new branched purine C-nucleosides, we tried to prepare 3-amino-4-(3,4-bis(benzyloxy)-5-(benzyloxymethyl)tetrahydrofuran-2-yl)furan-2-carboxamide involving the LDA-promoted cyclization of cyano ether with furan C-nucleoside which are not the mixture of α and β anomer, only one β form compound. From the 3-amino-4-(3,4-bis(benzyloxy)-5-(benzyloxymethyl)tetrahydrofuran-2-yl)furan-2-carboxamide, we obtained unknown C-nucleosides. We will introduce biological property of these compounds.

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Reactivation of paraoxone-inhibited acetylcholinesterase by monoquaternary pyridinium oximes with N-alkylbromide side chains

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Organophosphorus nerve agents cause neurotoxicity through the inhibition of acetylcholinesterase (AChE) in the human body. Thus, various oxime reactivators were discovered to reactivate the inhibited AChE. Pralidoxime (2-PAM) is one of these representative oxime antidotes. However, its reactivation ability, as well as its action on the inhibited AChE of the central nervous system is not sufficient, and therefore the discovery of new oxime reactivators is required. Here, oximes with N-bromoalkyl groups were synthesized, and their reactivation potency on AChE inhibited by paraoxon was evaluated.

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Stimulus Induced Targeted Drug Delivery with Mesoporous Silica Nanoparticles by Biocompatible Peptide Gatekeepers

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Among the drug delivery carriers, mesoporous silica nanoparticles (MSN) have received wide attention due to their tunable pore morphology, high specific surface area, easy surface modification/ bioconjugation for targeting and physiochemical stability. They can host the therapeutic compounds due their void cores, as extra reservoir for drug storage. In recent years, colloidal stability and biodegradability of the nanocarriers have received significant attention for biomedical applications. In the present work, we have developed colloidal and biodegradable raspberry type mesoporous silica that possess fluorescent property for biomedical applications. Drug can be loaded into the pores of the carrier at large quantity. Recently, non-covalent gatekeepers have received significant attention towards encapsulation stability. Hence, we installed a biocomptable protein gatekeepers on the surface of drug loaded carriers. The GST-affibody possess important role in undergoing degradation in the excess intracellular glutathione (GSH) environment. Further, this affibody can be conjugated with different types of antibody to target specific cancer cells to achieve a stable and biocompatible carrier for biomedical applications.

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N-Arylations of Sterically Hindered NH-Nucleophiles: Cu-Mediated Syntheses of Diverse N-Aryl Indole-2-carboxylates

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The syntheses of various N-aryl-substituted indole-2-carboxylates have been accomplished. Using CuO/K2CO3/pyridine conditions for 2-bromopyridine derivatives and CuI/N,N'-ethylenediamine/K3PO4 for bromobenzene derivatives, the desired N-arylations of indole-2-carboxylates were performed in good to excellent yields. These stoichiometric Cu-mediated conditions enable the coupling of indole-2-carboxylates with various arylbromides, which have been not so successful, due to the steric bulkiness of NH-nucleophiles and weak nucleophilicity. These results will expand the scope of metal-catalyzed N-arylation using heterocyclic amines with steric bulkiness and weak nucleophilicity.

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Chemotherapeutic potential of Hsp90 and biological evaluation of a novel Hsp90 inhibitor

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Heat shock protein 90 (Hsp90) is an ATP-dependent molecular chaperone that plays an important role in regulating many proteins involved in signaling pathway and cell proliferation. Once identified in 1987 as one of the most abundant intracellular proteins, Hsp90 has received considerable attention and emerged as an attractive cancer therapeutic target, due to its chaperoning function of the substrate proteins. The substrate proteins, referred to as client proteins includes many oncology targets such as p53 mutants, Raf1, Bcr-Abl, EGFR, Her2, Met, Cdk4, Akt, HIF and MMP2. In this regard, inhibition of Hsp90's chaperoning function induces simultaneous blockage of several signaling pathways in tumor cells so as to overcome the inevitable drug resistance of conventional cancer therapeutic agents. Therefore, the potential therapeutic benefits associated with Hsp90 modulation emphasize the importance of identifying novel Hsp90 inhibitors.In this study, we discovered that JJH-5-136 disrupted Hsp90 chaperoning function and impaired the growth of cancer cells. The result suggested that JJH-5-136 could serve as a novel Hsp90 inhibitor to improve anti-cancer effect in cancer chemotherapy.

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Design and Synthesis of Potent & Selective DRAK2 Inhibitors

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Death-associated protein-kinase-related 2 (DRAK2) is expressed especially by lymphocytes and is a member of the death-associated protein (DAP)-like family of serine/threonine kinases, which induce apoptosis when overexpressed by cell lines. DRAK2 protein blocks the in vivo mechanism of action of TGF-beta inhibits the growth of cancer, and induces cell growth of metastatic breast cancer. DRAK2 kinase protein is an important molecular target for the growth of triple negative breast cancer cells. We performed a High Throughput Screening (HTS) of 11,564 compounds of KRICT library and in silico screening. Also, we investigated the literature and known scaffold. Herein we report the discovery of potent and selective DRAK2 inhibitors.

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Novel drug delivery system for cancer therapy that dual targeting SSTRs and Cathepsin B

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The currently available anticancer agents frequently cause unwanted normal cell death mainly owing to their lack of selectivity for cancer cells. In addition, molecular imaging agents for tumors exhibit low target-to-background ratios. As a consequence, elegant methods that more specifically target cancer cells need to be developed for the improvement of chemotherapeutic efficacy and diagnosis. In a recent effort aimed at improving the tumor selectivity of therapeutic and imaging agents, we designed, synthesized and explored the effectiveness of a dual-targeting delivery system that targets cancer cells more selectively. The new delivery system is composed of a synthetic ligand (octreotide) of somatostatin receptors, a dipeptide substrate for cathepsin B, and a fluorophore or an anticancer agent. The fluorophore-conjugated delivery system was found to be applicable for specific fluorescence imaging of cancer cells that express both somatostatin receptors and cathepsin B. In addition, the anticancer agent containing delivery system leads to the death of cancer cells specifically. In contrast to cancer cells, normal cells that do not produce both somatostatin receptors and cathepsin B at high levels are unaffected by the delivery system. The new dual-targeting approach has the capability of overcoming obstacles associated with current chemotherapeutic and imaging methods.

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Rational Design, Synthesis And In-Vitro Anticancer Activities Of New Anilinoquinolines As Conformationally Restricted Sorafenib Congeners With Potential RAF Kinase Inhibitory Effects

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Two new series of C-5 and C-6 picolinamide based 2-anilinoquinolines have been designed and synthesized as antiproliferative sorafenib analogues. Fourteen compounds of the synthesized derivatives were selected for preliminary appraisal of their cellular anticancer activities against a panel of 60 human cancer cell lines at National Cancer Institute (NCI, USA). Based on the promising results of both compounds 6d and 6j, they were further tested at 5-dose testing mode. The obtained data revealed that compound 6j is the most potent derivative with submicromolar GI50 values over a number of cancer cell lines. Furthermore, the RAF Kinase inhibitory activity for the best compound 6j along with its corresponding positional isomer 10a was performed. Such assay results demonstrated that the C-6 is the proper position for picolinamide moiety to achieve RAF inhibitory activity.

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Search for the bioactive compounds from Myagropsis myagroides

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Myagropsis myagroides is a member of the family of Sargassaceae and its extract has shown various biological activities. The organic solvents extracts of M. myagroides has shown biological activities such as antioxidant activity, anticholinesterase activity. From the 100% ethyl acetate extract of M. myagroides, solvent partition fractions showed strong BuChE inhibitory and antioxidative activity. Finally, two cmpounds, O1-S1-13(compound A) and O1-S1-21-5(compound B) were isolated. The molecular formular of compound A was determined as $C_{11}H_{15}O_2$ by high resolution ESIMS. The structure determination of compoound B was attempted using various NMR experiments. The progress of the structure determination of Compounds A and B will be presented. Generally, compared to compound A, compound B showed higher DPPH radical scavenging activity and BuChE inhibitory activity. For compound B, DPPH scavenging activity was 73.4% at 100 μg/mL and RC50 value was 30.0 ± 0.02 μg/mL. Also BuChE inhibitory activity of compound B was 72.8%at 100 μg/mL and RC50 value was 4.76 ± 0.02 μg/mL. In conclusion, the two compound A and B from M. myagroides showed good antioxidant activity and BuChE inhibitory activity.

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약물 전달체인 Iodine이 결합된 실리카 나노 볼의 체내 유동성 및 표적 지향성 향상을 위한 pH 감응 미셀 도입

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동국대학교 신소재화학과

이 연구의 목적은 pH 에 감응하는 고분자 미셀을 도입하여 암 진단을 위한 방사성의약품의 약물전달체로 사용할 실리카 나노 볼의 표적지향성과 체내 약물 전달능력을 향상시키는데 있다. 실리카 나노 볼의 큰 비표면적은 다양하고 많은 약물을 담지하기에 적합하다. 또한 실리카 나노 볼은 체내에서 낮은 세포독성과 낮은 면역 거부반응을 가지고 있어 약물 전달체로서 널리 연구되어지고 있는 반면 분산도가 작아 체내에서 유동성이 낮은 단점이 있다. pH 감응형 고분자 Methyl ether poly(ethylene glycol)-poly(β-amino ester) block copolymer (MPEG-PAE)는 중성 조건에서 미셀의 형성하지만 약 산성 조건에서 이온화에 의한 미셀 붕괴가 특징이다. 이 특징을 이용하여 약물을 미셀 화 하면 약 산성 조건인 암세포 주변 환경에서 약물을 방출 할 수 있다. 그 뿐만 아니라 미셀은 수용성 분산도가 높아 실리카 나노 볼의 낮은 분산도를 보완하여 약물 전달체로서 가능성을 향상 시킬 수 있다. MPEG-PAE 는 분광학적 분석장비 (1H-NMR, 13C-NMR, FR-IR)을 통해 합성여부를 확인 하였다. 양전자단층촬영기(PET)의 방사성 추적자로 이용할 수 있는 양전자 방출핵종인 I-124 를 표지할 전구체로서 안정동위원소인 I-127 이 결합된 실리카 나노 볼은 졸-겔법을 이용하여 합성하였고, Bolton-Hunter 시약을 이용하여 I-127 을 실리카 나노 볼에 결합 시켰다. 분광학적 분석장비 (I-NMR, XRD, FR-IR)와 전자주사현미경(SEM)을 통하여 합성 여부를 확인하고 실리카 나노 볼의 직격이 30 nm 임을 확인하였다. 최종적으로 I-127 이 결합된 실리카 나노 볼을 pH 감응형 고분자로 미셀 화 하였고 지용성 평가를 통해 확인한 결과 실리카 나노 볼의 수용성 분산도가 향산된 것을 확인 할 수 있었으며 수력학적 크기의 변화를 통해 미셀이 약 산성 조건에서 붕괴되는 것을 확인 하였다.

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Development of Butyrylcholinesterase Inhibitors Using Xanthotoxol Derivatives

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We are looking for new candidate compounds applied as cholinesterase inhibitor. A series of xanthotoxol hybrid molecules were synthesized and their *in vitro* cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated. Xanthotoxol itself exhibits low inhibitory activity against both cholinesterases, but hybrid molecules demonstrated only BuChE inhibitory activity. Specifically, the IC_{50} values of 9-(benzyloxy)-7H-furo[3,2-g]chromen-7-one and 9-(3-chlorobenzyloxy)-7H-furo[3,2-g]chromen-7-one for BuChE were shown to be 1.89 ± 1.28 and 1.51 ± 0.93, respectively. They were effective inhibitors against BuChE and their activity is comparable to that of galantamine (IC_{50} = 1.7 ± 0.9 μM against AChE and IC_{50} = 9.4 ± 2.5 μM against BuChE). Xanthotoxol hybrid molecules can be novel candidate compounds applied as cholinesterase inhibitor.

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Clicked Synthesis of Purpurinimide Derivatives for Photodynamic Therapy

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Photodynamic therapy (PDT) is based on the accumulation of a photosensitizer (PS) in tumors, for which given exposure of light at an appropriate wavelength generates reactive oxygen species (ROS, e.g. singlet oxygen) that results in tumor destruction.Photodynamic study of PSs having various functional groups, those can generate shift of wavelength of maximum absorption and biological efficiency, will cause the more convenience about the prediction and control of the photodynamic properties of PSs.In this study, purpurinimide methyl ester derivatives were synthesized using N-propargyl-purpurinimide methyl ester as starting material. The derivatives were synthesized by 1,3-dipolar cycloaddition of N-propargyl-purpurinimide methyl ester containing a terminal triple bond and azide derivatives containing various functional groups. The click reaction, which was carried out using 10 mol% of copper(I) iodide in acetonitrile with an addition of diisopropylethylamine (DIPEA).Each derivative was characterized by a combination analysis using 1H-NMR and IR spectroscopies for structure determination, configurations and functional groups as well as UV-vis spectroscopy for shift of wavelength of maximum absorption.For photodynamic effect of the derivatives, photoactivity was investigated by MTT assay against A549 and HeLa cell lines. And then, each photodynamic result was compared with previous studies for the cationic chlorins.

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Synthesis and characterization of covalent bonded chlorin derivatives on graphene oxide nanosheets for photodynamic theraphy

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Photodynamic therapy (PDT) is a relatively new cancer modality that uses light, photosensitizer (PS), and oxygen for the treatment of various forms of cancer using photodynamic action. The PDT treatment derives great promise from the dual selectivity that is produced by both a preferential uptake of the drug by the diseased tissue and the restriction of carefully regulated light absorption onto the specific tumor sites.Graphene, a very recent rising star material, having an atomically thin, 2D honeycomb lattice that consists of sp2-hybridized carbons, exhibits remarkable electronic, thermal, optical, and mechanical properties. Particularly, graphene oxide (GO), graphene's hydrophilic derivative, has been found important potential applications in drug delivery due to their large specific surface area and abundant functional groups (epoxide, hydroxyl, and carboxyl groups).GO nanosheets were prepared by a modified Hummers' method. Chlorin derivatives having versatile functional groups (carboxyl, hydroxyl, aldehyde, amine) were synthesized from chlorophyll-a paste followed by extraction, oxidation, and imide formation. The chlorin derivatives were covalent bonded on the GO nanosheets through various synthetic methods contain coupling reactions (-COO- bond), click reaction (triazole ring formation), and N-alkylation (N-C bond) reaction. Finally, the covalent bonded chlorin derivatives on the GO nanosheets were characterized using a combination analysis by FT-IR, NMR, UV-vis, Raman spectroscopies, XPS and TGA analyses, and TEM images.

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Comparison study of Photoactivity of MPPd-Oxime derivative and HPPH(Photochlor)

김혜정* 심영기[1,*] 윤일[2]

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Photodynamic therapy (PDT) is based on the accumulation of a photosensitizer (PS) in tumors, for which subsequent light irradiation using an appropriate wavelength generates cytotoxic agents (reactive oxygen species, e.g. singlet oxygen) result in tumor destruction.In this study, we introduced an oxime group, which has shown good activity as antifungal agents, and have synthesized a new PS, 2-hexyl-oxime-methyl pyropheophorbide-d (HPPd-oxime derivative) for a comparison study of photoactivity with 2-(1-hexyloxyethyl)-2-devinyl pyropheophorbide-a (HPPH, photochlor?) which is a representative PS under application for a FDA admission.HPPd-oxime derivative was synthesized from chlorophyll-a paste followed by an extraction, elimination, oxidation, oxime addition, and finally O-alkylation. HPPd-oxime derivative and HPPH were characterized by a combination analysis of UV-vis absorption and 1H-NMR spectroscopies, and high resolution FAB mass spectrometry. Replacement of nitrogen atom on HPPd-oxime derivative caused a red-shift of both absorption and fluorescence emission bands compared with those of HPPH, which apparently due to electronegativity change. Finally, photoactivity results of HPPd-oxime derivative and HPPH were obtained using MTT assay against A549 and HeLa cell lines.

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The Discovery of 2,5-Isomers of Triazole-pyrrolopyrimidine as Novel Selective and Potent Janus Kinase 2 Inhibitors

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Members of the Janus kinase (JAK) family are potential therapeutic targets. Abnormal signaling by mutated JAK2 is related to hematological malignancy, such as myeloproliferative neoplasms (MPNs) and tyrosine kinase inhibitor (TKI)-resistance in non-small cell lung cancer (NSCLC). We discovered a potent and highly selective JAK2 inhibitor based on the structure of 4-(2,5-triazole)-pyrrolopyrimidine. (1) Among all triazole compounds, 2,5-triazole regioisomers more effectively inhibited JAK2 kinase activities than other isomers with substitutions of various alkyl groups at the R_2 position, except for methyl substituted 1,5-triazole, which was more potent than the corresponding 1,4- and 2,5-triazoles. (2) None of the synthesized 1,4-isomers inhibited the three JAK family members. (3) Compounds with phenyl or tolyl group substituents at the R_1 position were completely inactive compared with the corresponding methyl substituted analogues at the R_1 position. As a result of this structure-activity relationship, 54 substituted with a cyclopropylmethyl moiety exhibited significant inhibitory activity and selectivity. (IC_{50} = 41.9 nM, selectivity fold JAK1/2 10.6 and JAK3/2 58.1). Compound 54 exhibited equivalent inhibitory potency of wild type JAK2 and the V617F mutant. Moreover, 54 inhibited the proliferation of HEL 92.1.7 cells, which feature JAK2 V617F, and gefitinib-resistant HCC827 cells; compound 54 also suppressed STAT3 phosphorylation of Y705.

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Development of folate conjugated Fe_3O_4 nanoparticles for dual functions : diagnosis and treatment of cancer

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동국대학교 화학과

Isotope-magnetic NPs for dual modality PET/MRI imaging provide an opportunity to combine the power of MRI and PET, which has better anatomical resolution with the sensitivity for diagnosis of cancer.Chemotherapy is the most major therapeutic approach among conventional treatment. However, many chemotherapeutic agents can freely diffuse in both normal cell and cancer cell. The non-specific cytotoxicity presents severe side effects. For solution of this drawback, Nanosized drug delivery can lead enhanced accumulation in tumor through the enhanced permeability and retention (EPR) effect.In this present work, nanocomposites were designed and successfully synthesized using Folic acid conjugated Fe_3O_4 NPs and ^{68}Ga radioisotope dual applications of diagnostic imaging agent in Positron Emission Tomography (PET) and Magnetic Resonance Imaging (MRI). Also, Doxorubicin(DOX) as antineoplastic agent was loaded to the NPs for treatment of cancer.The ^{68}Ga-SCN-NOTA-folate-Hydrazine-Fe_3O_4 NPs (^{68}GaNFHFCNP) as targeted compound were synthesized via surface modified Fe_3O_4 NPs and NOTA as bi-functional chelating agent with ^{68}Ga radioisotope from an in-house generator. DOX was loaded via the intermediate DOX-Fe^{2+} to the NPs. Thus ^{68}GaNFHFCNP could exhibit synergic property such as the magnetic behavior and radio activity for diagnosis and cytotoxicity for treatment.

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인삼의 신규가공법을 통한 유효성분 및 피부암 억제 활성 극대화 연구

김관태 최필주 김태정 함정엽*

한국과학기술연구원(KIST) 천연물연구소

인삼은 다양한 질병의 예방과 치료, 건강증진을 위해 전통적으로 사용되어 왔고 지금도 널리 사용되고 있는 한약재로 최근 들어 중국을 비롯한 세계 각국에서도 주목 받고 있는 약용 식물이다. 특히 인삼에 포함된 사포닌인 진세노사이드를 활용한 항산화, 항암, 항염증, 항바이러스, 기억력 개선, 면역증진, 신경조절, 간 보호, 혈당저하 및 지방흡수 조절작용 등의 연구결과가 지속적으로 보고되고 있으며, 이렇듯 다양한 생리활성연구는 그 폭이 더욱 넓어지리라 판단된다. 한편, 여러 가공인삼 중 가장 잘 알려진 홍삼에는 진세노사이드 Rg3, Rk1, Rg5 등이 포함되어 있는데, 이로 인해 기존의 인삼과 비교하여 항암 활성이 월등하고 혈관 이완 작용, 혈소판 응집 억제 효과 등의 생리 활성이 있음이 밝혀져 왔고 새로운 약리 활성에 대한 연구가 계속 활발히 진행 중이다. 또한 이렇게 인삼을 가공하여 활성을 증진시킬 수 있는 바, 새로운 가공방법도 계속해서 보고되고 있다. 현대 사회에서는 암으로 인한 사망률이 급격히 증가하는 추세이고 이는 사회적, 경제적으로 엄청난 비용이 발생됨으로써 국가적으로 문제가 되고 있는 상황이다. 여러 암 중 피부암은 과거에는 국내 유병률이 높지 않은 암이었지만 최근 그 빈도가 늘고 있다. 자외선 노출 과다, 환경 오염 등의 이유로 국내에서도 증가 추세에 있는 피부암은 전이가 잘 되고 기존 항암제로 억제하기 어려운 난치성 특징이 있어 위험한 암이다. 이에 본 연구에서는 새로운 가공처리 방법을 이용하여 진세노사이드 Rg3, Rk1, Rg5 의 함량을 높인 인삼추출물을 이용하여 난치성 암종인 피부암에 대한 항암활성 효과를 확인하였다.

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Regioselective bromination of 1,10-phenanthroine derivatives

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Recently bromine substituted 1,10-phenanthroline and their metal complex have received considering attention because their important intermediates in synthetic and medicinal chemistry. The direct and selective bromination of phenanthrolines have reported in low yield by phi-bond deficient aromatics containing nitrogen. A simple synthesis of 3-bromo-1,10-phenanthroline derivatives by reaction with NBS or Br2 in the several conditions is presented herein. The 3-bromo-1,10-phenanthroline underwent various nucleophilic substitution or Suzuki coupling to give 3-substituted 1,10-phenanthroline.

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Quinoline Derivatives as Kinetic Stabilizers of Transthyretin to Prevent Amyloidogenesis

박황규 최성욱*

충남대학교 신약개발학과

Transthyretin (TTR) is a homotetrameric protein composed of 127-amino-acid, β-sheet-rich subunits. The established physiological functions of TTR are to bind to and transport the thyroid hormone thyroxine (T4) and holo-retinol binding protein in the blood and cerebrospinal fluid (CSF). TTR is one of more than 30 nonhomologous human amyloidogenic proteins, whose misfolding and/or misassembly appears to elicit the proteotoxicity and cell degeneration, which cause the amyloidoses.TTR fibril formation requires the rate-limiting tetramer dissociation and misassembly of partially denatured monomeric subunits. Small molecules that bind to T4 binding site stabilize the ground state of tetrameric TTR and raise the kinetic barrier for dissociation, imposing kinetic stabilization on TTR and preventing aggregation.Tafamidis has recently completed Phase II/III trials for the treatment of Transthyretin Type Familial Amyloid Polyneuropathy (TTR-FAP) and demonstrated a slowing of disease progression for the V30M TTR mutation. Herein we show that the quinoline derivatives to design for binding unoccupied T4 sites of the tetramer were synthesized and evaluated possibilites as kinetic stabilizers of WT TTR and V30M TTR mutation compared with Tafamidis.

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Synthesis of fluorescent probes based on quinolone sensing of Cu^{2+} ions and acidic pH

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충남대학교 신약개발학과

Synthesized quinolone derivatives turn up with a fluorescence enhancement at specific environment. The fluorescence intensity of a probe was enhanced in the dependent on Cu^{2+}-concentration, and it can selectively detect Cu^{2+} among various other metal cations including Zn^{2+}, Hg^{2+}, Ni^{2+}, Co^{2+}, Fe^{3+}, Cd^{2+} and Pb^{2+}. Also, the fluorescence intensity of pH probes was enhanced Under acidic condition due to its protonation. The design strategy for the probes are based on inhibited isomerization of quinolone derivatives.

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Synthesis of [C-11]Raclopride Through By Using of Strong Organic Base, 1,8-bis(tetramethylguanidino)naphthalene

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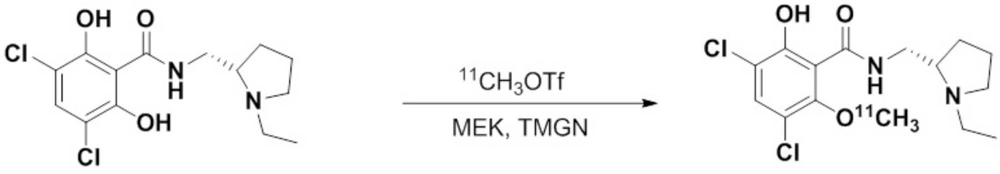
짧은 반감기를 가지는 C-11 으로 표지된 방사성의약품인 [C-11]raclopride 와 [C-11]DTBZ 등은 방향족 알콜을 포함한 전구체에서 일반적으로 강한 무기 염기성 시약 (NaOH, KOH, NaH 등)을 이용하여 [C-11]methyliodide 와 반응하여 합성한다. 상대적으로 친핵성이 약한 방향족성 알콜을 지닌 전구체들 ((S)-O-desmethylraclopride 또는 9-O-Desmethyl-DTBZ)은 강한 염기성 촉매가 필요하게 되며, 반응성을 높이기 위해 전구체와 염기를 비교적 장시간 선처리 한 후에 표지 반응을 수행한다. 무기 염기 촉매들은 유기 합성반응에서 사용할 경우 대부분 유기용매에서 용해도가 낮기 때문에 수분을 포함하게 되어 부반응의 원인이 되며, 수분의 함량을 낮출 경우에는 에멀젼 형태로 반응에 참여하여 불규칙한 합성 수율을 초래하게 된다. 본 실험에서는 유기 용매에 높은 용해도를 가지면서도 methylation 반응에 유리한 강한 염기성을 가지는 촉매 (1,8-bis(tetramethylguanidino)naphthalene, 상용명 TMGN)를 [C-11]raclopride 합성에 활용하여 높은 수율과 안정적인 반응성을 확보할 수 있는 지 조사하였다. 예상대로 TMGN 은 방사화학적 수율이 4.85(+/-)0.03 Gbq 을 나타내어 기존의 방법 (3.65(+/-)0.33)보다 우수한 방법임을 확인할 수 있었다. 용해도가 매우 높기 때문에 30 분 이상 용해 시켰던 반응 단계를 거치지 않고 합성을 진행할 수 있었고, 기존 합성방법에 비해 30 분 이상의 시간을 절약하였고, 반감기가 20 분인 C-11 동위원소 표지반응에서 매우 유리한 방법으로 여겨진다.



$[^{11}C]$Raclopride

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Analysis of Phospholipids, Lipid A and Sterols from Outer Membrane Vesicles Shed by *Acinetobacter baumannii* DU202

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Acinetobater baumannii DU202 (*A. baumannii*) is a gram-negative bacterium and well known resistant to various antibiotic drugs as multidrug-resistant bacteria (MDR). Recently, quantitative proteomic analysis of *A. baumannii* has been reported to cell wall and plasma membrane fractions including outer membrane vesicles (OMV) and outer membranes (OM). The OMVs of gram-negative bacteria are composed mainly of proteins, lipids, lipopolysaccharide (LPS) and sterol. In several cases, they contain either RNA or DNA, and are associated with various biological functions for their growth, development and survival such as immune response systems, secretion and transfer of contents to host cell. Therefore, to comprehend the structural characterization and function of OMV and OM in *A. baumannii* is important. In this study, we established the analytical method to effectively analyze extracted phospholipids, Lipid A and cholesterol levels from OMV and cell of *A. baumannii* using UPLC/Q-TOF MS^E, MALDI-TOF MS and GC-MS, respectively. Also, to investigate the different biogenesis pathway, novel biological roles of OMV and potential biomarker between OMV and cells, we studied the significant properties and various function of OMV and performed multivariate statistical analysis such as PCA and S-plot model of OPLS-DA.

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Charaterization of N- and O-linked Glycans from Glycoproteins by MALDI-MS and MS/MS

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Glycosylation is important role in signal transduction between cells, and various biological processes. Biosimilar is a clone of a biotherapeutic products that have been developed by leveraging biotechnology, such as gene recombination and cell culture techniques. Therefore, glycosylation analysis is necessary during various stages of a biotherapeutic product’s lifecycle and one of the most critical tools in the characterization of biotherapeutic proteins.In this study, N-glycans are enzymatically released by N-glycosidase F(PNGase F). O-glycans are chemically released by β-elimination. they are purified by SPE(solid-phase extraction)-PGC. The permethylation of sialylated glycans results in the conversion of all hydroxyl groups into methoxyl groups and serves to render glycans hydrophobic which may increase the signal intensity in mass measurement. We revealed the characterization of N- and O-glycans released from glycoproteins by using matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) and tandem mass spectrometry (MALDI-MS/MS) with 2,5-dihydroxybenzoic acid (2,5-DHB) as the matrix.

Charaterization of *N*- and *O*-linked Glycans from Glycoproteins by MALDI-MS and MS/MS

In Young Park[1,2], Jang Mi Jin[1], Hyun Joo An[2], and Young Hwan Kim[1,2*]

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Performance Evaluation of Domestic MALDI-TOF MS on Microorganism Identification

방글 박인영[1] 김영환*

한국기초과학지원연구원 생의학오믹스연구팀 [1]충남대학교 분석과학기술대학원

Application of mass spectrometer is now expanding in recent years. Especially, Mass spectrometer takes on a growing role in medical areas such as discovering markers for assessment of disorders, evaluation of colorectal cancer and of virus resulting in cervical cancer by applying MALDI-imaging. Due to wide introduction of a system to detect pathogenic microorganism based on MALDI-MS that goes back to five years ago, it is now applied in detection of pathogenic bacteria. Biotyper by Bruker, VITEK MS by Biomerieux and AXIMA-IDPlus by Shimazdzu are now on the market worldwide. Economic and social costs in recent years caused by Middle East Respiratory Syndrome (MERS) in South Korea urge a management system with capacity to detect contagious diseases in more accurate and faster way. In the mean time, Korean startup ASTA invented Korea's first MALDI-TOF mass spectrometer that identify pathogenic microorganism, and it will be available now on the market. One of projects conducted by Korea Basic Science Institute (KBSI) is supporting improvement in domestic MALDI-TOF MS. This result as a part of project reports compares microorganism identification performance of domestic and foreign MALDI-TOF MS.

Performance Evaluation of Domestic MALDI-TOF MS on Microorganism Identification

Geul Bang, In Young Park and Young Hwan Kim*

Biomedical Omics Group, Korea Basic Science Institute, Ochang 363-883, Korea

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Design, synthesis and biological evaluation of Diarylurea derivatives as potential anticancer agents

Mahmoud Mahmoud Mohamed Gamal EIDin 유경호[1] 오창현[2,*]

과학기술연합대학원대학교(UST) 의약화학 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터 [2]한국과학기술연구원(KIST) 바이오소재연구센터

A novel series of 2,5-disubstituted-1,3,4-oxadiazole containing urea 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 compared to sorafenib. At a single dose concentration of 10 ?M, many target compounds exhibited cytotoxic effect with more than 100% inhibition over different cell lines of different cancer types. For example, compound 1e showed 184% inhibition over Colo-205, and 137.9% inhibition against SK-Mel 2. Compound 1j inhibited the growth of Colo 205 colon cancer cell line, SK-Mel 2 melanoma cell line and MDA-MB-231/ATCC breast cancer cell line by 140%, 132.87% and 122.63%, respectively. The inhibition % of compound 1m were 154%, 125.42%, and 126.57% against NCI-H522, NCI-H460 non small cell lung cancer cell lines, and U 251 CNS cancer cell line. We are currently waiting for 5-dose results and the remaining one dose results.

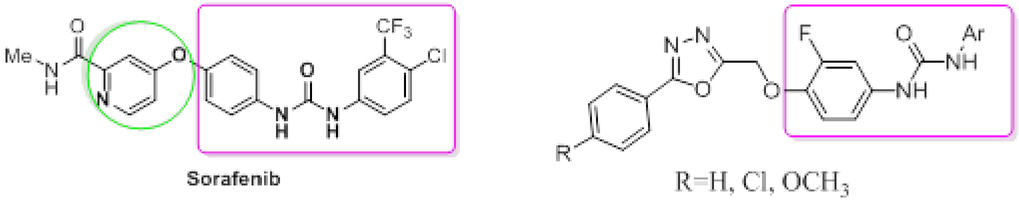

Figure 1. Structure of the target compounds and Sorafenib

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Synthesis of [^{68}Ga]Gallium Labeled Benzopyran Derivative

정순재 유국현*

동국대학교 화학과

The benzopyran ring is widely found in a number of natural products such as flavonoids. These natural products have demonstrated numerous biological activities such as antiviral, anti-inflammatory, anti-allergic, anti-mutagenic and anti-carcinogenic activities. In this study, a Ga-68 labeled benzopyran derivative was synthesized for investigation as a potent imaging agent for breast cancer. The reference compound was synthesized starting from 2-hydroxy-5-nitroacetophenone via six steps, and confirmed through ^{1}H NMR spectroscopy and mass spectrometry. The radiolabeling reaction was monitored using a radio-TLC and the radiochemical and purified by HPLC.

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Novel 2,4-diarylaminopyrimidines as ALK inhibitors

Gangadhar Rao Mathi **황종연[1] 윤창수[2] 정희정[3] 하재두[4] 조성윤[4] 김형래[4,*] 김필호[5,*]**

과학기술연합대학원대학교(UST) 의약화학 [1]한국화학연구원 신약연구본부 [2]한국화학연구원 신약연구본부 의약화학연구센터 [3]한국화학연구원 의약화학연구센터 [4]한국화학연구원 난치성질환치료제연구센터 [5]한국화학연구원 난치성질환치료제연구그룹

Anaplastic lymphoma kinase (ALK) serves as a potent target for innovative combination therapies based on selective small-molecule inhibitors of its use as an oncoantigen for tumour vaccination. After the first ALK inhibitor, crizotinib (xalkori) developed by Pfizer, developed resistance, various efforts to overcome drug resistance issues have been actively pursued. In 2014, the second-generation ALK inhibitor ceritinib was approved by the US FDA for the treatment of patients with ALK-positive metastatic NSCLC, who were previously treated with, or resistant to crizotinib.In order to develop novel ALK inhibitors, a series of new 2,4-diaminopyrimidines were synthesized and investigated for their biological activities against ALK wild type as well as mutants to discover preclinical candidates. Compared with ceritinib, the biological activities obtained with our compounds were promising, providing an in-depth understanding and gave new insights in the further development to produce selective and potent ALK inhibitors. The design, synthesis, and SAR of these compounds will be described.

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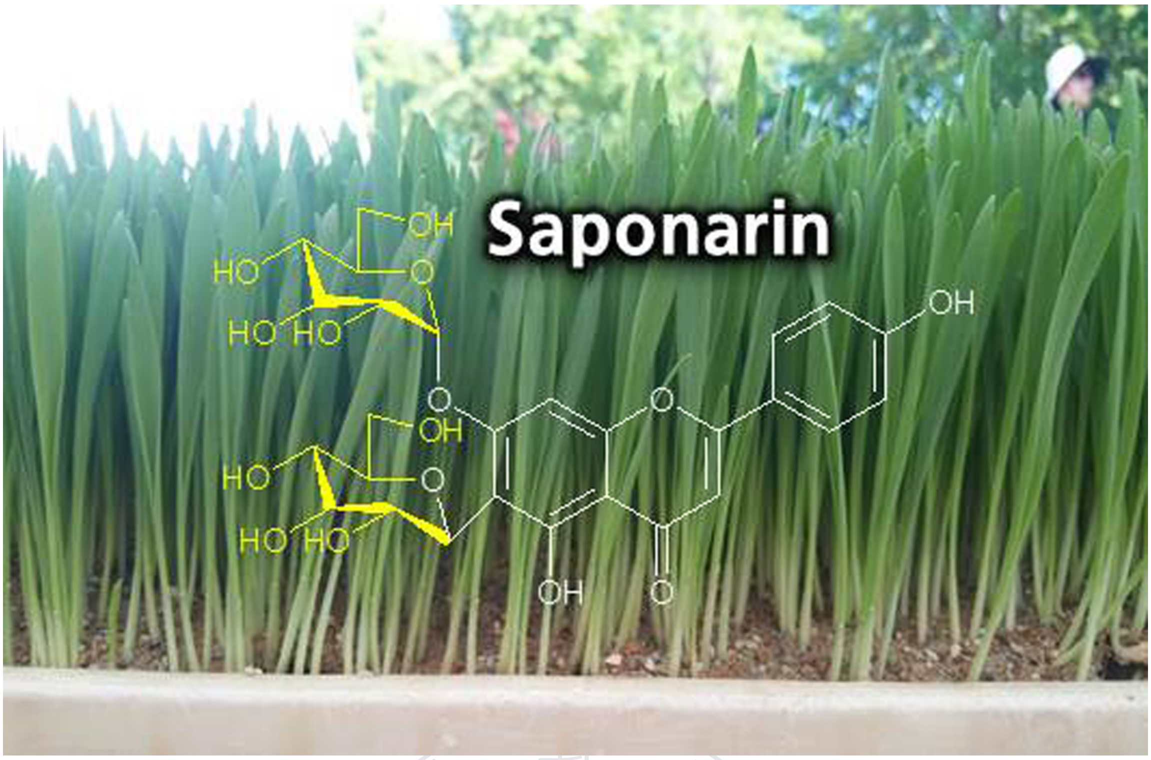
Saponarin from barley seedling attenuates adipogenesis and cholesterol metabolism in 3T3-L1 cells by regulating AMPK and PPARγ activity

서우덕

농촌진흥청 국립식량과학원

Mechanism of saponarin (SA), which isolated barley seedling (BS), on adipogenesis metabolism was investigated. SA was highly purified from BS by column chromatography and determined its molecular structure by ultra performance liquid chromatography (UPLC)-QTOF-Ms/Ms and nuclear magnetic resonance (NMR) analyses. SA reduced the lipid accumulation as well as attenuated intercellular triglyceride (TG) content in mouse adipocytic 3T3-L1 cells. SA reduced the expression of the preadipocytes differentitation regulator genes such as peroxisome proliferator-activated receptor gamma (PPARγ), sterol regulatory element-binding protein-1c (SREBP-1c) activities and induced AMP-activated protein kinase (AMPK) phosphorylation without cytotoxicity. Moreover, SA was inhibited adipocytes genes expression for activator protein 2 (AP-2) and adipose triglyceride lipase (ATGL). These results indicate that SA inhibited in lipid accumulation and gene expression of adipogenic factors and decreased the TG and cholesterol level in adipocytes. The intake of BS might provide the metabolic benefits of lipid and cholesterol control. Further human studies may confirm this effect.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Recent conjugation strategies of fluorophores and ligands for tumor imaging

하용황 최현경[1,*]

중원대학교 의약바이오학과 [1]중원대학교 의약화학과

Conjugation between various small fluorophores and specific ligand has become one of main strategies for bioimaging in disease diagnosis, pharmacokinetics, surgery, etc. Herein, we reviewed recent studies about molecular imaging techniques with cellular and animal level and synthetic strategies for various fluorophores. Various organic fluorophores, especially NIR probes, have been employed for connection with specific ligands. Types of ligands were small molecules, peptides, and antibodies, and aptamers, which have specific affinity for cellular receptor proteins, cancer-specific antigens or enzymes, and nucleic acids. This review may be helpful in selection of cancer-specific ligands and fluorophores, and expending for further developing new conjugation strategies in various cellular and animal condition.

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Phosphor-converted three-band white LED fabricated by coating K_2SiF_6:Mn^{4+} and $SrGa_2S_4$:Eu^{2+} phosphors onto the commercial blue LED

여별이 허영덕[*] 조영식

단국대학교 화학과

By coating the mixtures of the green-emitting $SrGa_2S_4$:Eu^{2+} and red-emitting K_2SiF_6:Mn^{4+} phosphors onto the blue-emitting InGaN chip, phosphor-converted three-band white LED is fabricated. The fine color tuning of three-band LED is obtained by varying the different amounts of $SrGa_2S_4$:Eu^{2+} and K_2SiF_6:Mn^{4+} phosphors. The phosphor-converted three-band white LED with $SrGa_2S_4$:Eu^{2+} and K_2SiF_6:Mn^{4+} phosphors shows excellent color rendering which can be applied for display as a white light source.

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Carbon Nanotube Nanocomposites with Highly Enhanced Strength and Conductivity for Flexible Electric Circuits

김한샘 신원상[1,*]

단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

Carbon nanotubes (CNTs) have an important role in nanotechnology due to their unique properties, retaining the inherent material flexibility, superior strength, and electrical conductivity, unless the bottleneck of CNTs persists and the aggregated structure is overcome. Here, we report on the highly enhanced mechanical and electrical properties of the CNT-chitosan nanocomposites through homogeneous dispersion of CNTs into chitosan solution using a high-pressure homogenizer. The optimal condition is a 50% (w/w) chitosan-CNT film, providing about 7 nm thickness of homogeneous chitosan layer on CNTs, a good tensile strength of 51 MPa, high electrical conductivity under 16 Ω/sq, and a stable bending and folding performance. This CNT-chitosan nanocomposite with highly enhanced properties is an amenable material to fabricate structures of various shapes such as films, sensors, and circuits and also enables a simple and cost-effective approach to improve the performance of a device that presents the first flexible and soft electric circuits yet reported using only CNT-chitosan as the conductor.

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Morphology and thermoelectric properties of Copper Selenid

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학부 [2]이화여자대학교 화학과

Thermoelectric materials allow for direct converting heat into electricity and vice versa. It is a challenge to develop thermoelectric materials with superior performance. The properties of thermoelectric materials are evaluated by the dimensionless figure of merit (ZT). Generally, a high efficient thermoelectric material should possess a high Seebeck coefficient, high electrical conductivity and low thermal conductivity. Other words, it should behave as a “phonon-glass-electron-crystal” with a high charge carrier mobility and a low lattice thermal conductivity. Superionic conductors with liquid-like behavior can be considered an extension of the phonon-glass electron-crystal concept and phonon-liquid electron-crystal (PLEC) thermoelectrics. Copper selenide (Cu2-xSe) is representative material as the liquid-like behavior of superionic conductors. Here, we synthesized uniform surfactant-free Cu2-xSe nanoplates and nanowires by changing synthetic condition. The size of nanoplates can be varied from 1 µm to 5 µm. We consilidated Cu2-xSe using spark plasma sintering (SPS) and evaluated their thermoelectric properties. Cu2-xSe nanoplate with ~1 µm size sample exhibited a ZT value of ~0.14 at 695K

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Highly Stable Transparent Conducting Electrodes based on Copper Nanowire@Graphene Core@Shell Nanostructure

안유미 이윤구*

대구경북과학기술원(DGIST) 에너지시스템공학전공

Transparent conducting electrodes (TCEs) have been known and well-studied as an essential element of various optoelectronic devices. Vacuum-deposited Indium tin oxide (ITO) has been widely used in a variety of optoelectronic devices. However, it has several drawbacks such as brittleness, low optical transmittance, and high processing temperature. Recently, researchers have shown that CuNW TCE can possess excellent electrical conductivity, optical transparency, and mechanical flexibility. However, it still has an issue regarding a long-term stability. For instance, CuNW is easily oxidized when exposed to air even at room temperature. Thus, it is necessary to suppress the oxidation of CuNW in order to enhance the long-term stability of CuNW TCE. Recently, we have developed highly stable and conductive TCEs based on a copper nanowire@graphene (CuNW@G) core@shell nanostructure. The CuNW@G core@shell nanostructure was successfully prepared by a low temperature PECVD (LT-PECVD) process at temperatures as low as 400 °C for the first time. The CuNW@G TCE exhibited excellent optical and electrical properties comparable to conventional ITO TCE. In addition, it showed remarkable thermal oxidation and chemical stability because of the tight encapsulation of the CuNW with gas impermeable graphene shells. Furthermore, the potential suitability of CuNW@G TCE was demonstrated by fabricating bulk heterojunction polymer solar cells. Polymer solar cells with CuNW@G TCE exhibited higher power conversion efficiency than those with CuNW TCE because of significantly enhanced anti-corrosion property.

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Reduction of Marine Bio-Fouling on Solid Substrates by Bio-Inspired Silica Coating

정연우 김수엽[1] 박수경 유정해 강성민*

부경대학교 해양바이오신소재학과 [1]부경대학교 수산생물학과

Control of marine bio-fouling has been of interest because non-specific adhesion of fouling organisms on marine vessels increased fuel consumption. Moreover, marine ecosystem has been disturbed by the migration of fouling organisms. To control marine bio-fouling, various studies have been conducted, and as a result, surface properties such as hydrophilicity and roughness were identified as the factors affecting marine bio-fouling. In this study, a bio-mimetic approach for reducing adhesion of marine organisms was investigated. The immobilization of cationic polymer on various solid substrates followed by silica coating resulted in super-hydrophilic surfaces, and the surfaces were found to be effective to reduce the initial attachment of marine diatoms. * This work was supported by the Korea Foundation for the Advancement of Science & Creativity (KOFAC), & funded by the Korean Government (MOE).

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BSA as additive : A simple strategy for practical applications of PNA in bioanalysis

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서울대학교 화학부 [1]서울대학교 화학과

Peptide nucleic acid (PNA) is an artificially synthesized oligonucleotide composed of natural nucleobases and pseudo-peptide backbone. Owing to the electrically neutral backbone, hybridization of PNA with its complimentary DNA or RNA with high affinity and specificity is possible. Therefore, PNA can be employed as a potent tool for molecular biology and genetic diagnostics. In spite of advantages of its application, its poor solubility in aqueous solution induces self-aggregation or nonspecific adsorption on hydrophobic solid surface. Here, we employed bovine serum albumin (BSA) as an additive to prevent the nonspecific adsorption of PNA on a hydrophobic surface and to enhance its solubility in aqueous media and thus, improved the sensing performance of GO/PNA based DNA sensor. In addition, the portion of the effective PNA strands for target binding could be increased without any disturbance on hybridization with a complementary target. This is the first report utilizing BSA for high yield of available PNA in its application by preventing nonspecific adsorption and for signal enhancement in GO/PNA based sensor system. We believe that the current study will offer great opportunities to broaden PNA application as useful tools in biomedical research.

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Football-shaped porous PCL microsphere scaffolds as a cell delivery system: Tuning of sphere- and pore-sizes using a combination of room temperature ionic liquid and camphene

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단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

PCL microspheres with a micro~macroporous morphology and cell active surface were developed as an injectable cell delivery system using room temperature ionic liquid and camphene. Room temperature ionic liquid (RTIL) and camphene were used, respectively, as a liquid mold and a porogen. The various-sized spheres from 250 to 650 ?m with various sizes and shaps of pore (or gabs) from about 0.1 to 100 ?m were formed depending on the camphene/RTIL ratio (0.8-2.6). To give cell activity, the surface of porous microspheres were further modified with with NGF-containing gelatin to have thin NGF/gelatin layer. PC12 cells attached and spread actively on microspheres and populated well within their macropores. The developed microspheres may be potentially applicable as a neuronal cell delivery scaffold for neuron tissue engineering.

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Luminescence spectra of Ce^{3+}-doped $LaAlO_3$ powders prepared by using CeF_3

최연희 이민호 정우식*

영남대학교 화학공학부

Ce(III)-doped lanthanum aluminate ($LaAlO_3$) powders were prepared by the calcination of a mixture of lanthanum oxide (La_2O_3), cerium fluoride (CeF_3) and alumina (Al_2O_3) powders in a nitrogen atmosphere, and characterized by X-ray diffraction, photoluminescence and scanning electron microscopy. The intense emission peak was observed at 420 (blue) nm and its intensity depended on Ce(III) concentration and calcination temperature. The results were compared with there on $LaAlO_3$:Ce^{3+} powders prepared from La_2O_3-LaF_3-CeF_3-Al_2O_3 and $LaFCO_3$-CeF_3-Al_2O_3reaction systems. The powders obtained by using La_2O_3-LaF_3-CeF_3-Al_2O_3 system showed the most intense emission.

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Synthesis of high surface area alumina powders from hydrolysis of partially nitrided alumina powder

정주희 정우식*

영남대학교 화학공학부

High surface area alumina powders were prepared by the hydrolysis of partially nitrided alumina (PNA) powder. The PNA powder was synthesized by the carbothermal reduction-nitridation reaction of a mixture of Al_2O_3 and carbon powders under a flow of nitrogen. Alumina powders were characterized by XRD, SEM, and BET. The morphology of alumina powders depended on hydrolysis temperature and duration. The alumina powders are expected to be used for preparing ceramics with improved hardness and wear resistance or for membranes or catalytic materials.

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Crystal structure and luminescence spectra of $Eu_{x-1}Ba_xAl_2O_4$ (x = 0 - 0.98)

이민호 최연희 정우식*

영남대학교 화학공학부

$Eu_{x-1}Ba_xAl_2O_4$ (x = 0 - 0.98) powders were prepared by the solid-state reaction of a mixture of Eu_2O_3, $BaCO_3$ and Al_2O_3 at 1400 °C under a flow of 10 vol% H_2/N_2 and characterized X-ray diffraction, Raman and infrared spectroscopy, field-emssion scanning electron microscopy. With increasing concentration of Ba^{2+} ion, the phase of $Eu_{x-1}Ba_xAl_2O_4$ was transformed from monoclinic to hexagonal. $Eu_{0.4}Ba_{0.6}Al_2O_4$ and $Eu_{0.6}Ba_{0.4}Al_2O_4$ powders were refined by the Rietveld method. In luminescence spectra of $Eu_{x-1}Ba_xAl_2O_4$, the peak diminished with increasing value of x up to 0.4 but became more intense at higher values. The position of peak by concentration of Ba^{2+} ion was blue-shifted from 520 (green) to 505 (bluish green) nm.

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Solution-Processed Bismuth Ferrite Thin Films for Non-Volatile Ferroelectric Memory Application

이지혜 윤명한[1,*]

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Ferroelectric materials have drawn growing interests in the field of ferroelectric random access memory (FeRAM) application because of low-power consumption, fast read-write performance, high integration density compared with conventional flash and dynamic random access memory devices. Particularly, bismuth ferrite (BFO), one of the rare multiferroic materials possessing both magnetic and ferroelectric characteristics, is a potential candidate for the application of next generation FeRAM due to large remnant polarization even at room temperature. However, the conventional BFO films exhibit several limitations such as high leakage current and unsecure Bi composition due to the high-temperature annealing. Herein, we report metal oxide thin film transistor-based non-volatile memories employing the solution-processed BFO thin films. The bilayer of ferroelectric BFO and insulating AlOx was introduced for the insulating film in order to lower the gate leakage current while the ferroelectric based polarization was activated. It was verified that the solution-processed BFO exhibit decent ferroelectric properties in terms of high polarization value and large capacitor memory window. Our study demonstrates that solution-processed BFO materials can be successfully incorporated into all solution-processed oxide thin-film transistors towards the realization of ferroelectric based memory devices.

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Dual-Wavelength Irradiation and Dox Delivery for Cancer Cell Ablation with Photocatalytic Pr Doped TiO_2 /NGO Hybrid Nanocomposite

최명호 민달희[1,*]

서울대학교 화학부 [1]서울대학교 화학과

Photosensitive semiconductors, titanium dioxide (TiO_2) has been continuously emphasized as the most promising material for various photocatalytic applications due to its strong oxidizing power, high chemical inertness, guaranteed stability and low cost. Moreover, low cytotoxicity and FDA approval makes it as a promising photocatalytic therapeutics reagent. However, a large band gap of TiO_2 (>3.2 eV) restricted its usage only under UV light, which has been a barrier for general therapeutic biomedical applications.Herein, hybrid nanocomposite of praseodymium doped TiO_2 nanocrystals and graphene oxide nanosheets are prepared by facile hydrothermal treatment. As-synthesized Pr-TiO_2/NGO hybrid nanocomposite exhibits enhanced photocatalytic activity under visible light irradiation by the intact graphene oxide and doped lanthanide mediated band gap narrowing compared to TiO_2. Moreover, high payload and controlled release of doxorubicin by charge reversal of hybrid nanocomposite at endosomal pH and near-infrared irradiation mediated efficient photothermal conversion provide highly favorable features in therapeutic applications. Through the combination of these three distinctive therapeutic modalities, highly efficient trimodal cancer cell ablation is demonstrated.

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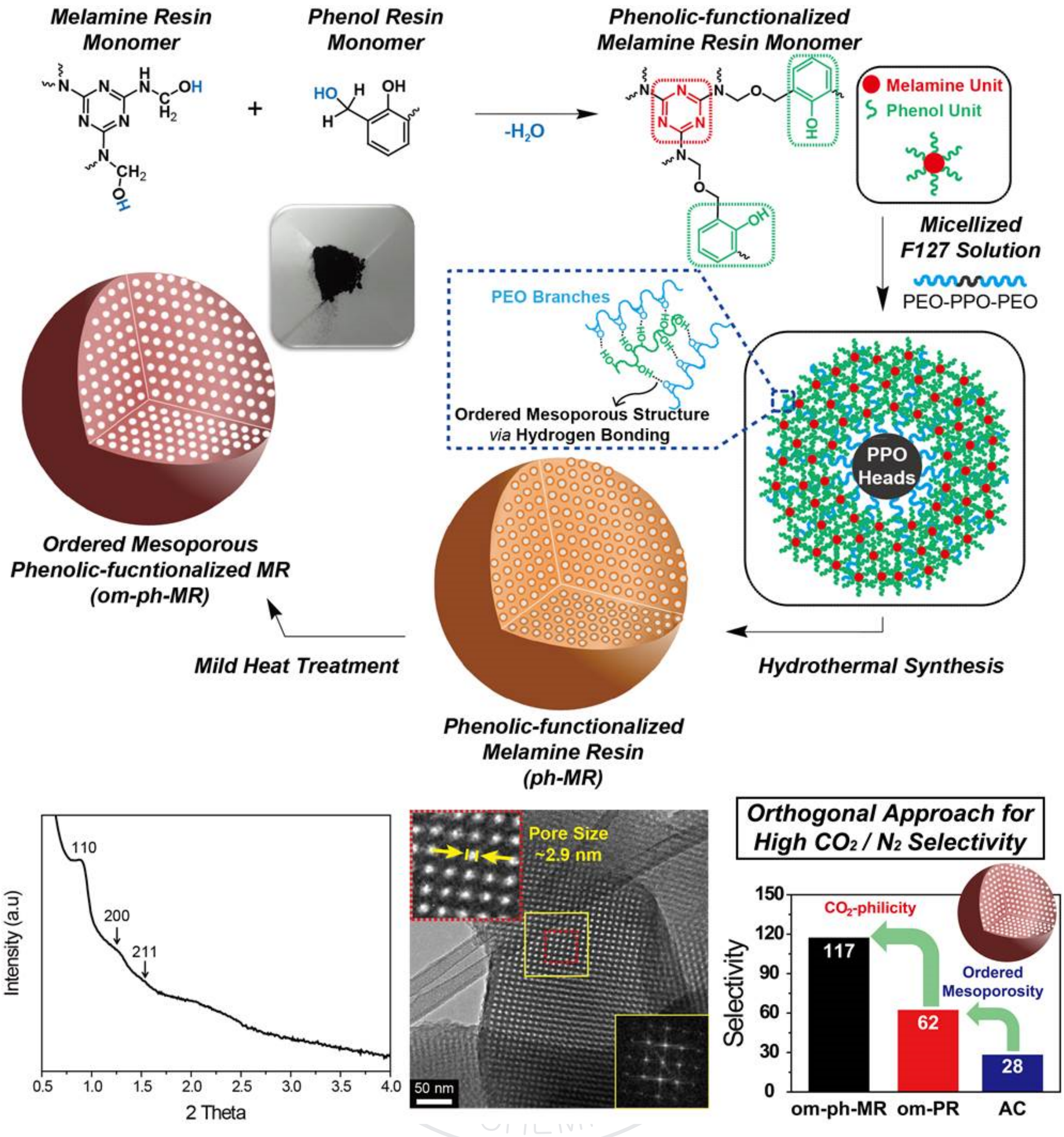
Combined CO2-philicity and Ordered Meso-porosity for Highly Selective CO2 Capture at High Temperatures

이지훈 최장욱*

한국과학기술원(KAIST) EEWS

Various dry sorbents have been lately introduced as promising media to capture carbon dioxide (CO2) at post-combustion stages. However, it is still desirable to further improve their performance in diverse aspects, and high temperature selectivity of CO2 over other gases is clearly one of them. Here, we report a co-assembly approach to turn nonporous melamine resin to a highly ordered mesoporous polymeric network (Space group: Im-3m) containing high nitrogen content (~18 at%). This mesoporous network shows anomalously increasing CO2/N2 selectivity with temperature rise, with the selectivity at 323 K reaching 117 (Henry method). This selectivity behavior is attributed to a combined effect of the high nitrogen content allowing for high binding affinity with CO2 and well-defined meso-pores (2.5~2.9 nm) accelerating to release N2 with temperature rise. The given orthogonal approach can be a general rule in designing dry sorbents with excellent selectivities at high temperatures.


Melamine Resin Monomer
Phenol Resin Monomer
Phenolic-functionalized Melamine Resin Monomer
-H2O
Melamine Unit
Phenol Unit
Micellized F127 Solution
PEO-PPO-PEO
PEO Branches
Ordered Mesoporous Structure via Hydrogen Bonding
PPO Heads
Hydrothermal Synthesis
Phenolic-functionalized Melamine Resin (ph-MR)
Mild Heat Treatment
Ordered Mesoporous Phenolic-fucntionalized MR (om-ph-MR)
Intensity (a.u)
2 Theta
110
200
211
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Pore Size ~2.9 nm
50 nm
Orthogonal Approach for High CO2 / N2 Selectivity
Selectivity
150
120
90
60
30
0
CO2-philicity
Ordered Mesoporosity
117
62
28
om-ph-MR
om-PR
AC

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미세유체 칩을 이용한 섬유아세포의 증식 및 이동 평가

고하니 **Tian Tian** 이석우*

공주대학교 화학과

본 연구에서는 포토리소그래피 기법과 복제 주물 기법을 통해 다양한 패턴의 미세 구조를 갖는 미세유체 칩을 제작하였다. 미세유체 칩 내에서 섬유아세포를 증식시킨 후 포스트에 압력을 가하여 세포층에 인위적인 상처가 형성되도록 하였으며, 압력을 제거한 후 섬유아세포의 증식 및 이동을 관찰하였다. 포스트에 가해지는 압력에 의해 구동하는 미세유체 칩의 기능은 형광 물질을 이용하여 규명하였으며, 섬유아세포를 미세유체 칩에 배양한 후 압력에 따라 인위적인 상처를 형성하는 것은 광학 현미경을 통하여 관찰하였다. 상처 형성 후, 12 시간 간격으로 동일한 위치의 세포에 대한 광학 현미경 이미지를 촬영하여 세포의 증식과 이동을 관찰하고, 증식 곡선을 도시하여 정량적인 평가를 수행하였다. 본 연구에서 제작한 미세유체 칩은 간단하며, 쉽게 제작가능하여 다른 세포의 증식 및 이동의 평가에 활용될 수 있을 것이다.

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Combinational Therapy based on Functionalized Graphene Oxide

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서울대학교 화학부 [1]서울대학교 화학과

Graphene Oxide (GO) possess the graphitic carbon structure domain of graphene in centre area but abundant carboxylic/hydroxy oxygen-containing functional groups in peripheral edge region, thus are more applicable for biological study with high solubility in physiological solution and become a promising candidate for biosensor platform and therapeutic agent.Here, we develop a simple, simultaneous anti-cancer drug and functional siRNA delivery system based on functionalized GO. SiRNA and DOX loaded GO complex facilitates therapeutic efficacy to cancer cells through the down-regulation of target gene expression and DNA cleavage activity of DOX. The functionalized GO with poly allylamine (PAA) induce the successful endosomal escape by sponge effect, enhancing not only the efficient nuclear uptake and cytotoxicity of DOX compared to free DOX but also RNAi mediated specific cleavage of mRNA. It is believed that a novel chemo-gene combinational therapeutic system is capable for superb anti-cancer or viral disease treatment.

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Poly(MAA-*co*-EGDMA)를 주형으로 한 중공 ATO 구의 합성 및 특성 규명

권유성 고하니 이석우*

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본 연구에서는 poly(MAA-*co*-EGDMA)를 주형으로 사용하여 중공 ATO 구를 합성하여 특성을 규명하는 연구를 수행하였다. 주형 물질인 poly(MAA-*co*-EGDMA)는 AIBN 을 개시제로 사용하여 MAA(methacrylic acid)와 EGDMA(ethylene glycol dimethacrylate)의 공중합 반응으로 합성하였으며, 평균 520 ㎚ 크기의 구형 입자로 얻어졌다. Sn/Sb 염을 이용하여 제조한 ATO(antimony doped tin oxide) 전구체 용액을 증류수에 분산된 poly(MAA-*co*-EGDMA) 분산액에 적가하여 poly(MAA-*co*-EGDMA) 표면에 ATO 전구체의 쉘을 형성하였다. 복합재료를 800℃에서 소성하여 중공 ATO 구를 얻었다. FT-IR 을 이용하여 작용기를 규명하였으며, FE-SEM 과 PXRD 분석으로 각각 형태, 크기 및 결정 구조를 관찰하였고, TGA/DSC 분석으로 열에 의한 화학 반응을 규명하였다. 중공 ATO 구와 분말 ATO 의 전기저항을 측정하여 전기 전도도의 차이를 규명하였다.

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One-pot preparation of TiO_2/Cu_2ZnSnS_4 heterojunction and its photocatalytic activity

김성덕 박용광 부충헌 정동운*

원광대학교 화학과

Cu_2ZnSnS_4 (CZTS) semiconductor was synthesized by reacting CuO, ZnO and SnO with ethanolamine, 2-methoxyethanol and thioglycolic acid. Anatase TiO_2 particle was dispersed into the CZTS precursor solution, so that TiO_2/Cu_2ZnSnS_4 heterojunction was created through the nucleation of Cu_2ZnSnS_4 onto the TiO_2 surface. The photocatalytic efficiencies of TiO_2/Cu_2ZnSnS_4 heterojunction samples with different TiO_2:Cu_2ZnSnS_4 ratios were investigated. The photocatalytic efficiency of TiO_2/Cu_2ZnSnS_4 heterojunction sample was superior to that of the pure CZTS and the efficiency decreased with increasing the TiO_2:Cu_2ZnSnS_4 ratio. The highest efficiency obtained from the 1:1 sample exceeded that of P-25 by about 1.5 times.

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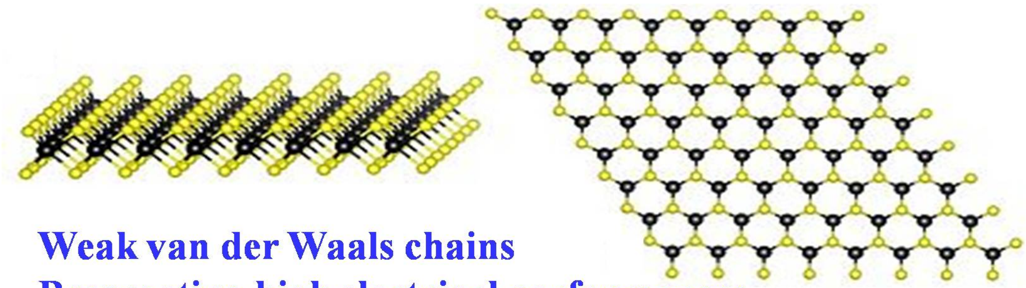
Synthesis and Electrical/Optical Characterizations of Monolayer MoS_2 by Chemical Vapor Deposition

홍광택 김성진[1,*]

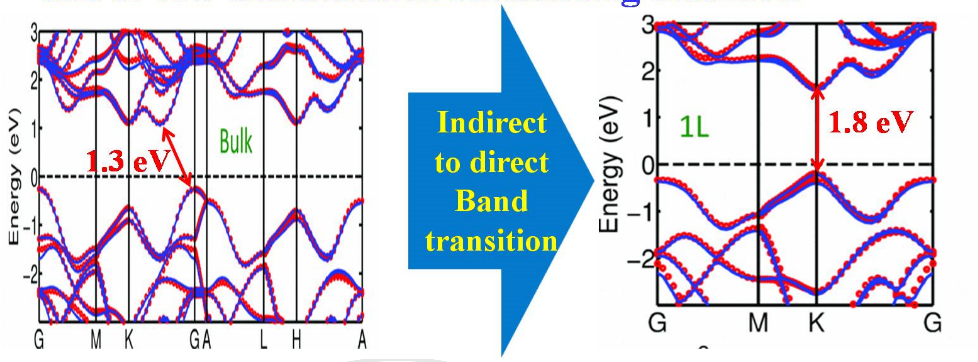
이화여자대학교 나노과학부 [1]이화여자대학교 화학과

The transition metal chalcogenides are widely studied in recent years. These materials show a superior electrical, optical and mechanical properties compared to traditional bulk materials. The most famous material among transition metal chalcogenides, MoS_2 have been investigated in diverse objects, such as FET devices and sensors. This material shows that transition from indirect to direct band gap when their layers are reduced from multilayer to monolayer. We synthesized various shapes of monolayer and also isolate triangular shape monolayer of MoS_2 by Chemical Vapor Deposition (CVD) method. The samples are also characterized by microRaman Spectroscopy, Photo-Luminescent (PL) emission and other characterization tools. We also fabricated the electrical device for extracting intrinsic electrical properties of monolayer MoS_2.



Weak van der Waals chains

Prospecting high electrical performances due to low dimensional conducting channels



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Cathode Material for Lithium-Sulfur Battery : Ordered Mesoporous Metal Oxides

최윤석 오세민 김지만*

성균관대학교 화학과

Lithium-Sulfur batteries are one of the most up-and-coming batteries for it's low cost, abundance, safeness, high theoretical specific capacity (1,675mAh/g) and high energy density (2,600Wh/kg) which are 3-5 times more than those of conventional lithium ion batteries.Despite of its considerable superiority as next generation energy device, Li-S batteries still have some obstacles hindering practical application.Sulfur and discharge products (Li_2S, Li_2S_2) are electrical insulator which causes low conductivity and poor rechargeability.Furthermore, polysulfide anions (Li_2S_n, $4 \leq n \leq 8$) formed during charge/discharge processes easily dissolve in organic electrolytes used in Li-S batteries. This can cause rapid capacity fading because of active mass loss during cycle.To overcome these problems, majority of studies have focused on porous carbon materials not only to impart sulfur conductivity but also to capture polysulfide by physisorption, capillary force. In this work, we introduce new possibility of mesoporous metal oxides(MO_x) as a sulfur host material. Because of high surface area and intimate contact with sulfur, mesoporous MO_x could effectively boost conductivity. Also, for its small sized porous nature, they would trap sulfur and effectively limit polysulfides dissolution.We anticipate that mesoporous MO_x-S composites as cathode materials in lithium-sulfur batteries will exhibit improved cyclic stability and high rate performance.Ordered mesoporous MO_x (TiO_2, MnO, NiO) were synthesized by nano-replication method via ordered mesoporous silica template (KIT-6). The materials are characterized by X-ray diffraction (XRD), N_2 adsorption/desorption measurements, scanning electron microscopy (SEM), and electrochemical electrochemical investigation was performed.

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In-depth investigation of the interaction between DNA and nano-sized graphene oxide

임예지 민달희[1,*]

서울대학교 화학부 [1]서울대학교 화학과

Graphene oxide (GO) is a single-layer of graphite oxide which has oxygen-containing functional groups including hydroxyl and carboxylic acid groups. GO has been harnessed in diverse biological applications, such as drug delivery, enzyme activity assays and biosensors. Among the numerous applications of GO, optical biosensors have been developed based on the preferential binding of single stranded nucleic acid on GO and fluorescence quenching capability of GO. More recently, researchers started to employ nano-sized GO (NGO) which is smaller than micro-sized large GO (LGO) for live cell imaging of various biomarkers and intracellular RNA. However, compared with the expanded applications of size-controlled NGO, in-depth study for the interaction between DNA and NGO was not sufficiently carried out.Herein, we investigated the length dependent interaction of DNA with NGO and compared the result with the case of LGO. By using three different DNA strands having varying lengths, we discovered kinetics and capacity of DNA adsorption, kinetics and sensitivity of sequence specific desorption of DNA, and relative strength of DNA interaction with NGO compared to LGO. We believe that the present study will provide useful information on the effect of GO size to its interation with DNA, which are important in the development of robust biosensors based on GO and DNA in the future.

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Direct cellular delivery of human proteasomes to delay tau aggregation

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서울대학교 화학부 [1]서울대학교 화학과

Mesoporous silica nanoparticle (MSN) is promising as a transfection agent and a drug carrier. MSN has been studied as delivery vehicle for molecules ranging from small chemicals such as doxorubicin to bio macromolecules such as DNA or proteins. MSN has many advantages as a drug delivery system due to 1) the ease of tuning the pore size (2 nm to 30 nm), 2) the possibility of diverse functionalization, and 3) the ability to protect the encapsulated molecules from enzymes such as nucleases or proteases.In this study, a novel silica nanoparticle was synthesized and applied to proteasome delivery. The proteasome is the primary machinery that degrades ubiquitin conjugated proteins, including many proteotoxic proteins implicated in neurodegeneration. We demonstrate that the successful delivery of exogenous proteasomes enhance the UPS-Proteasome system which degrade misfolded or damaged proteins. UPS-Proteasome system induces decrease in the tau aggregation, known as a key factor in Alzheimer’s disease. Our MSN based proteasome delivery shows effective degradation of tau protein in HEK293-derived cell line. We observed the degree of tau degradation is dependent on the concentration of MSN-proteasome complex. We believe that the delivery of exogenous proteasomes using our MSN with large pores will become a useful therapeutic strategy to treat the Alzheimer’s disease in the future.

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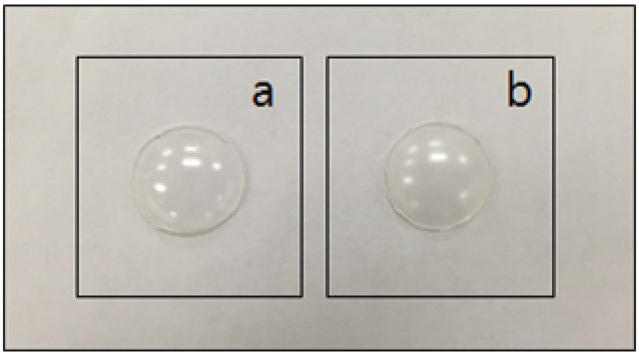
Fabrication and characterization of silicon-hydrogel ophthalmic lens containing amide group as additive

김득현 성아영*

대구가톨릭대학교 안경광학과

The high functional silicon hydrogel ophthalmic lens using amide group and HEMA as additives were manufactured and also the physical properties of the produced hydrogel lens were measured. For copolymerization, the mixture was heated at 130 ℃ 2hrs. and also, EGDMA and AIBN was used as cross-linker and initiator, respectively. The ophthalmic polymer by using thermal polymerization process for silicon hydrogel lens was manufactured and the results of physical properties showed that the water content of sample was in the range of 49.15~74.21% and 63.87~65.16%, respectively. The water content of sample containing acryl amide group increased as the ratio of additive increased. And in case of sample containing HEMA, the water content of sample decreased. The produced copolymer is suitable for silicon hydrogel ophthalmic lens with high water content.



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Development of Polyvinyl Alcohol (PVA) Nanofibrous Hydrogel for Tissue Engineering

TRAN HUNG TRI 윤명한[1,*]

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Recently, hydrogels have emerged as a leading candidate material for tissue engineering scaffold because they are biocompatibility, structurally similar to the natural extracellular matrix, and capable of promoting cellular adhesion and proliferation. However, most of hydrogel materials exhibit substantial difficulty in terms of controlling microscale geometrical and structural parameters, which are particularly important in three-dimensional culture for multiple cell-line co-culture and ultimately tissue regeneration. Here, we developed transparent PVA nanofiber-based hydrogel prepared using the conventional electrospinning method. Our PVA nanofiber hydrogel are transparent but insoluble in water via physical transformation instead of chemical cross-linking which may cause cytotoxicity. In conjunction with a variety of physical and chemical characterizations, the excellent viability and decent axonal outgrowth of neuronal culture was demonstrated on top of this new type of hydrogel. These results suggest that PVA nanofibrous hydrogel could be a promising 3D scaffold for cell culture and tissue engineering even compatible with delicate neuronal tissues.

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A New Layered Mixed-metallic Thiophosphate, $Ag_{1-x}(Ta_x/Zr_{1-x})PS_6$ (x=0.13)

차하늘 윤호섭[1,*]

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In the middle of searching for new soluble inorganic polymers consisting of group 4 metals using the reactive halide-flux technique, a new mixed-metallic layered thiophosphate, $Ag_{1-x}(Ta_x/Zr_{1-x})PS_6$ (x=0.13), has been found and the crystal structure has been determined by single crystal X-ray techniques. The structure of the title compound is isostructural with the mother compound, $AgTiPS_6$, which is composed of the one-dimensional chain, $^{1}_{\infty}[MPS_6]^-$ (M=Ti, Zr, Hf). This chain is constructed with dodecahedral MS_8 and tetrahedral PS_4 units by sharing common sulfur atoms. MS_8 units are linked by sharing three S atoms and the PS_4 unit is bridging these MS_8 units. We have found that the amount of substituted group 5 metals can control the stoichiometry of the cation. Ag^+. In this presentation, the comparison between the title compound and related phases with alkali metals is given. The classical charge valence of the compounds should be described as $[Ag^+]_{1-x}[Ta^{5+}]_x[Zr^{4+}]_{1-x}[P^{5+}][S_2^{2-}][S^{2-}]_4$.

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Solid and Solution Two-step Synthesis of the New Chromium Sulfide Cluster, $CrS_6(C_3H_4N)_3$

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A new quaternary thiophosphate, Cs_2CrPS_6 has been synthesized with alkali metal halide flux. The compound contains the binuclear $[Cr_2P_2S_{12}]^{4-}$ cluster which are well separated from each other by Cs^+ cations. The anionic cluster is composed of pair of edge-sharing Cr-centered octahedra and two P-centered tetrahedra. The cluster anion, $[Cr_2P_2S_{12}]^{4-}$ is stabilized through the electrostatic interactions with the cation, Cs^+. In order to isolate the anionic species, Cs_2CrPS_6 has been dissolved in the polar solvents such as DMF and $(CH_3)_4NCl$ has been added. Greenish-blue thin plate crystals have been obtained at room temperature and the crystal structure has been determined by single-crystal X-ray diffraction techniques. The compound has been proved to be $CrS_6(C_3H_4N)_3$. The structure of $CrS_6(C_3H_4N)_3$ consists of $[CrS_6]^{9-}$ octahedral and three $[C_3H_4N]^{3+}$ cations. The $[CrS_6]^{9-}$ anion is capped by three $[C_3H_4N]^{3+}$ cations to form the neutral $CrS_6(C_3H_4N)_3$ cluster. We propose that a productive route toward some of the soluble transition metal thiophosphates could be the solubilization of materials prepared by high-temperature solid state reactions.

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Multilayer Films Composed of Carbon Dioxide-responsive Oligoamines

우세은 홍종달*

인천대학교 화학과

This poster describes the synthesis of well-defined biodegradable oligoamine (denoted to OA-II) based on natural basic amino acid (lysine) and oligoamine patches. They contain an intermediary number of cationic groups (11 amino groups) to allow sufficiently strong, but reversible binding to anionic surface. The amine functionality of OA-II reacts with CO2 to form negatively charged carbamates by binding covalently with CO2. The overall charge of OA-II can be switched between cationic and anionic by CO2 complexation and carbamate formation in the ordinary range of pH5.5- pH7.5. The CO2 response of OA-II was studied by measuring the conductivity of an aqueous OA-II solution at pH7 on exposure to CO2 or N2 respectively. Moreover, Layer-by-layer multilayer self-assembly of OA-II polycation with polyacrylic acid (PAA) was studied by using UV-visible spectrometry and ellipsometry.Future work is directed towards the study of CO2 -responsive charge switching of (OA-II/PAA)n multilayer films, which would affect the permeability of monovalent or divalent anions and cations through the CO2-responsive membranes, for their application in designing sophisticated modern materials for biotechnology, filtration systems and sensors.

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Dielectric studies of$Y_{2/3}Cu_3Ti_{3.95}In_{0.05}O_{12}$ ceramic derived from non-aqueous chemical route

SINGHLAXMAN 이영일* 이한솔

울산대학교 화학과

The giant dielectric constant material $Y_{2/3}Cu_3Ti_{3.95}In_{0.05}O_{12}$ (YCTInO) has been synthesized by non-aqueous chemical route using metal nitrate and solid TiO_2 in ethylene glycol monomethyl ether. X-ray powder diffraction (XRD) study of the material sintered at 1050^oC for 15 hrs reveals the single phase cubic perovskite structure. Scanning electron microscopy (SEM) image of the material show the bimodal nature morphology and the grain size are found to be in the range of 0.9 ~ 3.0 μm. Energy dispersive X-ray spectroscopy (EDX) shows the presence of Y, Cu, Ti, In and O which confirm the purity and stoichiometry of the material. The dielectric property of this material was studied in the frequency range of 0.1 Hz -100 kHz in the temperature range from $30\text{-}160^oC$. The material exhibited the dielectric constant value of 7.8×10^3 at 100 Hz.

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Direct double stranded DNA detection based on graphene oxide

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서울대학교 화학부 [1]서울대학교 화학과

Herein, we develop a new method for direct detection of dsDNA which does not require denaturation process based on the invasion capability of peptide nucleic acid (PNA) and preferential binding of single-stranded PNA (ssPNA) over DNA/PNA duplex to graphene oxide (GO). When dye-conjugated PNA probe combine with target dsDNA, dye-conjugated PNA showed intense fluorescence signal even at low concentration of target DNA. As GO is an efficient nano-quencher which adsorbs single stranded PNA followed by long range energy transfer from dye, it could quench background fluorescence signal of the free PNA. By measuring the fluorescence of PNA probe, dsDNA could be analyzed quantitatively. Moreover, the high binding affinity of PNA for GO allows to overcome the drawbacks of conventional DNA probe and make the field of limited GO based sensor broader. We believe that this new direct GO-based dsDNA sensor will be a widely applicable tool in the field of DNA diagnostics.

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Fabrication and photocatalytic study of ZnO coated $ZnFe_2O_4$ particles

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강릉원주대학교 화학과

With growing demand for clean and comfortable environment, purification technologies with high efficiency and low cost reduce the pollutant contents of wastewater are urgently needed. In this study, a facile and efficient approach for the fabrication of ZnO coated $ZnFe_2O_4$ particles with a good core-shell structure has been demonstrated. The synthetic protocol involves the coating of successive layers of Citric Acid on to a magnetic core using a sol-gel method at room temperature followed by the deposition of Zinc Oxide nanoparticles on the surface of the $ZnFe_2O_4$ particles through a chemical reduction route. The ZnO coated $ZnFe_2O_4$ magnetic photocatalyst exhibited high photocatalytic activity in the degradation of Rhodamine B (Rh.B) under visible light. Moreover, ZnO coated $ZnFe_2O_4$ photocatalyst show Significantly enhanced photocatalytic properties than in the previous report concerning photodegradation of Methylene Blue (MB) in aqueous solution.

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Beam Induced Size- and Shape-controlled Synthesis of Pt Nanoparticles at Room Temperature

장지선 송재희[1,*]

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Metal nanoparticles are of special scientific and technological interest due to their unique chemical and physical properties. Among metal nanocrystals, Pt nanomaterials have been widely utilized in many industrial and technological applications, including fuel cell technology, gas sensing, hydrogen storage technology, fine chemical synthesis, and many oxidations and reductions.We present a facile one-pot preparation route for the production of platinum nanomaterials via a simple proton beam irradiation process at room temperature. Size- and shape-controlled Pt nanomaterials were prepared in an aqueous phase-based solution without the addition of any harsh reductants. We observed that the size and morphology of the Pt nanoparticles were easily varied by changing the proton beam current and duration time. It was also observed that the addition of isopropyl alcohol to the reaction mixture played a vital role for the morphology-controlled synthesis of Pt nanomaterials.

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An Effective Route for Room Temperature Synthesis of Platinum Nanoparticles Dispersed on Multi-walled Carbon Nanotubes

장지선 송재희[1,*]

순천대학교 기초의화학부 [1]순천대학교 화학과

The applications and scope of carbon nanotubes (CNTs) have been dramatically expanded since their discovery due to their unique structural geometries and physical/chemical properties. In particular, carbon nanotubes and their hybrid materials are attractive candidates for use as biological nanomaterials, electronic display nanodevices, and catalysis because of their structural characteristics and promising electronic, optical, and mechanical properties. Pt-based nanoparticles are widely used as a catalyst for application in fuel cells, where they are homogeneously dispersed on various types of carbon supports. In this study, a new synthesis route to decorate multi-walled carbon nanotubes (MWCNT) with platinum nanoparticles is presented via a simple proton beam irradiation process at room temperature. The characterization of the Pt nanoparticles and MWCNT-Pt composites has been done by using UV-Vis absorption spectroscopy, TEM and EDS analysis.

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Highly porous magnetic nanoparticles for the remediation of environmental pollutants

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한국기초과학지원연구원 서울서부센터 [1]한밭대학교 화학생명공학과

Highly porous magnetic nanoparticles (HPMNPs) were successfully synthesized by a successive coating of dopamine and iron oxide on magnetic nanoparticle. The structure of the HPMNPs was characterized using field-emission scanning electron microscopy, transmission electron microscopy, and Brunauer-Emmett-Teller (BET) and Barrett-Joyner-Halenda (BJH) methods were used to identify the specific surface area and pore-size distribution, respectively. The catalytic efficiency of the HPMNPs for the reduction of 4-nitrophenol to 4-aminophenol was tested in the presence of $NaBH_4$ at room temperature. The reduction was completed within 9 min. The high surface area and magnetic property of HPNMPs lead to exhibit excellent sorption property for heavy metal removal such as Cu(II), Pb(II), Cr(VI), and As(V) and recyclability to be use as a promising candidate for drinking water purification.

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Bur-like iron oxide capsules for visible light-driven photocatalysts with high performance

전효경 진예진[1] 최원산[2] 이하진*

한국기초과학지원연구원 서울서부센터 [1]이화여자대학교 화학나노과학과 [2]한밭대학교 화학생명공학과

Bur-like iron oxide (IO) capsules with and without gold nanoparticle core were synthesized by heat treatment of resin particles coated with needle-like IO nanoparticle under various temperatures. The IO capsule structure was characterized using scanning electron microscopy, transmission electron microscopy and X-ray diffraction measurements. The photocatalytic activity of the bur-like IO capsules was tested based on the decomposition of methylene blue (MB) under visible light irradiation at room temperature. For the IO capsules produced at 400℃, over 95% of MB dye was decomposed during 80 min. Further photocatalytic performances will be investigated with various bur-like IO capsules synthesized under different synthetic condition such as calcination temperature, number of growth cycle of IO and involving gold nanoparticles.

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A Facile Method for Fabrication of Superhydrophobic and Superoleophilc Composites and Application for Oil/Water Separation

임용택 김상헌 이하진[1] 최원산[*]

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With the increasing industrial oily wastewater and the frequent oil spill accidents, selective removal of oils from oil/water mixture continues to be the hot issue of research. Various materials such as sponges, metal meshes, and fabrics have been used for oil/water separation. Recently, considerable efforts have been focused on fabricating superhydrophobic and superoleophilic materials for oil/water separation using simple methods. In this respect, sponge and mesh were used as templates and coated with hydrophobic calcium carbonate ($CaCO_3$) and polydimethylsiloxane (PDMS) in xylene simultaneously by our proposed approach. This simple coating led to the increase in specific surface areas and superhydrophobic property of the sponge and the mesh. Our method to prepare superhydrophobic surfaces is very simple, facile, and scalable. The resulting superhydrophobic mesh or sponge exhibited outstanding performances for oil/water separation.

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Portable Sponge/Polymer Brush Composites for Environmental Remediation

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Contamination of water resources with heavy metal ions is considered as the most severe environmental accident, which cause serious damage to human beings and environment. Cases of serious side effects have been reported since they are accumulated in the human body along the food chain. Due to effectiveness of adsorption process, numerous adsorbents have been proposed for efficient removal of heavy metal ions or organic pollutants in waste water. However, previously reported adsorbents and adsorption process are not suitable for small scale enterprise and individual user. Development of a portable heavy metal ion remover which can be used even by untrained user is highly demanded. Sponge is portable, easy to use, and ubiquitous materials. Polymer brushes possess advantages of numerous reaction sites and pH-responsive behaviors for control of adsorption/desorption. Thus, highly porous sponge composites decorated with polymer brushes was developed for fast and efficient removal of heavy metal ions or organic pollutants in waste water or drinkable water.

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Superhydrophobic Cu Meshes with Multifunctions for Oil/Water Separation and Aqueous Pollutant Purification

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Superhydrophobic surfaces with various morphologies such as needle-like (NL), hairy like (HL), arch-like (AL), and needle-pine-like (NPL) structures were fabricated on Cu mesh templates by controlled oxidation and subsequent chemical modification with low surface energy materials. Initial chemical etching of the Cu substrates resulted in the formation of micropothole structures which contribute to a significant increase in trapped air in the nanostructures. To endow visible-light driven photocatalytic function, polymer/Ag/AgX layers were subsequently developed on Cu/CuO mesh. A combination of the filter layer (Cu/CuO mesh) and the photocatalyst layer (Cu/CuO/polymer/Ag/AgX mesh) was demonstrated to be used for oil/water separation and pollutant purification.

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Graphene Nanoplatelets doped indium via mechano-chemical reaction

전인엽 백종범[1,*]

울산과학기술대학교(UNIST) 에너지 및 화학공학부 [1]울산과학기술대학교(UNIST) 에너지공학부

We successfully implemented, for the first time, the doping of an indium (In) at the edge of graphene nanoplatelets (GnPs) through a mechanochemical approach by using graphite and In that are in a solid state. In doping at the edges of GnPs as well as the characteristic of InGnPs were confirmed via various analysis techniques. The content of In through energy-dispersive X-ray spectroscopies (EDS) was approximately 0.78 at.% (6.76 wt.%). Besides, we can confirm that the ball milling is very powerful approach to generate enough kinetic energy that can hold even post-transition metal ant then it can form C-In bond which is not known. Additionally, InGnPs display outstanding electrocatalytic performance with excellent long-term stability as well as tolerance against CO poisoning and methanol crossover for the cathodic oxygen reduction reaction (ORR) due to In doping.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of molybdenum diselenide nanosheets for energy storage application

이원재 백승민*

경북대학교 화학과

Recently the sodium-ion batteries (SIBs) have been attracted special attention in the both scientific and industrial fields, owing to the natural abundance of sodium and the easy excess to sodium sources. In this study, the molybdenum selenide ($MoSe_2$) nanosheets were synthesized via a chemical exfoliation technique, and used as an anodic material of SIBs. The X-ray diffraction patterns show that the basal spacing of exfoliated $MoSe_2$ was expanded up to 1.16 nm because of the intercalation of water molecules in the interlayer spaces. In the electron microscopy studies, the $MoSe_2$ nanosheets were observed as very thin layers, which can be distinguished from bulk materials due to their contrast differences. The electrochemical charge/discharge experiments clearly showed that the present $MoSe_2$ nanosheets had relatively high discharge capacity and coulombic efficiency in the half cell test.

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Fabrication of RuO_2 Hollow Nanostructures for Electrochemical Supercapacitor Applications

장수진 백승민*

경북대학교 화학과

In these days, as electronic devices and electric vehicles are growing as an essential part of our life, high energy density, long cycle life, high power density are demanded. Among the various energy storage devices, supercapacitors, compared with second rechargeable batteries, have received considerable attention owing to their promising application. Among the transition metal oxides, ruthenium dioxides is especially regarded as the one of the most promising electrode materials for supercapacitor applications due to high conductivity, short diffusion path and high specific capacitance. In this study, we are quite successful in fabricating the hollow structures by using layer-by-layer assembly technique. Scanning electron microscopic images of samples show ruthenium dioxides nanosheets were assembled in a controlled manner onto the polymer particles. The morphology of ruthenate hollow sphere can be confirmed by transmission electron microscopic images, supporting that ruthenate hollow sphere maintains its spherical morphology even after calcinations reaction. The electrochemical energy storage properties using cycling voltammetry were also examined.

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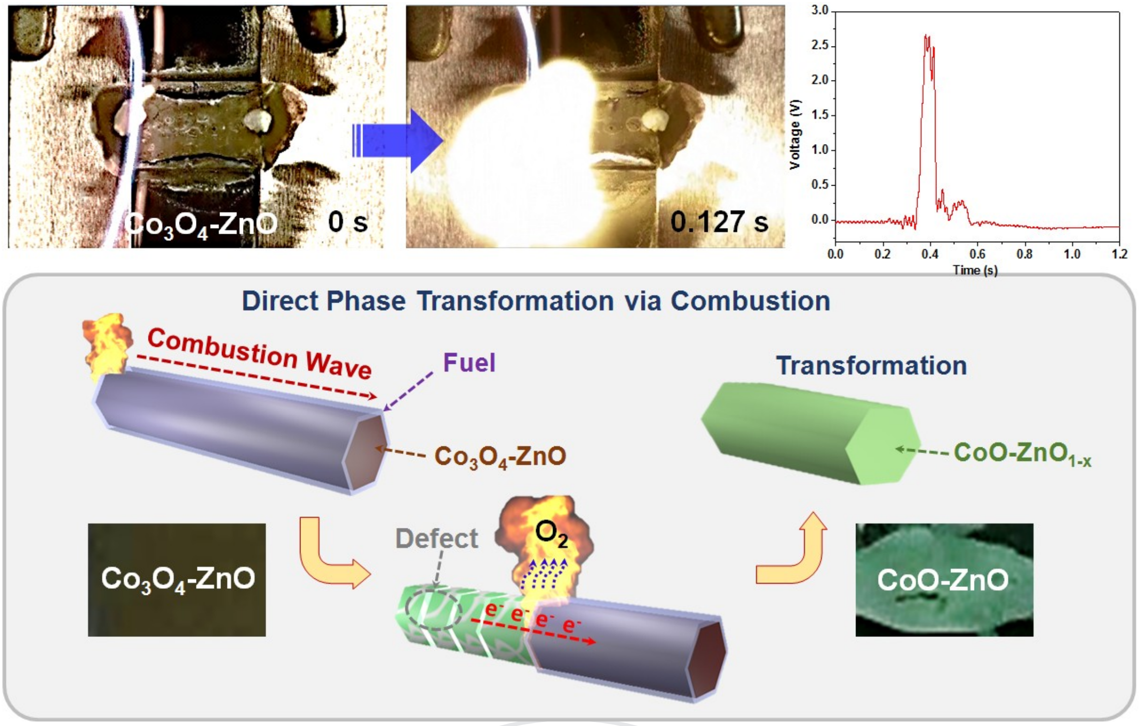
Phase Transformations of Metal Precursors via Combustion from Thermopower Waves and Their Chemical-Thermal-Electrical Energy Conversion Property and Enhanced Catalytic Property

이강열

고려대학교 기계공학부(BK21+)

The study of combustion at the interfaces of materials and chemical fuels has led to developments in diverse fields such as materials chemistry and energy conversion. Recently, it has been suggested that thermopower waves can utilize chemical-thermal-electrical-energy conversion in the hybrid structures comprising nanomaterials and combustible fuels to produce enhanced combustion waves with concomitant voltage generation. In this study, we present for the first time the direct phase transformations of Co-doped ZnO and Bi precursor via instant combustion waves and its applications to thermal-electrical energy conversion and photo-catalysis.


Co_3O_4-ZnO
0 s
0.127 s
Voltage (V)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Time (s)
Direct Phase Transformation via Combustion
Combustion Wave
Fuel
Co_3O_4-ZnO
Transformation
CoO-ZnO_{1-x}
Co_3O_4-ZnO
Defect
O_2
e^- e^- e^- e^-
CoO-ZnO

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Synthesis of the new mixed-metallic phosphates, $Na_xM_8P_6O_{35}$ family

염대규 윤호섭[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 화학과

The new mixed metallic phosphates, $Na_{3.52}Ti_{1.38}Nb_{6.62}P_6O_{35}$ and $Na_{3.09}Ti_{1.72}Nb_{6.28}P_6O_{35}$, have been prepared with the use of the metal halide. These compounds have been structurally characterized by single-crystal X-ray diffraction techniques. They are isostructural and the structure is composed of the metal phosphate framework and Na^+ ions in the vacant sites. The framework is constructed from corner-sharing MO_6 octahedra connected to the PO_4 tetrahedra. There are eight crystallographically independent transition metal(M) sites. All of these sites are occupied with mixed Nb/Ti. The occupancies of each metal site are not uniform. While the occupancies of Nb are dominant from the site 1 to the site 5, this is reversed from the site 6 to the site 8. The occupancies of the six Na sites are not equal. The Na1 to Na3 sites are fully occupied by Na^+ ions, whereas Na4 to Na6 sites are partially empty. The classical charge valence of the title compound can be represented by $[Na^+]_{3.52}[Ti^{3+}]_{1.38}[Ta^{5+}]_{6.62}[P^{5+}]_6[O^{2-}]_{35}$ and $[Na^+]_{3.09}[Ti^{3+}]_{1.72}[Ta^{5+}]_{6.28}[P^{5+}]_6[O^{2-}]_{35}$

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The Strategy for Efficient and Effective for Supercapacitors

이근식 이효영[1,*]

성균관대학교 화학과 [1]성균관대학교 화학과, CSMM

Supercapacitors consisting of electrical double layer capacitors offer fast charging-discharging rates and the ability to operate for millions of cycles. These devices can be applied for power hybrid electric vehicles and portable electronic equipment. In order to obtain a high performance supercapacitor, there are several factors that must be achieved including high specific surface area (SSA), high electrical conductivity, and high diffusion rate of the electrolyte due to an appropriate pore volume. Also it is important that vertically oriented or aligned electrode materials with a suitable pore size and distribution to facilitate high mobility of electrolyte ions for short paths and ease of access of electrolyte ions.In this talk, we report the strategy for high SSA electrode materials using graphene on supercapacitors. We developed a novel strategy using an anti-solvent to fabricate non-stacked reduced graphene oxide (NSrGO) from non-stacked graphene oxide (NSGO). Through a conventional thermal reduction process, NSGO can be easily turned into NSrGO to give a high surface area and simultaneously ultrahigh pore volume.[1] Further, to get high diffusion rate of electrolyte, it needs controlling the pore volume. To solve the critical problems, we developed on activated non-stacked reduced graphene oxide (a-NSrGO) electrodes that have high conductivity and high SSA with a wide pore distribution (from macro- to micro-pores) for the best-fit energy storage performance, which have a high SSA with intrinsic graphene conductivity and a fast diffusion rate of the electrolyte.[2] The high performance of the a-NSrGO supercapacitors is attributed to their specific appearance and enlarged pore distribution with high SSA. The other way to unique approach, we report a novel method to produce highly dense and vertically aligned rGO (VArGO) involving simple hand rolling and cutting.[3] Furthermore, the vertically aligned structure of the VArGO electrode yielded the highest electrolyte ion diffusion in the cell, leading to a great improvement in electrochemical characteristics to a degree suitable for supercapacitor applications.

These are expected to find application in conventional supercapacitor devices.References[1] Adv. Mater., 2013, 25, 4437-4444.[2] RSC Adv., 2015, 5, 60914?60919.[3] ACS Nano, 2104, 8, 4580-4590.

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Synthesis and Characterization of Porous Carbon Nanosheets by Direct Carbonization of Organic Salts

이지영 이영아[1] 유정준[2] 조우경[1] 김봉수* 윤하나[2,*]

한국과학기술원(KAIST) 화학과 [1]충남대학교 화학과 [2]한국에너지기술연구원 에너지저장연구실

Porous carbons are highly useful as electrodes in supercapacitors, Li-ion battery anodes, catalyst supports, CO_2 adsorbents or hydrogen storage carriers. In particular, synthesis of porous carbons by direct carbonization of organic salts have attracted much attention due to their advantages of a simple synthetic process, well-developed pores, and no need for use of excess activating agents. Servila et. al recently reported interconnected carbon nanosheets by direct carbonization of potassium citrate and sodium citrate and mesoporous carbon by direct carbonization of iron citrate which show good performances for a supercapacitor. However, a thoughtful study on the synthetic mechanism of the porous carbon nanosheets are still insufficient. Here, we report interconnected porous carbon nanosheets synthesized by direct carbonization of potassium citrate and sodium citrate and their electrochemical performance. Also, we observe the morphology changes of the organic salt precursors depending on the temperatures to elucidate the synthetic mechanism of the porous carbon nanosheets. [Acknowledgement]This work was conducted under the framework of Research and Development Program of the Korea Institute of Energy Research (KIER) (B5-2498).

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Synthesis of Dual Reactive *N*-Methacrylated Pyrrole Monomer for Conductive Material Composites

이주윤

한국교통대학교 교양학부 - 화학

Electrically conductive polypyrrole (PPy) has been demonstrated as a promising material for numerous applications such as sensors, tissue engineering, light emitting diodes, batteries, electrochromic devices, electromagnetic shielding, and corrosion inhibition. Due to the lack of reactive functional groups in pyrrole monomer itself, however, much intensive efforts have been devoted to chemically introduce pendent functionalities into PPy backbone skeleton. In a study related to this interest, polymerizable group-endcapped pyrrole derivatives as a dual active monomer could be desirable to architect three-dimensional (3D) conductive quasi-composites by grafting copolymers. Here, a new functional pyrrole monomer with a polymerizable methacrylate moiety, 3-((3-(1H-pyrrol-1-yl)propanoyl)oxy)-2-hydroxypropyl methacrylate (Py-N-MA), is presented, and this dual reactive Py-N-MA is electropolymerized into methacrylate-endcapped PPy (PPy-N-MA) as a telechelic polymer capable of further polymerization with different vinyl monomers.This work was supported by Korea National University of Transportation in 2015.

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Electrochemical performance of ordered mesoporous carbons with different carbonization temperature in supercapacitor

원종구 이창현 황윤경 JINXING 김지만*

성균관대학교 화학과

The electrochemical capacitors, also known as supercapacitors, are energy storage devices using electrochemical double layer capacitors(EDLC) or pseudo-capacitors. Supercapacitors can be alternative approach to solving increasing power demands of energy storage device, electric vehicles, and fuel cell vehicle because they can deliver energy at high rates and store high power compared to batteries. There are two properties to increase electrochemical performance in electrodes of supercapacitors : 1) high-capacitance material that have high surface area or pseudo-active species is needed to ensure high energy density. 2) high electrical conductivity material is a key factor to ensure high rate capability. Ordered mesoporous carbons have been known as candidate electrode materials because of its huge specific surface area, electrical conductivity, chemical stability, controllable porosity and pseudo-active sites for a variety of redox reactions. However, ordered mesoporous carbons have relatively low electrical conductivity due to amorphous phase. To improve electrical conductivity, we control carbonization temperature of ordered mesoporous carbon. In our study, ordered mesoporous carbons(CMK3) were synthesized by hard template method through impregnation the carbon precursor into the template(SBA-15) then carbonization at 900℃, 1200℃, 1350℃, and 1450℃. The as-synthesized ordered mesoporous carbons were characterized by X-ray diffraction (XRD), N2-sorption isotherm, Raman, and scanning electron microscope (SEM).

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Synthesis of $Li_{1.6}Mn_{1.6}O_4$ from mesoporous β-MnO_2 using flux method

채창완 박윤봉*

충남대학교 화학과

Mesoporous silica is useful in variety of applications including catalysis, adsorption, photonics, and electronics. The interest in such ordered mesoporous systems results from their interesting framework topologies, high surface area, and controllable pore size and volume. Furthermore, $Li_{1.6}Mn_{1.6}O_4$ is the most suitable for recovery of lithium from seawater because it has high selectivity, large adsorptive capacity, and high chemical stability for lithium ions. In this research, we have studied the effect of controlling surface areas and pore sizes of the adsorbents for the purpose of improving the lithium adsorption efficiency. The mesoporous $Li_{1.6}Mn_{1.6}O_4$ with high surface area and narrowly dispersed pore size has been synthesized from mesoporous β-MnO_2 through flux method. The synthesis of mesoporous β-MnO_2 was carried out by impregnating a mesoporous silica template (KIT-6) possessing a highly ordered 3D pore structure with an aqueous solution of manganese. The Li^+ extraction experiments were performed in an acidic solution and then the Li^+ uptake experiments were achieved in Li-enriched solution. The physicochemical properties of the $Li_{1.6}Mn_{1.6}O_4$ and $H_{1.6}Mn_{1.6}O_4$ were characterized by X-ray powder diffraction (XRD), brunauer-emmett-teller(BET), inductively couple plasma-atomic emission spectroscopy (ICP-AES) and thermogravimetric analysis (TGA)/differential thermal analysis (DTA).

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Template Free Synthesis of Boron Nitride Sheets

유정보 전도연 곽성근 HongYounghoonAndrew 김유진[1] 정수진 허남회[*]

서강대학교 화학과 [1]서강대학교 화학

Like graphite, hexagonal boron nitride (BN) has a layered structure, which can thus be exfoliated as mono-layered BN sheets. We report a novel method to fabricate the BN sheets, which were prepared by direct reaction between MgB_2 and NH_4Cl at 450 ^oC in an evacuated quartz ampule. The formation of BN sheets were accomplished at low temperature without any templates. The BN sheets were fully characterized by X-ray diffraction, transmission and scanning electron microscopy, X-ray photoelectron spectroscopy, and UV-visible spectroscopy. The BN sheets exhibit distinctive broad luminescence signals from 250 to 700 nm, which was excited at 200 nm. Another notable feature is that the BN sheets uptake the CO_2 gas in the low pressure range between 0.01 - 1 bar at 25 ^oC. The CO_2 absorption capacity is about 0.40 mmol/g at 1 bar. Details on the synthesis and properties of the BN sheets will be presented.

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Graphene oxides modified with Pd nanoparticles as effective catalysts for the reduction

김지당 최현철*

전남대학교 화학과

sp^2 carbon nanostructures has received of attention due to their unique physical and chemical properties. Especially, graphene is a two-dimensional material with a single atomic layer of carbon atoms arranged in a hexagonal lattice. Due to its unique structure, graphene exhibits unusual optical and electronic properties. Pd-based compounds have high catalytic activity. However, the applications of Pd nanoparticles remain limited by disadvantages in terms of their easy aggregation and the difficulty of catalyst product separation. So, try to overcome these problems, nanocomposites composed of Pd nanoparticles dispersed on suitable substrates have been intensively studied. In this study, we prepared Pd-decorated graphene oxide by introducing thiol groups on graphene surfaces. Surface thiolation is an effective way to obtain dispersed metal nanoparticles on the surface of graphene. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The reduction kinetics of 4-nitrophenol is also investigated by ultraviolet-visible (UV-vis) measurement.

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오존처리에 의한 탄소나노튜브의 표면개질 방법 고찰

박태진* **Stanislaus S. Wong[1]**

한국원자력연구원 방사성폐기물처분연구부 [1]SUNY Stony Brook

탄소나노튜브는 6 각형 고리로 연결된 탄소, 즉 벤젠이 연결되어 벌집모양을 갖는 긴 대롱 모양을 이루게 된다. 따라서, 이론적으로 탄소나노튜브의 표면은 벤젠과 유사한 특성을 가지게 된다. 하지만, 실제 탄소나노튜브의 경우 그 표면에 무결정성 탄소층 등이 존재하기 때문에 온전한 물성 확인과 응용을 위해선 먼저 탄소나노튜브의 표면을 정화해야 한다. 아울러, 나노규모의 탄소나노튜브에 기능성 재료를 연결하여 복합 특성을 기대하기 위해선 탄소나노튜브의 표면개질이 반드시 필요하다. 본 연구에서는 탄소나노튜브의 표면정화 및 표면개질을 동시에 처리할 수 있는 오전처리방법(ozonolysis)에 대해서 간략하게 알아보고자 하였다. 더불어, 오존처리된 탄소나노튜브에 촉매 및 양자점(quantum dot)을 연결, 그 복합특성을 확인하는 연구를 살펴보았다.

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Ultrafast Removal of Anionic and Cationic Heavy Metals at Dirking Water Level Using Hierarchically Structured Carbonate Adsorbent

Md. Shahinul Islam Mahfuza Mubarak[1] 최원산[2] 이하진[*]

한국기초과학지원연구원 서울서부센터 [1]이화여자대학교 화학나노과학과 [2]한밭대학교 화학생명공학과

This report presents impractical applicable, iron oxide coated hierarchical magnetic IO@$CaCO_3$ synthesized via a hydrothermal method. This material shows very faster removal rate of both the anionic As(V), Cr(VI) and cationic Pb(II) compare to any conventional adsorbent reported so far. Only 9 min is required for complete removal (99.99%) of As (V) along with other toxic metals from waste water. Also, exhibited excellent adsorption capacity of As(V), Cr(VI) and Pb(II) 184.1, 251.6 and 1034.6 mg $g^{?1}$, respectively at broad pH range. The adsorption of heavy metals involved ion-exchange between the metal ion species and negatively charged groups, including surface hydroxyl groups, sulfate, carbonate and carbonate-like species. Along with batch adsorption technique, column-based filtration method for the removal of heavy metals in aqueous system was also being testified. Moreover, the effects of various pH and ionic strength on adsorption of heavy metals were evaluated. Moreover, IO@$CaCO_3$ adsorbent showed excellent recyclability property.

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Catalytic activity of Ag-decorated graphene oxides in the reduction of 4-nitrophenol

김지당 최현철*

전남대학교 화학과

The recent increase of interest in carbon materials has opened new ways for producing arrays of novel functional nanomaterials. Among them, graphene is a two-dimensional material with a single atomic layer of carbon atoms arranged in a hexagonal lattice. Due to its unique structure, graphene exhibits unusual optical and electronic properties. In this study, we prepared Ag-decorated graphene oxide by introducing thiol groups on graphene surfaces. Thiol groups were utilized as linkers to secure the Ag nanoparticles without agglomeration. The samples mainly were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The Ag-decorated graphene oxide exhibits high catalytic activities for the reduction of 4-nitrophenol.

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Enhanced Electrochemical Performance of Lithium-Sulfur Battery by TiO_2 Layer Coating on Ordered Mesoporous Carbon Cathode

오세민 최윤석 JINXING 김지만*

성균관대학교 화학과

Various kinds of materials such as conducting polymer, graphene, inorganic oxide have been presented as a solution for physical barrier to impede the dissolution of polysulfide in lithium-sulfur battery. In this work, another efficient physical barrier was built by coating of TiO_2 layer over Ordered Mesoporous Carbon (OMC) cathode with sol-gel method. TiO_2 layer was amorphous nature identified by XRD and UV-reflectance and very thin examined by SEM and TEM. The material was investigated as cathode for lithium-sulfur battery. The electrode of TiO_2 coated OMC exhibited the enhanced electrochemical performance of battery. TiO_2 coating resulted in higher discharge capacity and capacity retention compared to OMC electrode. Thin layer of TiO_2 possibly facilitates the reduction of sulfur which is captured within TiO_2 barrier. Consequently, higher amount of sulfur is utilized in electrochemical reaction of lithium-sulfur battery.

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Conductivity Enhancement of Poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) Induced by Ionic Exchange with Ionic Liquid Additives: Density Functional Theory Calculation

박성진 장윤희[1,*]

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Poly(3,4-ethylenedioxythiophene):Poly(styrenesulfonate) (PEDOT:PSS) is a flexible, transparent and solution-processible conducting polymer. But, its conductivity is not satisfactory for its electronic application. Recently, excessive amount of PSS inhibits the packing and alignment of the PEDOT chains. Recently, ionic liquid (IL) additives have been used to improve conductivity of PEDOT:PSS, but the detailed mechanism has not been clearly understood. Only hypothesis is that an ionic exchange helps the alignment and packing of the PEDOT chains. Therefore, we herein carry out density functional theory (B3LYP/6-31++G**) calculations of exchange free energy between PEDOT:PSS oligomer and a series of IL pairs in aqueous phase using Poisson-Boltzmann solvation model. Moreover, we also monitored the PEDOT chains along the ionic exchange process. Indeed, we find that high-performance IL additives induce an spontaneous "ionic exchange" with PEDOT:PSS. With such exchange, the PEDOT chains would decouple from entangled PSS, and evolve into a rather extended, aligned, closed packed structure resulting in a 5000-fold improvement of their electrical conductivity. This result provides a guideline for a design of high-performance IL additives: weakly-bound IL pairs inducing a spontaneous exchange with PEDOT:PSS would increase conductivity of a PEDOT:PSS-based electrode.

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Controlled Regioregularity of Pentathiophene Based Copolymers for Solution-Processable Organic Thin Film Transistors (OTFTs)

김형남 김윤희* 안은수 이예슬

경상대학교 화학과

We developed new amorphous copolymer via Pd-catalyzed Suzuki coupling reaction. The copolymer has good solubility in common organic solvent such as chloroform, toluene, chlorobenzene. The polymer exhibit good thermal stability and high charge-carrier mobility and high on/off current ratio. The field effect mobility of OTFTs the advantages of cheap manufacturing and simple processing make them suitable for commercial applications. The facts important for obtaining high mobilities are the use of organic molecules with high structural order and an extended π-system as active layers.

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Controlling Emitting Dipole Orientation of Iridium Complexes for Highly Efficient Phosphorescent Organic Light-Emitting Diodes

안은수 이지은 LIU XIANQING 김윤희* 김장주[1],*

경상대학교 화학과 [1]서울대학교 재료공학부

In this study, we investigated the effect of main ligands of heteroleptic Ir complexes (HICs) on the emitting dipole orientation (EDO) in doped films and related the EDO to the angle between the transition dipole moments (TDM) of emission dipoles and the C2 axis of the molecules. For this purpose, we designed and synthesized four iridium complexes where the hydrogen atom(s) at different positions of the cyclometalated ligands of Ir(ppy)2 tmd were systematically replaced by methyl group(s) keeping the ancillary ligand the same as tmd.

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Tailored Magnesium Oxide as a Catalytic Template for the Preparation of Graphitic Mesoporous Carbon

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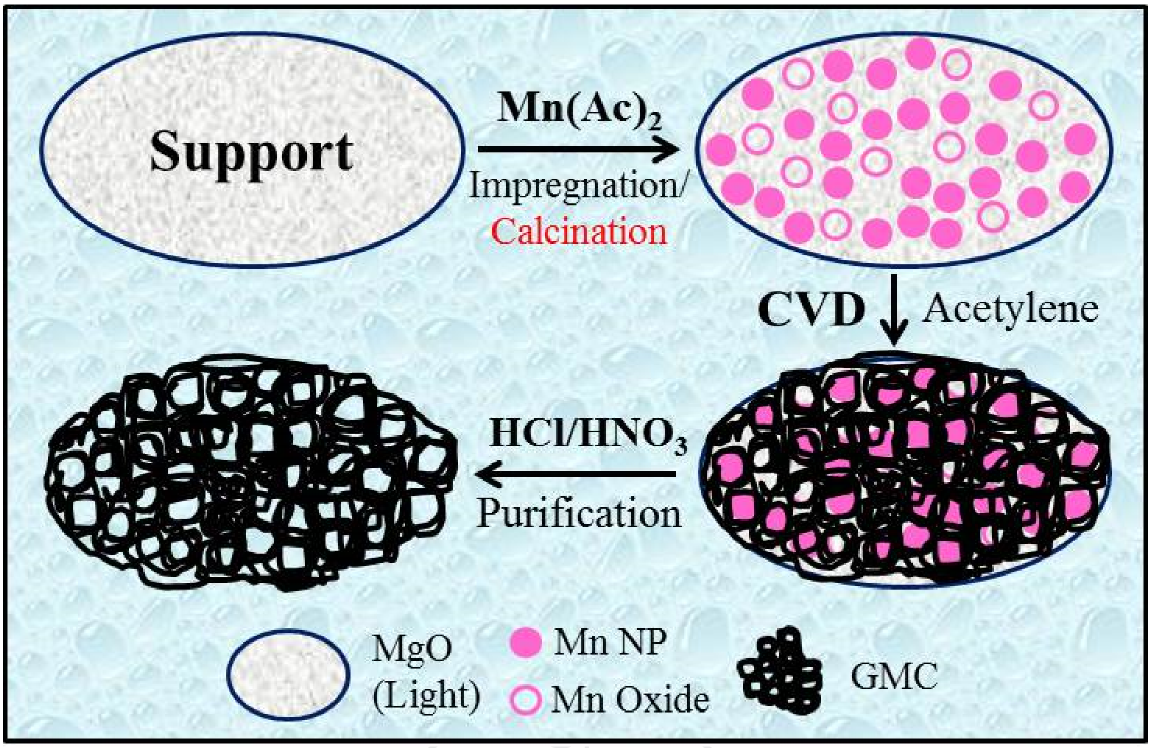
Manganese impregnated MgO was prepared by simple wet impregnation method. Mn/MgO was used as a catalytic template for the production of graphitic mesoporous carbon (GMC) using acetylene gas as carbon precursor by chemical vapor deposition (CVD) method. The metal concentration over the MgO and reaction temperature was optimized for the better formation of GMC. The deposited GMC was separated from the catalytic template by the acid treatment, and was investigated by various physico-chemical techniques such as XRD, N2 sorption, SEM, HRTEM, and Raman spectroscopy. The BET surface area of GMC is ca. 200 m2 g?1. The XRD pattern and Raman spectroscopic techniques revealed the crystallinity and the degree of graphitization of mesoporous carbon. Raman ID/IG value of GMC showed the high degree of graphitization. The XRD pattern also supports the formation of GMC is high purity with well graphitized. The interlayer distance of GMC is around 0.34 nm which matches well with the bulk graphite hexagonal structure. All the analytical results strongly support the prepared mesoporous carbon to be highly ordered, and well graphitic nature. Further, the results demonstrate that the GMC synthesized by using a Mn/MgO might be a promising contender for the large-scale synthesis. The produced GMC with high degree of graphitization might be an ideal candidate for nanoelectronic application like supercapacitors and so on.


Support
Mn(Ac)2
Impregnation/
Calcination
CVD
Acetylene
HCl/HNO3
Purification
MgO
(Light)
Mn NP
Mn Oxide
GMC

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The design of new D-A type copolymers for high-performance Organic Thin?Film Transistors

이예슬 안은수 LIU XIANQING 김윤희*

경상대학교 화학과

Two new D-A copolymers, PNDT-B and PNDT-TBT, were synthesized and characterized for use as active materials in OTFTs. The incorporation of NDT groups effectively extended the degree of π-conjugation in both systems. And the long alkoxy side chains of both polymers facilitated good solubility in common solvents. The structure and physical properties of polymers were characterized by DFT calculation, UV?vis absorption, cyclovoltammetry, TGA and DSC analyses. X-ray diffraction studies indicated a relatively highly ordered intermolecular structure in PNDT-TBT after annealing. This high degree of molecular order resulted from the crystallinity and increasing planarity, provided by the thiophene linker groups and the interdigitation of the long alkoxy side chains.

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Structural and optical investigation of Organic semiconducting materials with different end groups

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경상대학교 화학과

Organic thin film transistors (OTFTs) have attracted a lot of interest because of their potential as replacements for conventional silicon-based transistors in low-end electronic applications, as well as the possible applicability as base elements for the development of new opto-electronic products. OTFT active materials can be divided into two classes according to their processing methods, i.e., solution processing and vacuum deposition processing. Solution processed organic semiconductors have attracted considerable interest because of the low fabrication costs; deposition of semiconductor layer by ink jet printing, spin-casting, and dipping. They also have higher compatibility with plastic substrates than silicon based thin film transistor (TFT), and diverse potential applications, such as in driving circuits of large-area flexible display panels, new generation smart cards, integrated logic circuits, and sensors etc.We studied structural and optical investigation of Organic semiconducting materials with different end groups.

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A Facile synthesis of efficiently recyclable Ag coated Fe_3O_4@TiO_2 core-shell particles

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With growing demand for clean and comfortable environment, purification technologies with high efficiency and low cost to reduce the pollutant contents of wastewater are urgently needed. In this study, a facile and efficient approach for the fabrication of Ag coated Fe_3O_4@TiO_2 particles with a good core-shell structure has been demonstrated. The synthetic protocol involves the coating of successive layers of TiO_2 nanoparticles on to a magnetic core using a sol-gel method at low temperature followed by the deposition of silver nanoparticles on the surface of the Fe_3O_4@TiO_2 particles through a chemical reduction route. The Ag coated Fe_3O_4@TiO_2 magnetic photocatalyst exhibited high photocatalytic activity in the degradation of Rhodamine B (Rh.B) under visible light. Moreover, Ag coated Fe_3O_4@TiO_2 photocatalyst show flawless photocatalytic properties than in the previous report concerning oxidationreaction of 2,4,6-trichlorophenol (2,4,6 TCP) in aqueous solution. The renewable photocatalytic activity of the photocatalyst was also examined.*Keywords*: Ag coated Fe_3O_4@TiO_2, core-shell structure, magnetic photocatalyst, renewable photocatalytic activity, 2,4,6-triclorophenol

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Electrochromic device with separated porous electrolyte layers

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With a possible application for outdoor reflective information displays, electrochromic device is nonemissive, different from emissive types such as LCD and LED, and provides some considerable advantages such as excellent visibility outside and little viewing angle dependence as well as low driving voltage. However, most electrochromic devices render a phenomenon of image blurring through adjacent cells. This takes place as current paths through the electrolyte, and results in a serious problem against clear images displayed in an electrochromic device. In the past, to avoid the color blurring, a partitioning technique separating electrolyte was employed, which was costly and technically getting more difficult as the cell size decreased. In this study, some porous, separated electrolyte layers with various sizes were embedded in between both electrodes, by which it became available to induce the specific-oriented movement of the materials such as ions within the electrolyte. And it was found out that such a way of moving the materials within the electrolyte in a specific direction could greatly help minimize the image blurring.

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A spray drying approach for the fabrication of porous silicon-carbon nanotube micro particles for highly stable Li battery anode

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성균관대학교 화학공학과 [1]성균관대학교 화학공학부

Porous silicon-carbon nanotube micro particles have been successfully prepared by a spray-drying followed by calcination process. The particles were composed of carbon nanotube (CNT) networks, which were decorated by silicon nanoparticles (Si). The aqueous solution with CNT, Si, glucose and poly(vinylpyrrolidone)(PVP) was used for the spray-drying. The size and porosity of particle were controlled by the content of PVP and confirmed by scanning electron microscopy, Brunauer-Emett-Teller analysis and thermogravimetric analysis. Moreover, its electrochemical properties as Li battery anode were also characterized by galvanostatic charge-discharge test. The prepared Si-CNT particle showed high specific capacity with outstanding cyclic stability owing to its porous structure. The pores in the particle buffer the stress from the volume-variation of silicon and also facilitate the ionic diffusion, resulting in the high performance as a lithium battery anode.

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Preparation and Optical properties of barium titanates doped with lanthanum ions

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동국대학교 신소재화학과

Barium titanate is a versatile perovskite material which exhibits high dielectric constant, ferroelectric and electrical insulating property, and chemical and physical stability. Pure and lanthanum doped barium titanates were prepared by solution combustion method. XRD analysis indicates the formation of tetragonal barium titanates. The phonon frequency and band gap of barium titanates were estimated from the IR and diffuse reflectance spectra, respectively. The luminescence intensity was highly dependent on the concentration of lanthanum ions as well as the concentration of sensitizer and the intensity of excitation source. The results were utilized to discuss the luminescence mechanism.

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Synthesis of Copolymers with Different Alkyl Groups for Organic Solar Cells

LIU XIANQING 이지은 하연희 김윤희*

경상대학교 화학과

Alkyl side-chain engineering has shown considerable potential for the development of high-performance photovoltaic polymers. Indeed, the crystallinity of polymer in the solid state, and their solubility in organic solvents are directly controlled by the characteristics of the alkyl side chains of the polymer backbone. Proper selection of the tethering position, length, and bulkiness of these side chains is paramount for obtaining desired photovoltaic properties. To explore these effects, we synthesized copolymers and studied them with regard to chemical structure and photovoltaic performance. UV?vis spectroscopy and cyclic voltammetry studies showed that variations in alkyl chain length affect crystallization, light absorption, and the HOMO and LUMO energy levels. To know the impacts on the photovoltaic performance, we fabricated OPV devices with PC71BM as acceptor and measured the performance of these devices. Therefore, we can get significant result replacing alkyl groups.

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Structural and optical studies of Yttrium indates prepared by solution combustion method

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Pure and lanthanum doped yttrium indates were prepared by solution combustion method. XRD analysis indicates both c-type and hexagonal forms of yttrium indates can be prepared depending on the sintering temperature. The phonon frequency and band gap of yttrium indates estimated from the IR and diffuse reflectance spectra, respectively. The luminescence spectra showed peaks at 526 nm, 548.5 nm, and 662.5 nm. The effects of the concentration of activator and sensitizer on the luminescence intensity were studied. Furthermore, the effects of the excitation source intensity on the luminescence was investigated and their detailed analysis indicates that the luminescence occurs through the two-photon absorption process.

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Studies on fine structure analysis and enhanced electrochemical performance promoted by Ruthenium doping in $Li_2FeP_2O_7/C$ lithium ion batteries cathode materials

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울산대학교 자연과학대학 화학과 [1]울산대학교 화학과

After initial commercialization of the lithium ion batteries filed, lithium transition metal oxides ($LiMO_2$, M=transition metal) were widely used in cathode materials for an electronic devices. According to an increase of the demand, high cost and safety issues came to the fore. Although several cathode materials including olivine-structured $LiFePO_4$ and polyanion-based compounds have been considered as next generation lithium ion battery materials, most of them possess low operation voltage and discharge capacity. After that, Nishimura et al. first reported $Li_2FeP_2O_7/C$ which has highest reversible potential of 3.5V (vs. Li/Li^+) among all Fe-containing phosphate cathodes, its specific discharge capacity is 110mAh/g in 2.0V-4.5V (vs. Li/Li^+).We study on electrochemical performance and structural characteristics promoted by Ruthenium (Ⅲ) doping on $Li_2FeP_2O_7/C$. The $Li_2Fe_{1-x}Ru_xP_2O_7/C$ (x =0.00, 0.005, 0.01, 0.02, 0.03, 0.04, 0.08, 0.10) were prepared by simple sol-gel synthesis method. Doped ratio of ruthenium is measured by ICP-AES. Also, XPS measurements were conducted. The monoclinic P 21/c (14) space group crystal structures were determined by XRD and Rietveld refinement data. The morphologies were observed by FE-SEM, and HR-TEM, respectively. Also, electrochemical measurements such as A.C. impedance, cyclic voltammetry, galvanostatic charge-discharge were conducted. As a result, ruthenium doped LFPO/C have advantages of an increased specific capacity at various current density as well as a decreased polarization during the charge and discharge.

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Layered gadolinium hydroxides equipped with organic spacers for the selective detection of meta-vanadate in aqueous solution

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경희대학교 응용화학과

In the past, vanadium compounds were prescribed as therapeutic agents for anaemia, chlorosis, tuberculosis and diabetes. Generally, the vanadium compounds mainly exists as oxo-anion forms (vanadates) in dilute aqueous solutions, and the toxicity increases with the oxidation states. However, in aqueous solution, even non-toxic vanadium compounds can easily transform to vanadium pentoxide (V_2O_5) and trioxide (V_2O_3) which are distributed mainly to the bone, liver, kidney, and spleen. And these compounds may harm the human body, including the respiratory, circulatory and central nervous system, digestive system, kidneys, and skin diseases. In this study, we investigated Eu-doped layered gadolinium hydroxides (LGdH:Eu) modified with organic anions (carboxylate, sulfonate and sulfate groups) as a possible fluorescent sensor for selective detection of meta-vanadate in aqueous solutions. It is interesting that the sensitivity for the meta-vanadate could be significantly enhanced by the simple exchange reaction with non-conjugated organic groups, where no energy transfer process is expected. We propose that these organic spacers can highly increase the accessability of meta-vanadate ions into the interlayer spaces and consequently expand the energy transfer routes from vanadate groups. When LGdH:Eu-Org was ultimately exfoliated in formamide, the red emission of this luminescent colloid was detectable for meta-vanadate concentration lower than 5 ppm even with the naked eyes.

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Phase Transformation of SiO_2 coated Nano Ceramic Pigment

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한국세라믹기술원 엔지니어링 세라믹 센터 [1]한국세라믹기술원 엔지니어링세라믹센터 [2]한국세라믹기술원 도자세라믹센터

This work characterization of the coloration and thermal behaviors of SiO_2 coated β-FeOOH nanorods. Generally, nanoparticles have reduced their original properties at high temperature. For example, previously our groups demonstrated that the SiO_2-coated α-Fe_2O_3 nanoparticles retained their coloration after being heated to 1000°C. Especially, rod type β-FeOOH is easily tuned color change from redness to yellowness through various length of β-FeOOH. However, color of β-FeOOH was easily thransformed to dark brown α-Fe_2O_3 at 500°C. To improve thermal/color stability of β-FeOOH, which can be applied for core-shell structure. We selected the SiO_2 as shell for minimizing their oxidation and aggregation of nanoparticles. The SiO_2 is a common coating material due to its high stability and transparency. In particular, SiO_2 is a suitable material for use as an optical coating due to its transparency in the visible range. We studied the relationship between SiO_2 coating and phase/coloration of β-FeOOH nanorod. Details of the phase structure and optical properties of core-shell structures were characterized by UV-vis, TEM (transmission electron microscopy), CIE Lab color and XRD (powder X-ray diffraction).

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Effect of transition metal ion adsorption on the luminescence behavior of $GdVO_4$:Eu nanoparticles

김현섭 고두현* 변송호*

경희대학교 응용화학과

Gadolinium orthovanadate ($GdVO_4$)-based nanoparticles have attracted considerable attention for applications as a multifunctional bio-probe, simultaneously capable of fluorescent and magnetic imaging. In particular, when activator ions were doped into $GdVO_4$ matrices, they show efficient luminescence properties which is useful in bio-probe applications, because of a strong absorption of the VO_4^{3-} group followed by an efficient energy transfer from $GdVO_4$ to activator ions. Recently, we recognized that even small amount of transition metal ions, when adsorbed on the surface, can interfere the bio-probe function of $GdVO_4$ nanoparticles. In this study, the effect of transition metal adsorption on the luminescence behavior of Eu-doped $GdVO_4$ ($GdVO_4$:Eu) nanoparticles have been closely investigated for various kinds of transition metal ions (Co^{2+}, Cd^{2+}, Cu^{2+}, Mn^{2+}, Ni^{2+}, Pb^{2+}, and Zn^{2+}) with different concentrations in aqueous media. A significantly different decrease in intensity of the red emission of $GdVO_4$:Eu nanoparticles was induced depending on the transition metal cations. This behavior is explained by the different secondary inner filter effect (IFE) due to a different spectral overlap between the emission band of $GdVO_4$:Eu and the absorption band of transition metal cation. The most efficient filtering of $GdVO_4$:Eu emission was observed after adsorption of Cu^{2+} in aqueous solution.

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Preparation of ZnO-decorated CNTs and investigation of their photocatalytic properties for congo red

오명은 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have interesting mechanical, physical and chemical properties due to their strong covalent bonding combined with their unique 1-D nanostructures. However, further improvements in synthesis and post-processing are required to optimize their properties for practical applications. For instance, the strong tendancy of agglomeration, as well as a poor wettabily with nonorganic materials, are major problems for the fabrication of CNT-reinforced composites. To address these problems, surface and structure modifications of the CNTs by physical and chemical methods have been developed, including ball millng treatment, plasma treatments, polymer wrappings, electrochemical treatments, and surface functionalizations with functional groups. Among the various CNT dispersion methods reported, high-energy ball milling is used most commonly. In this work, we present the ZnO-decorated CNTs by high energy ball-milling treatment. The prepared sample was characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photocatalytic activities of prepared materials was evaluated by the conversion of congo red in aqueous solution under UV irradiation. The obtained results showed that ball milled CNT-ZnO displayed much higher photocatalytic activity compared to non-treatment material.

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Functionalization of ordered mesoporous carbon with sulfonic acid group for Na/SO$_2$ battery

황윤경 원종구 이창현 **JINXING** 김지만*

성균관대학교 화학과

Sodium-ion batteries have attracted great attention particularly in large-scale electric energy storage applications for renewable energy and smart gred because of the huge abundant sodium resources and low cost. However, it has some disadvantage like lack of battery performance and safety in the practical application. In this study, we report a synthesis of functioncalized ordered mesoporous carbon(OMC). And it is used to Na/SO$_2$ batteries as cathode material. The ordered mesoporous carbon(OMC) synthesized by hard template mathod throughout nano-casting. The carbon precursor into the template(SBA-15) followed by carbonization at 900℃. And then functionalize ordered mesoporouse carbon surface to see the effect of chemical properties of the surface. The synthesized material was identified by high angle X-ray diffraction(XRD), N2 adsorption-desorption isotherms, scanning electron microscope(SEM), FT-IR spectroscopy, thermogravimetric analysis, and electrochemical properties were analyzed by charge-discharge profile and cycle performance.

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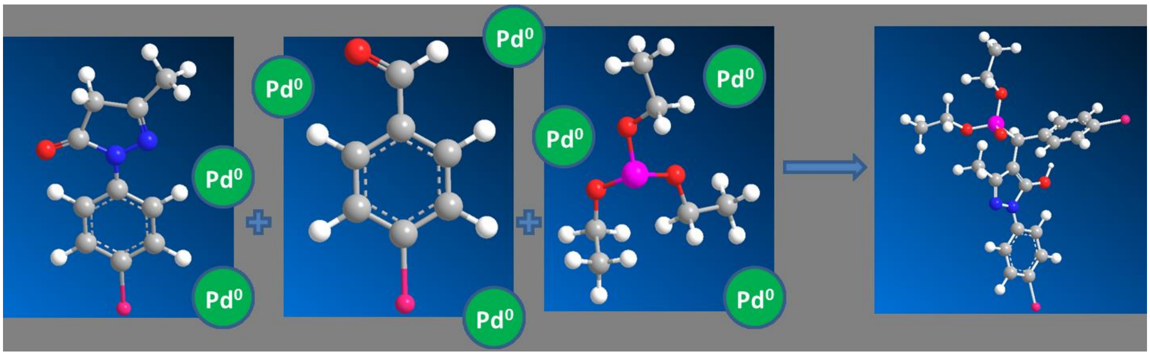
Biosynthesis and characterization of palladium nanoparticles and their catalytic application in multicomponent reaction

<u>BASAVEGOWDANAGARAJ</u> MISHRAKANCHAN 이용록[*]

영남대학교 화학공학부

Palladium nanoparticles (PdNPs) were synthesized using green method. An aqueous extract of *Perilla frutescens* leaf was used as a bioreductant to reduce Pd^{2+} ions to Pd^0 without any extra surfactants or capping agents. Polyphenols and flavonoids are believed to be actively involved in the reduction process. The formation of PdNPs was confirmed by UV-Vis spectra. Transmission electron microscopy revealed spherical nanoparticles, ranging in size between 10 and 17 nm (average ~13 nm). X-ray diffraction revealed reflections from the (1 1 1), (2 0 0), (2 2 0), (3 1 1) and (2 2 2) planes confirming the crystallinity of the nanoparticles with a face centred cubic (fcc) structure. Energy dispersive X-ray spectroscopy confirmed the presence of palladium. Fourier transform infrared spectroscopy suggested the role of polyols present in the *P. frutescens* leaf extract. The synthesized nanoparticles were used as a catalyst for the synthesis of pyrazolylphosphonate derivatives in high yield. The excellent catalytic performance of the synthesized PdNPs can be associated to their extremely small size and high dispersity, so the as-synthesized PdNPs will be applicable for future industrial processes.



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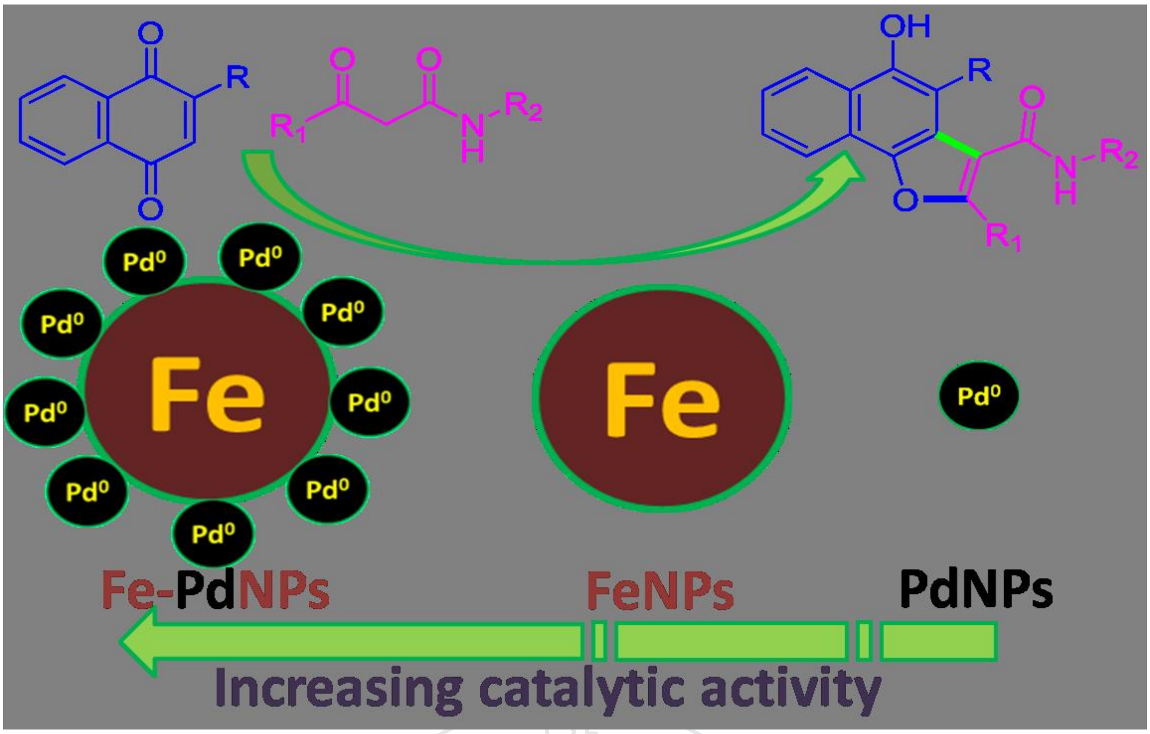
Green synthesis of Fe, Pd, and Fe-Pd bimetallic nanoparticles and their catalytic application for the construction of naphtho[1,2-*b*]-furan-3-carboxamides and benzofuran-3-carboxamides

MISHRAKANCHAN BASAVEGOWDANAGARAJ 이용록*

영남대학교 화학공학부

The surface adjustment of iron nanoparticles by secondary metals increases the reaction efficiency of bimetallic nanoparticles. The adsorption of secondary metals (e.g., Pd, Ag, Pt, or Ni) on iron can increase the reaction efficiency of iron nanoparticles. In addition, magnetic separation is a better option than filtration or centrifugation because it increases the reusability by preventing the loss of catalyst. Herein, we present a green and facile approach for the synthesis of Fe, Pd and Fe?Pd bimetallic nanoparticles using an aqueous bark extract of Ulmus davidiana and their application as magnetically recoverable catalysts for the [3 + 2] cycloaddition of 1,4-naphthoquinones or benzoquinones with β-ketoamides. The surface chemistry of the Fe-Pd bimetallic nanoparticles was determined by X-ray photoelectron spectroscopy. The morphology, size, crystallinity, weight loss, oxidation state, and ferromagnetic behavior of the synthesized nanoparticles were investigated. The bimetallic nanoparticles exhibited strong catalytic activity in high yield for the synthesis of naphtho[1,2-*b*]furan-3-carboxamides and benzofuran-3-carboxamides compared to their respective monometallic nanoparticles.


O
R
O
O
O
R1
N
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R2
OH
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R2
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Pd0
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Pd0
Fe-PdNPs
FeNPs
PdNPs
Increasing catalytic activity

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Dye-doped silica coated iron oxide nanoparticles for in vivo MR and fluorescence cancer imaging

이채동 김종민 박원철*

서울대학교 융합과학기술대학원 융합과학부

In this research, we prepared fluorescent silica-coated iron oxide nanocrystals for dual fluorescence and magnetic resonance imaging. The as-prepared core/shell nanoparticles were intended to improve the diagnostic accuracy and broaden the scope of the diagnosis. In the synthesis, the as-prepared iron oxide nanocrystals were coated with RITC (Rhodamine B isothiocyanate)-doped silica shell via reverse micelle method. Then the core/shell nanoparticles were analyzed to confirm the shape, size distribution and fluorescence by transmission electron microscopy (TEM), dynamic laser scattering (DLS) and photoluminescence (PL) spectroscopy each. By WST-1 assay, we confirmed that the as-prepared nanostructures are not toxic in cell levels. Finally, through in vivo MR and fluorescent imaging, we verified its possibility as bimodal imaging contrast agents for cancer diagnosis.

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Fluorescent silica-based mesoporous nanoparticles for ibuprofen drug delivery

서보경 유동건 박원철*

서울대학교 융합과학기술대학원 융합과학부

In this research, we synthesized Rhodamine B isothiocyanate (RITC)-doped core/mesoporous shell silica nanoparticles as theranostic nanocarriers. RITC-encapsulated silica nanoparticle cores were prepared by sol-gel process. The cores were grown to the desired size by controlling the conditions in the St?ber method and mesoporous shell was further added around the core by using cetyltrimethylammonium bromide (CTAB) as porous guiding agent. The shape, size and fluorescence of the as-prepared nanostructures were confirmed by using transmission electron microscopy (TEM), dynamic laser scattering (DLS) and photoluminescence (PL) spectroscopy. Ibuprofen loading and release experiments in buffer solution (pH 7.4) showed that these nanostructures were available for drug delivery system. In addition, cytotoxicity test and fluorescent imaging were conducted to investigate the cell-level behaviors in cellular level and confirmed its possibility as a theranostic nanocarriers

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Electrochemical oxidation of methanol by a multi-wall carbon nanotube modified electrode

오명은 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have drawn particular attention on account of both their scientific interest and their potential for technological applications. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO_2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and hydrodehalogenation. In this work, we demonstrate the efficient synthesis of the bimetallic (Pd-Pt) nanoparticles decorated CNTs. The prepared sample was characterized by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and cyclic voltammetry (CV). For the methanol oxidation the bimetallic (Pd-Pt) nanoparticles decorated CNTs exhibites high electrochemical activity.

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Simple Solventless Synthesis of Silver-Copper Bimetallic Nanoparticles with Core-Shell and Alloy Structures

최은진 이소희 김다솜 박원철*

서울대학교 융합과학기술대학원 융합과학부

Noble metal nanoparticles (NPs) have been extensively utilized owing to their novel optical, electronic, catalytic, magnetic and mechanical properties as compared to the corresponding bulk materials. In recent years, bimetallic NPs have also attracted considerable attention not only from the integrated properties by tuning the composition of the constituent elements but also from the new and unusual properties by mechanically alloying. Among many bimetallic NPs, Cu-based NPs incorporated with noble metals have a number of advantages compared to mono-element metallic NPs, such as much higher catalytic activity, better antibacterial ability, and relativity low-cost. In this study, we report a simple solventless synthetic protocol to produce Cu-based bimetallic NPs incorporated with Ag. Small-sized bimetallic nanomaterials are obtained by heat treatment, using salt powder as a template. Moreover, the structures of the NPs can be tuned by the reaction temperature, allowing for selection between hetero-structured core-shell NPs and homogeneous alloys. The size, structure, elemental distribution, and surface chemical identification of the Ag@Cu core-shell and AgCu alloy NPs were characterized by high-resolution transmission electron microscopy, field-emission scanning electron microscopy, energy-dispersive X-ray spectroscopy, high-angle annular dark-field scanning transmission electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy, and cyclic voltammetric measurement. The proposed synthetic procedure provides a simple and scalable approach for mass production and can be widely applied to prepare other single metal or alloy NPs.

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Photocatalytic activity of struvite-based catalyst

정지현 최현철*

전남대학교 화학과

Nitrogen (N) and phosphorus (P) are the indispensable elements for all living organisms. They play an irreplaceable role in the breeding, growth, and development of organisms. However, pollution problems related to the N and P discharge of wastewater commonly include eutrophication and dissolved oxygen depletion in water bodies as well as toxicity to the aquatic life. Therefore, the removal of N and P from wastewater is an important priority for maintaining water quality and alleviating environmental pressure. Various chemical and biological processes have been developed for N and P removal, such as metal precipitation, biological nutrient removal processes, enhanced biological phosphorus removal processes, and the struvite crystallization process. Among these processes, the struvite crystallization process is an ideal technique because it can simultaneously remove and recover P and N from wastewater. The applications of crystallization techniques are used in a wide range of industries such as pharmaceuticals, fertilizers, catalysts, sugar, and specialty chemicals. The objective of this study is to investigate the applications of crystallization techniques of struvite as photocatalyst.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrolyte concentration and cell gap dependent coloration efficiency of electrochromic device

송주희 아칠성*

한국전자통신연구원(ETRI) 스마트I/O플랫폼연구부

Electrochromism is a phenomenon represented by reversible color changes (such as coloration and decoloration) through electrochemical redox reactions in electrochromic materials. Electrochromic device has such advantages as low driving voltages (< 3V), bistability, easy control of light transmittance with a driving voltage, and sustenance of transparent state with power off. Also, it has various applications, which include: smart optical shutters, smart windows, electrochromic mirrors, reflective information displays, and so forth. This presentation will demonstrate how coloration efficiency changes in response to the variation of electrolyte concentrations and cell gap between two electrodes. The results show that coloration efficiency decreased as the cell gap got closer, and was not affected by electrolyte concentration while it varied from 0.01M to 1M. And WO3 was used as the cathodic electrode whereas the anodic side employed triarylamine-modified nanostructured TiO2. The used electrolyte was LiClO4. Along with coloration efficiency according to the cell distance and electrolyte concentration, other properties such as coloration range, switching speed, and bistability were also examined.

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Amine group functionalized carbon nanotubes for Hiyama-coupling reaction

정지현 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have received a considerable attention due to their unique chemical and physical properties, as well as their technological applications, and so have been extensively studied assupporting materials. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electrooxidation,selective hydrogenation, alcohol oxidation, Suzuki coupling, Hiyama-coupling, CO oxidation, and Fischer-Tropsch synthesis, etc. Palladium is an attractive catalyst for the hydrodehalogenationreaction because it enhances the division of carbon-halogen bonds and facilitates hydrogenation. In this study, we manufactured Pd-CNT by modifying amine groups on CNTs surfaces. Amine groups wereutilized as linkers to secure the Pd nanoparticles without aggregation. The catalytic effect of Pd-CNT was investigated about Hiyamacoupling reaction of 4-iodotoluene with trimethoxy phenyl silane in pxylene.The morphology and structure of prepared surfaces are also examined by transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS).

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Facile synthesis of ordered mesoporous metallic nickel

JINXING LICHENGBIN 이창현 황윤경 원종구 김지만[*]

성균관대학교 화학과

Nanostructured nickel have been widely investigated as current collector, magnetism, and catalyst as a result of their different properties compared to their bulk materials. All this research is mainly based on the successful synthesis of nanostructured nickels such as nanoparticle, nanowire. Porous metallic materials have also attracted considerable attention because they have several advantages such as increased catalytic capabilities due to high surface area, enhanced transport of reactants, and ease of catalyst recovery. Here, we demonstrate a facile method for the preparation of highly ordered mesoporous nickel using cubic mesoporous silica (KIT-6) hard template, followed by complete characterization of the mesoporous metallic nickel.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Rapid colorimetric detection of inflammation by Polydiacetylene (PDA) biosensor

송시내 임은경[1,*] 하갑

한국생명공학연구원(KRIBB) 바이오나노센터 [1]한국생명공학연구원(KRIBB) 바이오나노연구센터

Biosensors for point-of-care testing of critical illnesses are urgently needed, especially in many areas of poor healthcare infrastructure. Herein, we developed colorimetric biosensor for C-reactive protein (CRP) as a marker of inflammation detection based on polydiacetylene (PDA) liposomes that provides a promising colorimetric biosensor for point-of-care use. It is well known that diacetylene lipid monomers were self-assembled into vesicles and polymerized by UV irradiation, resulting in the formation of blue-colored PDA liposome with maximal absorption at 640 nm. Subsequently, PDA liposomes modified with anti CRP antibody for CRP detection. Color of PDA liposomes change from blue to red in response to a variety of environmental perturbations, such as temperature, pH as well as ligand-receptor interactions. Therefore, we can detect inflammation through unique bleu-to-red color transition of PDA biosensor.

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A new multi-functional conjugated polymer for using in high-performance bulk heterojunction solar cells

이상봉 김형남 박성종 김윤희*

경상대학교 화학과

We have synthesized a new conjugated polymer, the novel units brings not only superior charge transfer properites but also charge transport characteristics for efficient bulk heterojunction solar cells. the polymer exhibited sufficient highest occupied molecular orbital (HOMO) energy levels to ensure a high open circuit voltage (VOC) in solar cell applications. The lowest unoccupied molecular orbital (LUMO) energies were 1.0 eV above those of the PCBM n-type acceptor, which generated a driving force for energetically favorable electron transfer. The results show that the new copolymer is a useful material for preparing high-performance PSCs and organic photovoltaic applications.

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A series of new polymers with alternating Donor and Acceptor for Solar Cells based on Thin Polymer Films

이지은 천예림 하연희 김윤희*

경상대학교 화학과

Organic photovoltaic devices have gained abroad interest in the last few years due to their potential applications in large-area and low-cost solar cells. Various material concepts have been employed using small molecules, conjugated polymers, and combinations of inorganic and organic materials as the active layer have been used. Among them, solar cells based on thin polymer films are particularly attractive because of their ease of film formation via a solution process and mechanical flexibility. Although significant progress has been made, the performances obtained from polymer solar cells (PSCs) are still not satisfactory for commercialization. As a result of intensive investigations by many researchers, it is well known that by lowering both HOMO energy level and bandgap, both high short circuit current (Jsc) and open circuit voltage (Voc) can be achieved thus rendering high power conversion efficiency (PCE) upon thorough device and materials optimization. The recent trend in molecule design of organic photovoltaic cell tends to match electron donor and electron acceptor pair. This design concept has various advantages such as easy facile control band gap and to help facilitated charge transfer in molecule. Moreover, these D?A polymer can provide long-wavelength absorption in UV?visible range and it is thus possible to increase Jsc. In this study, we designed a series of new polymers with alternating donor and acceptor.

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Preparation and Characterization of Ferromagnetic Fe_3O_4 and Layer Silicate Porous Composite

황지연 최진주 이지호 윤주영 한양수*

(주)나노스페이스 나노물질연구소

Highly porous composite materials of ferromagnetic Fe_3O_4 and layer silicate were prepared by a simple coagulation-precipitation method. The magnetite (Fe_3O_4) particles with the average size of ~300 nm were firstly dispersed in the aqueous solution containing citric acid, followed by mixing with the pre-swelled layer silicate colloidal solution. Then the pH of mixed suspension was controlled in the range of 2~6 by adding acetic acid, leading to highly viscous gel-like phase in the acetic pH domain (pH ${}_3O_4$ Particles and negatively charged layer silicate ones. The gel-like products were separated by centrifugation, washed with the mixed solvent of distilled water and acetone, then dried at 120℃ for 2hr. The porous structure analysis using nitrogen adsorption-desorption isotherm revealed that the composite powders exhibited high specific surface area up to 450 m^2/g, which is mainly consisted of mesopores with the pore dimension of 5.0 nm.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Photocatalytic propertices CNT-ZnO nanocomposites

김은혜 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have received a considerable attention due to their unique chemical and physical properties, as well as their technological applications. Recently, there have been great interest in metal oxides decorated CNTs for applications in heterogeneous catalysts, fuel cells and biosensors. The most appealing metal oxide is a Zinc oxide(ZnO) because of low cost, non-toxicity, outstanding stability, great surface area, oxide is a wide bandgap semiconductor (E_g ~ 3.4eV) with important technological applications in several fields. When ZnO particles are illuminated with ultraviolet (UV) light, electron/hole pairs are generated. These electrons and holes can migrate and initiate redox reactions with water and oxygen, by which they degrade organic molecules absorbed on the surface of a photocatalyst. In this work, we demonstrate a novel and simple method for the synthesis of CNT-ZnO. The prepared CNT-ZnO was characterized by X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photocatalytic activity of CNT-ZnO was tested by congo red degradation process under ultraviolet light irradiation. The results showed that CNT-ZnO exhibited excellent stability in the photocatalytic process.

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Amperometric determination of L-CySH with CNT-SNO$_2$ nanocomposites

김은혜 최현철*

전남대학교 화학과

L-cysteine is a sulfur-containing amino acids which naturally contained with small quantities in a number of proteins and plays a important role in biological system. For example, it can be used as a prospective radiation protector, antioxidant, free radical scavenger, and cancer indicator. Its deficiency is associated with a number of clinical situations such as liver damage, skin lesions, hair depigmentation, edema, lethargy, muscle, fat loss, slowed growth, and AIDS. Owing to the reasons above, sensitive detection of L-cysteine is practically important. In this study, we synthesized tin oxide decorated on thiolated carbon nanotubes (SnO_2-CNT). Morphology characteristics of the SnO_2-CNT were investigated with transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Cyclic voltammetry (CV) and amperometry (at an applied potential of 0.45 V) were used to investigate electrochemical characteristics.

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Effect of Heteroatom-incorporation on Ordered Mesoporous Carbon for Na/SO_2 Batteries Cathode

이창현 원종구 황윤경 JINXING 김지만*

성균관대학교 화학과

In this work, we propose the Na/SO_2 batteries using the porous carbon as cathode. Among the porous carbons, the ordered mesoporous carbon (OMC) has remarkable characteristics, such as high specific surface area and large pore volume. Particularly, the modification of ordered mesoporous carbon by substituting some atoms with heteroatoms, such as nitrogen (N), oxygen (O), sulfur (S) and phosphorus (P) is an effective way to tailor the electrical and chemical performance of their surface. We were successfully synthesized by nano-replication method using a variety of carbon precursor (e.g. phenanthrene, 1,10-phenanthroline, sucrose, p-toluenesulfonic acid(p-TSA), 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide(DOPO)). The physical properties of heteroatom-incorporated OMCs were analyzed by X-ray diffraction (XRD), N_2-sorption isotherm and scanning electron microscope (SEM). In the electrochemical properties, sulfur incorporated OMC(S-OMC) exhibits a better cycle performances than the others OMC.

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Carbon monoxide removal activity on clay supported binary copper manganese oxide catalysts

이지호 김세희 이희숙 한양수*

(주)세일에프에이 기업부설연구소

Hazardous gas (CO) removal activity was investigated on clay supported binary copper manganese oxide catalysts (CMP), CMP-Kuni, CMP-S1ME, CMP-Lapo. The composite type porous catalysts were prepared by a wet chemical redox-precipitation method in the presence of colloidal clay particles, respectively. Among them CMP-Lapo exhibited the highest CO removal activity which could be explained by the largest surface area of > 350 m^2/g. According to the catalytic activity of CMP-Lapo as a function of heat treatment temperature the highest CO removal activity was observed at 300 ^oC. The highly dispersed CMP catalytic particles in porous matrix formed by the house-of-card structure of platelet clay particles and the amorphous like character of CMP particles seemed to be important role in the catalytic decomposition of CO.

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Mesoporous CO oxidation catalyst via Mn-pillared layer copper hydroxide

이지호 김세희 이희숙 한양수*

(주)세일에프에이 기업부설연구소

The manganese species (MnO_4^-) pillared layer copper hydroxide, $Cu_2(OH)_3(MnO_4)$, was prepared by a direct coprecipitation method and evaluated as a low temperature CO oxidation catalyst. In a typical preparation, copper acetate solution and $KMnO_4$ solution were titrated simultaneously into the pH-controlled base solution, which resulted in the formation of Mn-species intercalated copper hydroxide layer with basal spacing (d_{001}) of 7.2 Å. Thus prepared Mn-pillared layer compound was further thermally treated at around 300 ^{o}C to obtain porous (SBET ~ 90 m^2/g) $CuO/CuMn_2O_4$ mixed oxide catalyst, and it exhibited excellent CO removal activity ever at room temperature.

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Development of n-channel polymer semiconductors for the thin-film crystalline structure

하연희 천예림 조길원[1,*] 김윤희[*] 이상봉

경상대학교 화학과 [1]포항공과대학교(POSTECH) 화학공학과

we designed two new hybrid linear side chains by alternating the combination of hydrophobic alkyl chains (?R?) and hydrophilic oligo(ethylene glycol) chains (?O?). The microstructural ordering of the resulting polymers was altered according to the attached side chains, without disrupting the rigidity of the polymer main chain. Unipolar n-channel charge-transport behavior was observed for the resulting copolymers. These results demonstrate that hybrid side chains using oligo(ethylene glycol) are promising new solubilizing groups for high-performance organic semiconductor materials.

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Opto-physical Properties and Surface Analysis of Opthalmic hydrogel lens using Acrylated polydimethyl siloxane

김동현 성아영[1,*]

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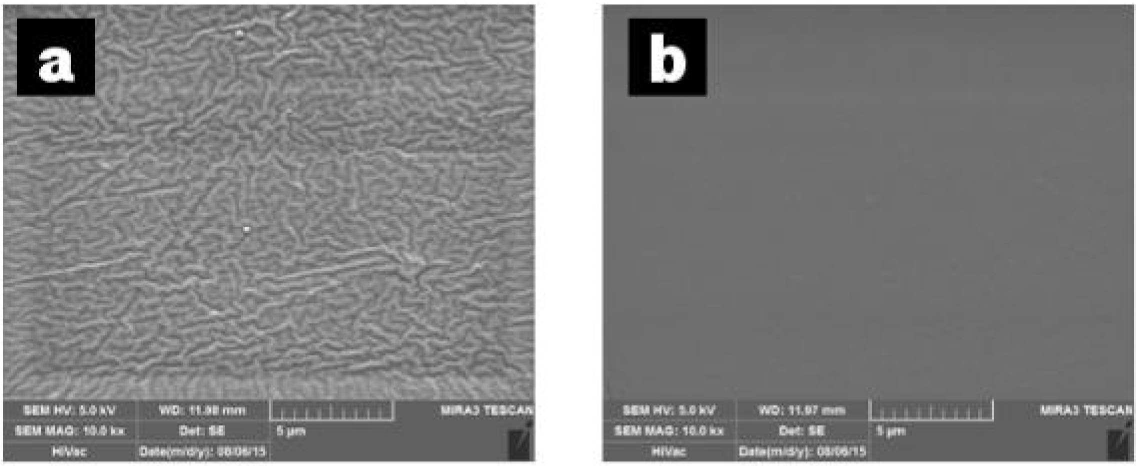
The materials for ophthalmic hydrogel lenses were polymerized by adding acrylated poly(dimethyl siloxane) to N,N-dimethylacrylamid, 2-Hydroxyethyl methacrylate and cross-linking agent ethylene glycol dimethacylate which are commonly used in ophthalmic hydrogel lenses. And also, the utility of acrylated poly(dimethylsiloxane) as a high gas permeability and visible light transmittance material for ophthalmologic devices by measuring the oxygen permeability, spectral transmittance and surface condition were investigated.(Fig. 1.) In case of the sample including silicone, smooth surface with some wrinkle pattern was observed. The oxygen permeability value of the lenses ranges from 25.04 to 27.90 x 10^{-11}(㎠ x ㎖ O_2)/(sec x ㎖ x mmHg). The visible light tansmittance of copolymerized ophthalmic lenses, was in the range 88~ 93%. The material containing siloxanyl methacrylate is expected to be able to be used usefully as a material for high oxygen permeability hydrogel lens. Fig. 1. Surface analysis of hydrogel lens sample by SEM (a: Inc. silicone, b: Inc. HEMA)



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Novel polymer for high performance bulk heterojunction solar cells

천예림 박성종 이상봉 김윤희*

경상대학교 화학과

Novel polymer for bulk heterojunction solar cells have attracted interest due to their potential application. In This work , We develop a polymer with good solubility, film-fabrication ability and thermal ability. It can pack closely to form crystalline structures that enhance charge carrier mobility. Considering above this factors, this material exhibits good properties with high PCE value. So this polymer can be promising donor material for high-performance PSCs.

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Calix[4]arene-spiropyran based receptor for metal sensors

이민혜 송창식*

성균관대학교 화학과

Design and development of efficient, sensitive and selective probe for metal sensor are an important research in biological, environmental and chemical science. Calixarenes is well developed and their unique topology offers a wide range of scaffolds enabling them to encapsulate many different metal ions. Even though, the various complexing units are available for the detection of metal ions (chelators, open-chain structures, crown-ethers, cryptands), calixarenes offer distinct advantages in term of selectivity and the easy incorporation of a various functional moieties into the skeleton. Calix[4]arene can be tuned to be sensitive and selective towards particular metal ions. Spiropyrans are photochromic compounds that can isomerize in response to UV/vis irradiation as a result of a reversible heterolytic cleavage of the spiro C-O bond followed by cis-trans isomerization which produces a metastable merocyanine. The zwitterionic open form of merocyanine exhibit negatively charged phenolic oxygen, that can act as a cheating site for a variety of metal ions. In addition, an increasing the binding sites into the spiropyran structure enhance the selectivity among various metal cations. The click reaction between azide and terminal alkyne catalyzed by Cu(I) has extensively facilitated the practical and efficient regiospecific formation of 1,4-disubstituted 1,2,3-triazoles. The triazole and its derivatives are utilizing the highly selective for the detection of various metal ions. Calix[4]arene-spiropyran offer significant promise due to the function of calix[4]arene and spiropyran units are bridged through 1,2,3-triazole. The present investigation mainly focuses on the design and synthesis of Calix[4]arene-spiropyran probe using click chemistry and their application in metal sensors.

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Enhancement in rate capability of disodium terephthalate by compositing with graphene for SIB anodes

김유신 표명호*

순천대학교 인쇄전자공학과

Organic compounds as anode material for sodium-ion batteries (SIBs) have been widely investigated because of low production costs and environmental friendliness. Disodium terephthalate (DST) is one of the most promising organic anode materials for SIBs, which has a theoretical capacity of 250 mAh/g. However, a relatively large amount of conductive additive is necessary because organic compounds have very low intrinsic conductivity. In this study, to improve the conductivity of an organic active materials, DST was composited with GO, and subsequently reduced thermally to form DST/rGO composite. Since rGO has relatively higher conductivity and larger surface area, the SIB using rGO-incorporated DST as an anode material is expected to show high rate capability and cycling stability. We have been attempting to control the microstructure of a DST/rGO composite by means of co-precipitation. In addition, the work on revealing the microstructure of DST/rGO composite and its effect on enhanced cell performance is currently in progress.

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Fabrication of Phosphorescence WOLEDs Based on Dimeric Phenoxazine Derivative for Hole Injection Layer

김승호 박종욱*

가톨릭대학교 화학과

Our hole injection material, namely, 10,10’-bis(4-tert-butylphenyl)-N7,N7’-di(naphthalen-1-yl)-N7,N7’-diphenyl-10H,10’H-3,3’-biphenoxazine-7,7’-diamine (1-PNA-BPBPOX) were adapted to white OLED devices for solution process. By incorporating adjacent blue and orange emitting layers in a multi-layer structure, highly efficient white emission has been attained. The device was fabricated with hybrid configuration structure. White devices were fabricated using a multilayer emission structure consisting of a single host layer. The red phosphorescent, tris(2-phenyl-1-quinoline)iridium(III) [Ir(phq)3], and the blue phosphorescent, iridium(III)bis[(4,6-di-fluorophenyl)-pyridinato-N,C2]picolinate (FIrpic), are doped into separate layers of N,N-dicarbazolyl-3,5-benzene (mCP) host. The FIrpic and Ir(phq)3 guest molecules are directly excited by direct recombination on these molecules. In the device, the maximum value of UV?visible absorption (UV-vis) of hole injection layer PNA-BPBPOX is 366 nm in solution state and 370 nm in film state, not showing absorption of visible light. When the device with BPBPOX was compared to the device with PEDOT:PSS a commercialized solution HIL material, luminance efficiency was 6.37 cd/A for PNA-BPBPOX and 0.66 cd/A for PEDOT:PSS for the optimized white device structure, showing 10 times as high efficiency.

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Improvement in Photocatalytic Activity and Thermal Stability of WO_x-Impregnated Disordered Nanoporous TiO_2

박수빈 **LIZHENGHUA**[1] 이현아 김지만*

성균관대학교 화학과 [1]성균관대학교 화학과

Titanium dioxide (TiO_2) has received a great attention in photocatalysis because of its high bandgap energy, non-toxicity, low-cost. Especially, nanoporous TiO_2 exhibits high activities and performances in photocatalysis fields due to its high surface area with large pore volumes. There are two kinds of nanoporous TiO_2, which are ordered and disordered nanoporous TiO_2. Disordered nanoporous TiO_2 is easier to prepare *via in-situ* hydrolysis of titanium glycolate spheres without employing any hard-templates than synthesizing ordered nanoporous TiO_2. In order to obtain high crystallinity of TiO_2 for high photocatalytic activitiy, post thermal treatment is necessary. In the previous research, however, it was observed that post thermal treatment led nanoporosity in disordered nanoporous TiO_2 collapsed by agglomerating TiO_2 primary particles. In this research, we investigated nano-propping effect of impregnated WO_x in the pores for hindering grain agglomerations. Impregnated WO_x obstructed TiO_2 grains from agglomeration, and improve the pore structure stability at high thermal treatment temperatures. Therefore, disordered nanoporous TiO_2 cooperated with WO_x showed large surface area and high crystallinity with large grains. It enhanced the photocatalytic activities of disordered nanoporous TiO_2.

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Metal Oxide Embedded Porous Carbon Composites using Metal-Organic Frameworks: Metal Oxide Form and Porosity Control Study

김의수 윤민영[1,*]

가천대학교 글로벌캠퍼스 화학과 [1]가천대학교 글로벌캠퍼스 나노화학과

Metal oxide nanoparticle embedded porous carbon composite materials have various uses, including as catalyst supports, sensor, and adsorbents, because of their good stability and unique porosity. Despite their importance, the procedures for the synthesis of metal-oxide nanoparticle embedded porous carbon composites have not been widely studied. We present a facile synthesis method for metal oxide embedded porous carbon compound via simple pyrolysis of metal-organic frameworks (MOFs, MIL-100). The porosity of the composite material was controlled by addition of carbon source (such as furfuryl alcohol) to the MOF. We found that the incorporation of an additional carbon source and further wash process can be used to control the chemical composition and pore structure of the resulting carbon materials. In addition, the composition and the rate of flowing gas during pyrolysis determine the oxidation state of the resulting metal oxides. The prepared composite materials were characterized by SEM, TEM, and PXRD analysis revealing that the nanoparticles have a single phase and uniform size. One of the prepared materials can be used as an electrode of Li-ion battery. Details of our recent work will be presented

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Plasmonic gold nanoparticles for sensitive photoacoustic imaging and visible-light induced graphene oxide reduction

KumarDinesh 이아름 강은미[1] 배유민[2] 임동권[3,*]

고려대학교 NBIT [1]승실대학교 화학과 [2]고려대학교 ku-kist 융합대학원 [3]고려대학교 KU-KIST 융합대학원

Strong light absorption and scattering properties in the visible and near-infrared (NIR) region have been extensively explored plasmonic gold nanoparticles for their use in numerous photochemical and biological applications. Here, we have highlighted the performance of gold nanostructures for visible light induced graphene oxide reduction at room temperature and hybrid graphene oxide based plasmonic nanoparticles (gold nanoparticles (AuNPs) and gold nanorods (AuNRs)) for sensitive photoacoustic imaging. The use of visible light with plasmonic nanoparticles (AuNPs) has been proved to be a simple, chemical free, and energy efficient method to produce r-GO.[1,2] The reduced graphene oxide prepared using visible light showed excellent fluorescence quenching properties and target detection capabilities. On the other hand, reduced graphene oxide coated gold nanorods (r-GO-AuNRs) due to the excellent NIR light absorption properties and highly efficient heat transfer process through the reduced graphene oxide layer, exhibits excellent photothermal stability and significantly higher photoacoustic amplitudes (in the 4-11 MHz operating frequency of an ultrasound transducer) than bare-AuNRs, graphene oxide coated AuNRs (GO-AuNRs), or silica-coated AuNRs, as demonstrated in both in vitro and in vivo systems. A four times higher magnitude of the enhanced electromagnetic field around r-GO-AuNRs can be generated compared with bare AuNRs or GO-AuNRs as suggested by finite-element-method simulation studies. The excellent optical stability of AuNRs along with its ability to amplify the photoacoustic amplitude (PA) signal intensity and a relatively straightforward surface chemistry of r-GO (via covalent or noncovalent modifications of the ligand on the r-GO layer, which is essential for drug delivery systems) anticipated r-GO-AuNRs to be an promising theranostic agent.[3] Therefore, the r-GOAuNRs can be useful for sensitive disease diagnosis, as vehicles for therapeutic drug delivery, and for NIR sensitive photothermal therapy.

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Fabrication and characterization size controllable TiO_2 hollow spheres for photocatalysts

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계명대학교 화학과 [1]보경직물 부설연구소

Nano sized TiO_2 hollow spheres (THS) were prepared by using a polystyrene (PS)@TiO_2 core shell spheres. This method involved the fabrication of monodisperse PS, sequential deposition of TiO_2 precursor via template-directed self-assembly. The result materials were characterizerd by transmission electron microscopy (TEM), X-ray diffraction (XRD), Brunauer-Emmett-Teller method (BET) analysis, termogravimetric analyzer (TGA) and photorcatalysis. TEM images showed well-defined PS and THS materials. The XRD peaks showed anatase structure and BET surface area is 76 m^2/g. TGA indicated the removal temperature of PS. Prepared THS were used as photocatalysts for the degradation of methylene blue under UV light irradiation.

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Synthesis of hollow silica spheres with hexagonal mesopores without thermal processes

이종탁 배재영*

계명대학교 화학과

Polystyrene (PS)@mesoporous silica core@shell composites were prepared by sol-gel method using polystyrene and cetyltrimethylammonium chloride (CTACl) as dual templates under room temperature. The sol-gel process of TEOS is directed exclusively onto the template, and well-defined mesoporous hollow silica spheres (MHSS) with radially oriented mesochannels are fabricated. MHSS were obtained by removing the polymer core and the templates without thermal processes. The product were characterized various method such as transmission electron microscopy (TEM), X-ray diffraction (XRD), fourier transform infrared (FT-IR) spectrometry, and Brunauer-Emmett-Teller (BET) analysis. TEM observations showed that the formation of the uniformed mesoporous hollow spheres with ordered radially oriented mesochannels. XRD peaks showed uniformed mesoporous structure. FT-IR spectrum indicated that organic materials were removed through absence of peaks. The nitrogen adsorption-desorption measurement exhibited that the pore size, BET surface area, pore volume of MHSS were 3.032 nm, 1262 m^2/g, 0.146 cc/g, respectively.

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Synthesis and Characterization of ladder-like structured Polysilsesquioxane

이재영 이종탁 배재영*

계명대학교 화학과

Polysilsesquioxane (PSSQs) is composite materials consisting of inorganic framework and organic functional groups. Their inherent dual characteristics offer various application. Ladder-like structured PSSQs was successful synthesized by direct hydrolysis and polymerization in the presence of catalyst at room temperature and normal pressure. Chemical composition and structureal analysis of the obtained PSSQs were charaterized using ^{29}SI-NMR, GPC, XRD and SAXS. A ladder-like structure having a molecular weight of 2100 was confirmed by the analysis results of XRD and ?68 ppm a T^3 peak of ^{29}Si-NMR.

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Preparation of cubic mesoporous silica at room temperature and functionalized with various functional groups

서원호 배재영*

계명대학교 화학과

Highly ordered mesoporous silica materials with cubic structure were prepared by sol-gel method using tetraethyl orthosilicate (TEOS) as a silica presursor and cetyltrimethylammonium chloride (CTACl) as a template. Functionalization of the functional groups were used by various silanes. The result materials were characterized by X-ray diffraction (XRD), transmission electron microscope (TEM) and N_2 sorption isotherms. The functional groups were analyzed by fourier transform infrared spectrometer (FT-IR). XRD patterns and TEM images showed well-ordered cubic structures in all of these silica materials and N_2-sorption isotherms indicated high surface area. According to FT-IR, an amino group, a mercapto group, a vinyl group, and a methacrylate group was confirmed that the functionalized on cubic mesoporous silica.

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Ca-doping Effects on Structure and Electrochemical Property of P2-type $Na_{0.67-2x}Ca_xMnO_2$

한수철 표명호*

순천대학교 인쇄전자공학과

Layered P2-Na_xMO_2(M=전이금속)는 충방전에 따라 단계적 상변이를 거치며, 이로 인하여 반복적 충방전 시 구조 불안정이 야기되고 전기화학적 성질도 열화되는 현상을 나타낸다. 본 연구 그룹에서는 이를 해결하고자 layered P2-Na_xCoO_2 의 Na^+ 자리에 Ca^{2+}를 치환(도핑)함으로써 산소 층사이에 강한 정전기적 인력을 유도함으로써 구조적 안정화를 기하고자 하였다. 충방전 결과 Ca^{2+}는 Na^+ layer 층에 항상 존재하며, Ca-O 사이의 강한 인력으로 인하여 구조적 변화가 억제되는 것을 확인하였다. 이에 따라 가역 용량 감소는 없으면서 capacity retention 이 향상된 $Na_{0.60}Ca_{0.07}CoO_2$ 를 보고하였다. 본 연구에서는 Mn^{3+}의 Jahn-Teller 효과로 구조적 불안정성이 더욱 심할 것으로 예측되는 layered P2-Na_xMnO_2 화합물에 Ca^{2+}을 치환 함으로써 치환에 따른 효과를 극대화 하고자 하였다. Na_xMnO_2 에 Ca^{2+}을 Na^+ Site 에 치환 함으로써 충방전시 발생하는 MnO_6 간의 Slippage 를 완화 시킬 수 있을 뿐만 아니라 Jahn-Teller distortion 억제도 가능 할 것으로 예상하였다. Ca^{2+}이 치환된 $Na_{0.67-2x}Ca_xMnO_2$ (x = 0, 0.01, 0.02, 0.03) 조성을 갖는 양극물질은 Solid state 방법을 이용하여 800°C 에서 열처리하여 합성되었다. X-ray diffraction 결과로 부터 Ca^{2+} 이온이 성공적으로 P2-type Na_xMnO_2(Hexagonal $P6_3$/mmc) 격자 내에 치환된 것이 확인되었다. 전기화학 실험에서는 1.5V ~ 4.0V 의 전압 범위에서 10mA/g 로 25 cycle 충방전 실험한 결과, Na_xMnO_2 와 비교하여 Ca^{2+}이 치환) 됨에 따라 capacity retention 및 reversible capacity 가 더 증가되는 경향을 보였다. 이상의 결과로부터 Na^+ 자리에 Ca^{2+} 치환은 layered P2-type Na_xMnO_2 에도 구조적 안정성을 부여하며 전기화학적 특성 향상의 가능성이 있음을 확인하였다

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Superhydrophobic surface coatings using silica particle/poly(trimethoxysilyl)propyl methacrylate nanocomposites to improve mechanical durability

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광운대학교 화학과 [1]광운대학교 화학센서연구실

Superhydrophobic surface coatings with high static water contact angle (>150°) have been receiving tremendous attention in recent years. The applications of superhydrophobic coatings are diverse due to their unique water-repellency, self-cleaning ability, and anti-biofouling property. Various methods have been proposed to fabricate superhydrophobic surfaces mimicking the lotus surface structure, including lithographic patterning, plasma etching, electrochemical deposition, electrospinning and chemical vapor deposition. However, these methods often require harsh synthetic conditions and complex fabrication techniques. In addition, the poor mechanical stability of such superhydrophobic coatings has been also severe limitation in their widespread applications. Herein we demonstrate on a one-step facile spray-coating technique to fabricate a superhydrophobic surface modified with silica particle/poly(trimethoxysilyl)propyl methacrylate nanocomposites. The superhydrophobic surface coatings prepared are characterized in term of water contact angles and surface roughness/morphology by using a scanning electron microscopy (SEM). Futhermore, abrasion resistance of superhydrophobic coatings prepared in this work is evaluated by a home-made scratch tester composed of a piece of sandpaper and weights with different masses.

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$Ni(dmamb)_2$를 사용한 MgO 기질 위의 NiO 박막의 적층 성장

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NiO 는 p 형 투명 전도성 막으로서 광학적 및 전기적 특성이 우수한 물질이다. 우리는 $Ni(dmamb)_2$ [nickel bis(1-dimethylamino-2-methyl-2-butanolate)]를 선구물질로 사용하여 MgO(001) 기질 위에 NiO 박막을 CVD 방법으로 적층 성장시켰다. $Ni(dmamb)_2$ 는 상온에서 액체이며 증기압이 75 ℃에서 213 mTorr 로 충분히 높다. 실험 중 기질의 온도는 250-400 ℃ 구간에서 25 ℃ 간격으로 변화시켰다. 침착한 박막은 X-ray photoelectron spectroscopy (XPS)로 NiO 임을 확인하였고, 박막의 조성은 energy dispersive spectroscopy (EDS)로 조사하였다. X-ray diffraction (XRD)과 reflection high-energy electron diffraction (RHEED) 분석은 박막이 결정성이 우수함을 보여 주었다. 박막의 두께는 scanning electron microscopy (SEM)로 측정하였고, transmission electron microscopy (TEM) 사진을 분석하여 NiO 박막이 MgO(001) 기질 위에 적층 성장했음을 확인하였다.

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Nitrogen and phosphorus co-doped cubic ordered mesoporous carbon as supercapacitor electrode material with extraordinary cyclic stability

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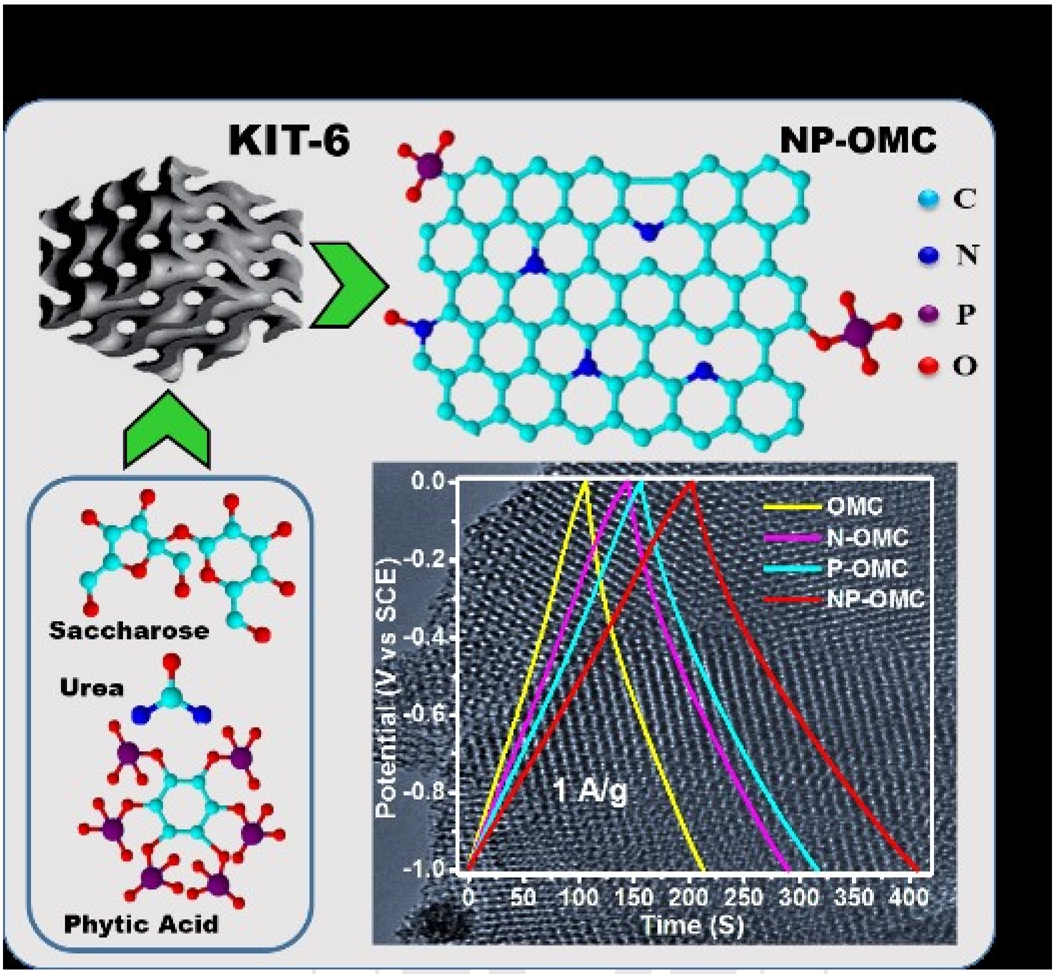
Heteroatom and porosity both have different, but definite effect on the electrochemical capacitance of carbon materials. These effects are studied in details by cubic ordered mesoporous carbons (OMCs) co-doped with N and P. 3-dimentional (3D) mesoporous silica, KIT-6 is utilized as a hard template to synthesize the cubic OMC. Interestingly, although the porosity parameters e.g. surface area and pore volume do not change much with N doping, a significant increase of these values is observed upon P doping. Moreover, the P content does not affect the N doping characteristics on co-doping of both N and P. When tested as supercapacitor electrode, the N-OMC despite much lower porosity parameters, exhibits similar specific capacitance compared with the P-OMC. High specific capacitance in NOMC arises mainly from the pseudocapacitive effect of doped N species, whereas high porosity parameters are the main reason for the specific capacitance shown by P-OMC. The synergistic contribution of both effects enables the NP co-doped OMC to show highest specific capacitance of 210 F g^{-1} at 1.0 A g^{-1}. Moreover, excellent retention of specific capacitance with more than 90 % of initial capacitance is observed for NP-OMC at high current density of 10 A g^{-1}. and also for 3000 charge-discharge cycles. This is mainly because of high-surface area hierarchical porous structures with uniform and ordered mesopores in the cubic OMC, which facilitate the unrestricted movement of electrolyte ions to access the active surfaces, as well as excellent synergistic effect of co-doping of N and P.


KIT-6
NP-OMC
C
N
P
O
Saccharose
Urea
Phytic Acid
OMC
N-OMC
P-OMC
NP-OMC
1 A/g
Potential (V vs SCE)
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
Time (S)
0
50
100
150
200
250
300
350
400

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Electrophoretic Deposition of MgAl Layered Double Hydroxide Monolayer Synthesized by One-Step Direct Growth Method

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성균관대학교 화학과

Monolayer nanoplates of MgAl Layered double hydroxide (LDH) were prepared by a facile one-step synthesis without exfoliation process. As-prepared MgAl-LDH monolayer nanoplates were grown in-plane only by applying formamide to weaken interlayer interactions of stacking. Tris(hydroxymethyl)aminomethane was used as a ligand to prevent from intercalation of CO_2 anion, and MgAl-LDH monolayer was fabricated with NO_3 anion species directly, even under CO_2-existing condition. The LDH monolayer nanoplates were electrophoretic deposited on nickel substrate for an orientated LDH thin film showing superior performance.

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A new fluorescence material produced from ammonium citrate for efficient optosensing mercury ions

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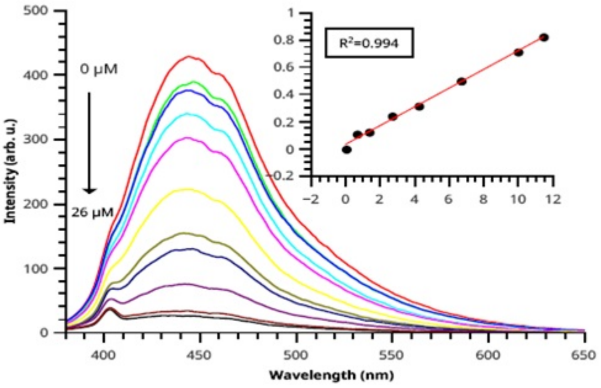
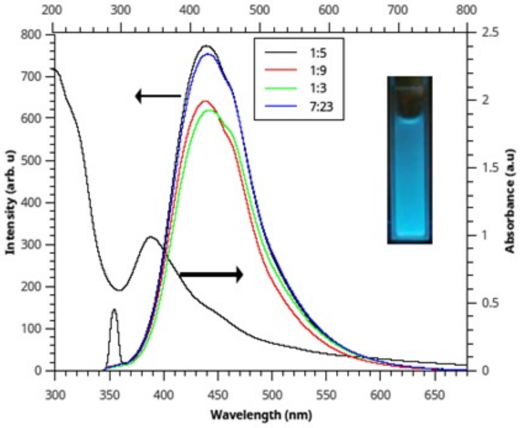
창원대학교 화학과 [1]Western Kentucky University

A new approach with simple, fast and most versatile is proposed for producing a promising fluorescence material from ammonium citrate. The synthetic procedure was performed using solid-phase reaction strategy at an extremely low temperature. The product were studied by XRD pattern, TEM image, FT-IR spectra, and XPS analysis. The prepared product possess nanoscale, water soluble, quantum yield of approximately 27%. Based on the quenching effect on fluorescence emission, the mercuric ions could be detected with a limit of detection of 0.06 ?M with high selectivity.The quenching effect of prepared materials by Hg+ ions (left); Emission and absorption spectra of prepared fluorescence material (right).





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A greener approach to zinc glycerolate and ZnO micro-flowers for water pollutant sensing

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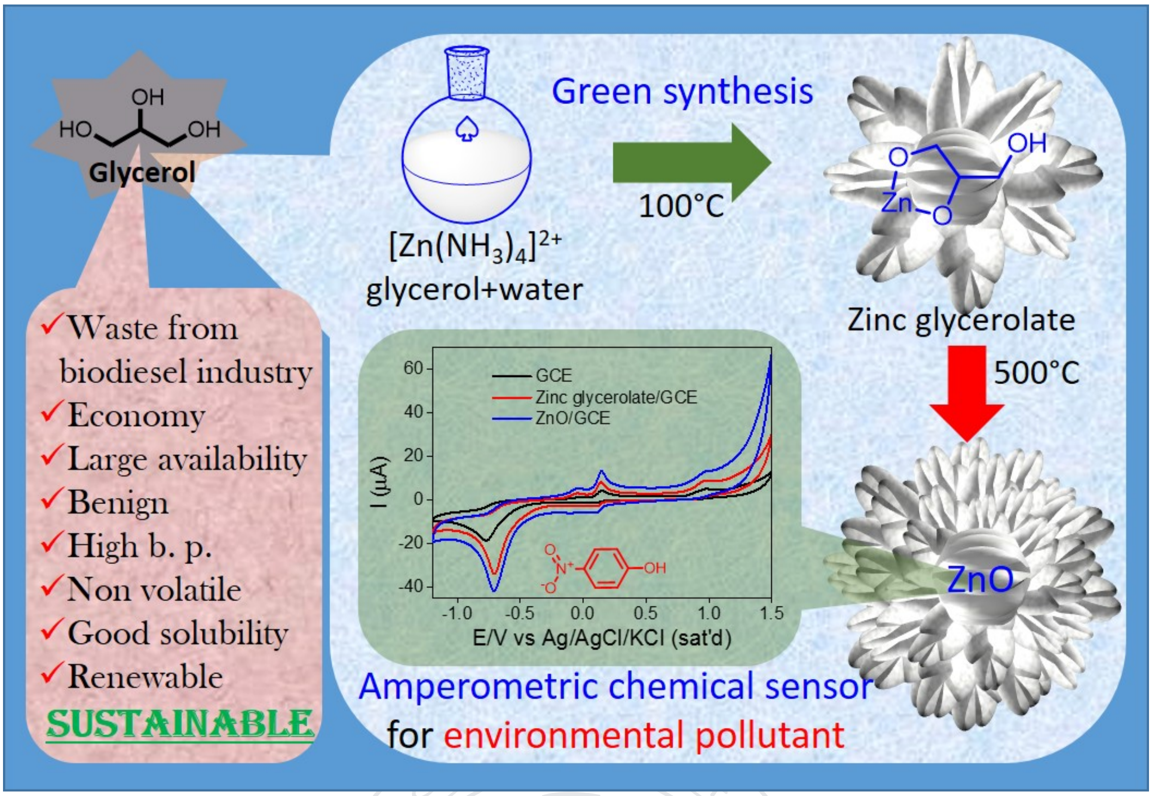
The solvent or reaction medium is one of the key players to decide the material’s morphology during synthesis. Glycerol is an environmentally benign solvent that have excellent chelating capability and also expected to control the morphology of the final material. Herein, aqueous glycerol is employed as a green solvent to synthesis zinc glycerolate and the corresponding ZnO micro-flower structures with an intention to develop a greener chemical process for inorganic material synthesis. A clear solution of zinc ammonium complex is used as a source of zinc, which converts to zinc glycerolate in the presence of glycerol. Glycerol plays a dual role as a reactant to form zinc glycerolate and as a solvent to control the morphology. The unreacted glycerol is recovered after the reaction and reused further, which make the current process more sustainable and economical. The flower-structured zinc glycerolate and ZnO are then used to modify a glassy carbon electrode to make a binder-free, non-enzymatic amperometric electrochemical sensor for p-nitrophenol that is a brutal environmental pollutant present in water. Excellent sensitivity, selectivity and stability of the modified electrode is found and can be a good alternative for the purpose.


OH
HO
OH
Glycerol
✓Waste from biodiesel industry
✓Economy
✓Large availability
✓Benign
✓High b. p.
✓Non volatile
✓Good solubility
✓Renewable
SUSTAINABLE
[Zn(NH3)4]2+
glycerol+water
Green synthesis
100°C
O
OH
Zn
O
Zinc glycerolate
500°C
ZnO
GCE
Zinc glycerolate/GCE
ZnO/GCE
I (μA)
60
40
20
0
-20
-40
-1.0
-0.5
0.0
0.5
1.0
1.5
E/V vs Ag/AgCl/KCl (sat'd)
O
N+
-O
OH
Amperometric chemical sensor
for environmental pollutant

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Up-conversion luminescence properties of YGdVO4:Yb/Er phosphor with various host material concentrations

정종원 GerelkhuuZayakhuu 오주현[1] 이용일[*]

창원대학교 화학과 [1]부경대학교 물리학과

Nanoparticles have been the subject of increased scientific interest, both for fundamental research and for a wide area of application. Upconversion is a process that generating higher energy emission from low energy of incident light. Many trivalent rare earth ions such as Er3+, Yb3+, Tm3+ and Pr3+ are doped as emission and absorption centers in these materials. The Yb3+ ion has simple energy level about 980nm. So, the Yb3+ ion was easily excited by 980 nm laser diode. When Er3+ attach to Yb3+, they generate effective energy transfer, because of agreement in emission range of Yb3+ and absorption range of Er3+.In this study, Er3+ and Yb3+ co-doped YGdVO4 phosphors were prepared by hydrothermal method, which was a fast, reproducible and easily scaled up chemical route for obtaining fine power of oxide. 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). Upconversion luminescence spectrum was measured by using 980 nm laser diode. Under 980nm laser diode excitation, the YGdVO4:Er3+, Yb3+ powder show the intense green upconversion emission, which is 2H11/2, 4S3/2 ? 4I15/2. The X-ray diffraction patterns of YGdVO4:Er3+,Yb3+ reveal that the sample have been successfully synthesized.The aim of this study is to compare the luminescence characteristics of GdVO4, YVO4, and YGdVO4 phosphors which were synthesized with three different host material concentration.

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Stacking density regulated ultrahigh capacity ternary metal oxide/graphene composite for LIB anode

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순천대학교 인쇄전자공학과

Graphene has emerged as the one most actively pursued material with limitless application in fields of energy production and storage. Regulating the stacking density of graphene layers can open new vistas and diverse possibilities, especially in energy storage materials. Various metal oxides (MO) or ternary metal oxides (TMO) intended for anode and cathode materials for LIB have been composited with graphene to enhance the electrochemical performance, stability, and longevity of the MO/TMO. In this work, we report the successful entrapment of Sn based ternary metal oxide ($CoSnO_3$) sandwiched between graphene layers. The stacking density of the graphene stacks was controlled by applying a novel procedure involving pre-aligning of oppositely charged graphene layers in solution. An electrostatic aligning of positively charged amine functionalized graphene (GN) with Co^{2+}/Sn^{2+} anchored graphene oxide (CSG) in an acidic solution results in a densely stacked composite (CSG/GN) sandwiching $CoSnO_3$ between graphene layers. This configuration provides excellent stability and an unprecedented capacity response during electrochemical cycling. A specific capacity response approaching ~1500 mAh.g^{-1} at a charge/discharge current density of 100mA.g^{-1} is achieved, which is unprecedented and surpasses the theoretical capacity of $CoSnO_3$ and $CoSnO_3$/graphene based LIB anodes. Composites synthesized under identical conditions avoiding the pre-aligning process result in sparse stacked composites showing lower capacity response (~600 mAh.g^{-1}) with poor electrochemical and structural stability. The origin of the ultrahigh capacity is believed to be arising from enhanced reversibility of a conversion reaction stabilized by the compact structure, which is facilitated by the pre-aligning process.

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Pyrene composited with Graphene oxide for versatile organic electrode materials in secondary ion batteries

정재항 표명호*

순천대학교 인쇄전자공학과

이차전지 전극소재로 일반적으로 사용되는 Inorganic crystalline material 들은 channel size 한계로 인하여 한 종류의 양이온에만 활성을 가지며, 또한 formula unit 당 1 전자 산화-환원반응으로 인하여 가역용량 증가가 제한적이다. 더욱이 Inorganic crystalline material 들은 양이온의 삽입/탈리 과정 중 구조적 변화가 수반되는 문제점을 가질 수 있다. 이에 반하여 비결정성 유기소재는 다전자 산화-환원 반응이 가능하고 구조 변화에 따른 stress 이완이 가능한 장점들을 갖고 있다. 본 연구실에서는 polycyclic aromatic hydrocarbons (PAH) 의 일종인 pyrene 분자로부터 수개의 unit 들이 결합된 oligopyrene 을 sodium ion batteries (SIB)의 cathode 로서 이미 적용하여, 높은 전압에서 가역적인 산화-환원반응을 확인하였고 안정적인 capacity retention 과 rate performance 를 얻었다. Oligopyrene 은 PAH ring 간의 conjugation 이 없어 polypyrrole 또는 polythiophene 와 달리 결합에 따른 HOMO level 증가가 거의 없으며 따라서 약 1V(vs Ag/AgCl)에서 가역적인 산화-환원이 발생함을 확인하였다. 본 연구에서는 pyrene 을 SIB 의 음극물질로 적용하여 다양한 이차전지 (Lib, SIB, KIB)에서의 성능을 확인하였다. Pyrene 은 1 전자 반응을 할 때의 이론용량은 133mAh/g 이지만 2 전자 반응이 가능하여 이차전지의 anode 로 적용시켰을 경우 큰 용량을 기대할 수 있다. Pyrene 은 흔히 사용하는 전해질과 같은 유기용매에 용해되고 낮은 전기 전도성을 가지고 있다. 또한 초기 실험 CV 결과 -1.5, -2.1V(vs SHE)에서 환원 peak 이 나타나지만 산화 peak 이 나타나지 않는 것으로 보아 환원반응 중 dimer 형성으로 인해 가역적인 산화-환원반응의 어려움을 확인하였다. 이를 보완 하기 위해 GO 와 함께 composite 시켜 전기 전도성을 높이고 인접한 pyrene 분자들의 dimer 형성을 막아 가역적인 산화-환원반응이 일어날 수 있게 개선하였다.

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Effect of Mo3+ concentration on the upconversion luminescence of NaLuF4:Mo3+/Er3+ phosphors

GerelkhuuZayakhuu 정종원 **B.T.Huy** 이용일*

창원대학교 화학과

Upconversion phosphors (UCPs) are a new class of materials that can convert near-infrared light into visible green emission by sequentially absorbing multiple photons. It is the most efficient host material to date for green (Yb3+/Er3+ doped) and blue (Yb3+/Tm3+ doped) upconversion phosphors. In this work, we introduce a transition metal ions, specifically molybdenum (Mo3+) ions doped in β-NaLuF4:Er3+ phosphors with different concentration (6-30%). β-NaLuF4:Mo3+/Er3+ phosphors were synthesized by a facile hydrothermal method. The characterization of the developed β-NaLuF4:Mo3+/Er3+ was performed by photoluminescence (PL), Field emission scanning electron microscope (FE-SEM) and X-ray diffraction (XRD). The results demonstrate a successful incorporation of Mo3+ ions in β-NaLuF4 phosphors. The maximum emission was observed in a sample containing 24% Mo3+ ions. The effect of Mo3+ on the upconversion luminescence of β-NaLuF4 phosphors were investigated in detail. In addition, these high quality upconversion phosphors have a potential for the application in the field of optical nanodevices, bioanalytic sensing, biomedicine and solar cell.

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Time and space-resolved imaging of metal-enhanced fluorescence on silver nanorods arrays

양원근 채원식*

한국기초과학지원연구원 대구센터

Recently, metal-enhanced fluorescence (MEF) study attracts multidisciplinary researchers in basic, biological, and environmental sciences. Plasmonics from metal nanostructures reveals new physical insights because of interesting physical phenomena such as electromagnetic fields accumulation and electron recombination pathway modulation. Involved photophysics enables us to detect fluorescent molecules with ultra-high sensitivity through the MEF concept. Here we considered how to increase fluorophor signal in the viewpoint of material morphology change. In this study, we investigated MEF property by using two-dimensional (2D) array of silver (Ag) nanorods. Electrochemically grown Ag nanorods arrays with controlled length, which were fabricated using porous alumina membranes as structure-directing templates by adjusting deposition time, were subjected to study MEF characteristics. Consequently, open-end tip configure of the Ag nanorods array shows remarkable enhancement of fluorescence signals compared to bulk emission intensity. Spatially-resolved fluorescence modulation and enhancement factors could be directly and uniquely estimated by monitoring fluorescence intensity and lifetime changes of fluorophores near the 2D Ag nanorod arrays.

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Application of Size-controlled Au and Au@SiO_2 nanoparticles for Improving Photocatalytic Activity of TiO_2

이지은 이완인*

인하대학교 화학과

Plasmonic photocatalysis has been an important issue for improving photocatalytic reactivity under solar light. The noble metal present on the TiO_2 surface induces the promotion of charge-separation by forming Schottky-junction that suppresses the recombination of e^-/h^+ pair. And especially, the LSPR effect formed by the noble metal can strongly enhance the electric field in the vicinity of the metal NPs. The enhanced electric field can boost the excitation of electrons from its VB to CB, thus enhancing the photocatalytic activity of TiO_2.Au nanoparticles (NPs) with different sizes were prepared. And corresponding Au@SiO_2 core-shell structures were synthesized by stober method. These nanoparticles were loaded on the TiO_2 surface and then analyzes plasmonic photocatalytic activities in decomposing salicylic acid (SA) in aqueous solution under UV-visible light. All of these plasmonic photocatalysts exhibit higher efficiency than bare TiO_2 systems. Among the Au/TiO_2 systems, Au3/TiO_2 exhibits the highest efficiency due to the space-charge separation effect of noble metals. And the gradual decrease of catalytic activity with the increase of Au NP size is emerged by the increased LSPR sensitization effect. However these effects by Au nanoparticles in the Au@SiO_2/TiO_2 systems are blocked by the insulating SiO_2 shell. Thus, in the Au@SiO_2/TiO_2 systems, the LSPR effect is the dominant factor in enhancing the photocatalytic activity. Au17@SiO_2/TiO_2 exhibits the highest efficiency among the Au@SiO_2/TiO_2 systems.

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Improvement of $CH_3NH_3PbI_3$/CuSCN Solar Cell By Interface Treatment

손미래 이완인[*]

인하대학교 화학과

Organo-lead halide perovskites have attracted much attention for solar cell applications due to their unique optical and electrical properties. However, the organic hole-transporting materials (HTMs) generally used are quite expensive because of complicated synthetic procedure and high-purity requirement. Hole transport material‘s research on perovskite solar cells is already in progress, but we can’t find the materials to replace spiro-MeOTAD yet. Thus we applied an effective and cheap inorganic p-type hole-transporting material to perovskite-based device. CuSCN is expected to be an promising HTM for perovskite solar cell, because conduction band (CB) of CuSCN is close to CB of spiro-MeOTAD and it exhibits a high hole conductivity. Furthermore, CuSCN is highly stable and economical material. However, the interface between perovskite layer and CuSCN layer control is a very important problem to study how to increase the efficiency by reducing the damage of perovskite because solvent used in CuSCN can cause damage to the perovskite layer. We make a diluted 5% spiro-MeOTAD boundary layer to the interface between the perovskite layer and CuSCN layer in order to protect perovskite layer. As a result we obtain an increased efficiency of 10.1% than It did’t have any treatment.

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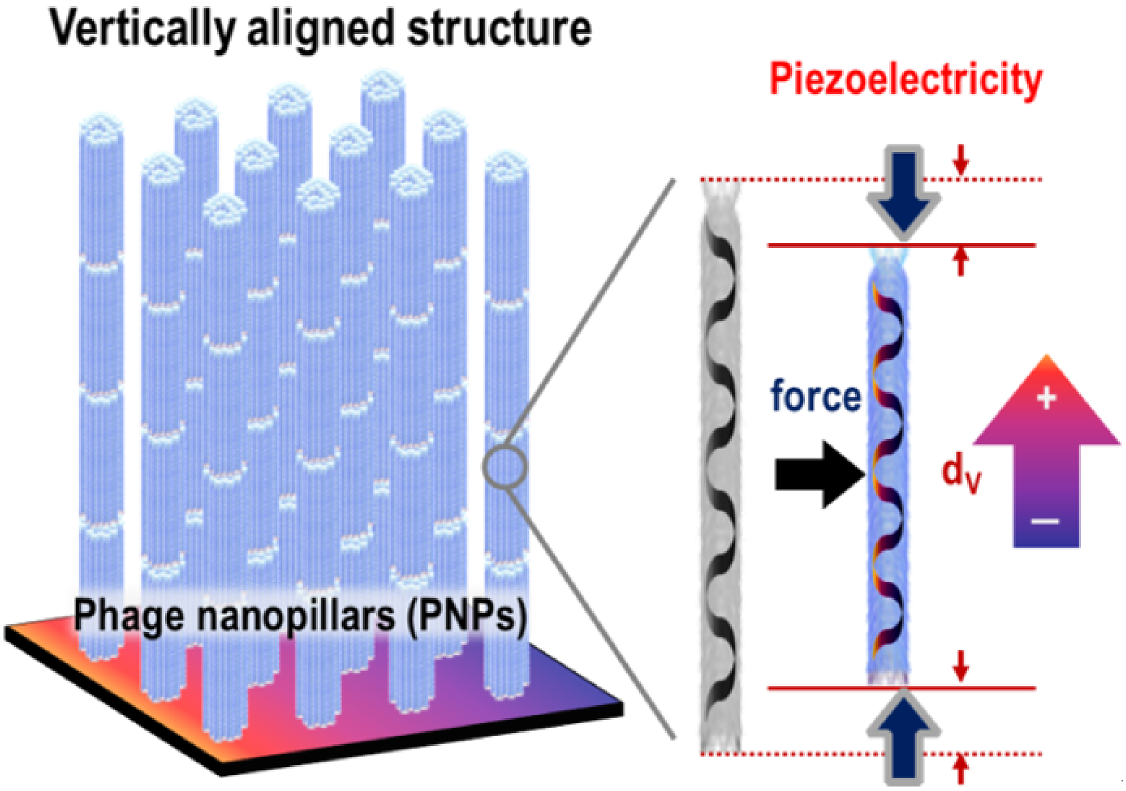
Bioinspired Nanogenerators Based on Vertically Aligned Phage Nanopillars

한혜지 오진우[1,*] 김춘태[2] 이소영[2]

부산대학교 차세대기판학과 [1]부산대학교 나노소재공학과 [2]부산대학교 나노융합기술학과

Energy harvesting from mechanical resources has attracted great attentions owing to the demands for a power supply of implantable and wearable electronics, operated in the power range of microwatt to nanowatt. Biomaterials have attracted great attentions as promising materials for energy harvesting owing to their non-toxicity and biocompatibility. M13 bacteriophages are relevant in this context because we can easily modulate their functions through genetic engineering. In this contribution, we show that M13 bacteriophage nanopillars work as efficient piezoelectric material and thereby can be used to provide the functional material in energy harvesting devices. The sufficient electrical power from phage nanopillars thus holds promise for the development of self-powered implantable and wearable electronics. The apparent versatility of M13 bacteriophage also suggests that phage nanopillars can serve as functional nanomaterials for numerous electronic and optoelectronic applications.


Vertically aligned structure
Phage nanopillars (PNPs)
Piezoelectricity
force
d_V
+
–

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Solvent-free synthesis of nitrogen-doped carbon sheets for CO2 adsorbent

이규형 이선혜 방소라 허남회*

서강대학교 화학과

We report a novel method to synthesize the nitrogen doped carbon sheets (N-doped carbon), which were prepared by solvent-free reaction between glucose and solid hydrazine (H3N+NHCO2-). Three different N-doped carbon sheets were obtained from annealing the reaction mixture under Argon atmosphere at 500, 700, and 900 oC, respectively. The N-doped carbon sheets were fully characterized by X-ray diffraction, transmission and scanning electron microscopy, IR spectroscopy, and Brunauer?Emmett?Teller (BET) measurement. All the N-doped carbon sheets have the CO2 adsorption capability. The CO2 uptake was examined in the low pressure range between 0.01 - 1 bar at 25 oC. Maximum CO2 absorption capacity is about 2.23 mmol/g at 1 bar. Details on the fabrication of the N-doped carbon sheets and their properties will be presented.

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DNA-Mediated Control of Nanogap and Au Shell Structures for Use in Plasmonic-Enhanced Solar Energy Conversion System

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DNA-mediated synthetic strategies enable to synthesis the nanogap controlled anisotropic plasmonic nanostructures in a high yield. The reaction conditions such as pH and NaCl concentration are critical role in determining the optical properties of the resulting nanostructures by changing the shell structures and intra-nanogap distance. We synthesized three noticeable plasmonic nanostructures [i.e., half-shell with sub-1.0 nm nanogaps, closedshell with a wide nanogap (2.1 nm) and star-shaped with an irregular nanogap (1.5-4.0 nm)]. The solution-based and single particle-based Raman measurements showed a strong relationship between the plasmonic structures and the SERS intensity. Especially, anisotropic half-shell with sub-1.0 nm intra-nanogaps showed a wavelength-independent and a highly sensitive surface-enhanced Raman scattering (SERS) response, indicating the strongly enhanced electromagnetic field in the nanogap and broad light absorption properties ranging from visible to NIR light.An understanding of DNA-mediated control for nanogap-engineered plasmonic nanostructures can provide new insights into the design of new plasmonic nanostructures. And also, the plasmonic nanostructures with open sub-1.0 nm nanogap can be used for various fields, such as SERS-based in-situ target detection or efficient plasmon-enhanced solar energy conversion system.References 1.H. Lee, S. H. Nam, Y. J. Jung, S. Park, J.-M. Kim, Y. D. Suh* and D.-K. Lim*, DOI: 10.1039/C5TC01915J J. Master. Chem. C, (2015).2.D.-K. Lim, K.-S. Jeon, J.-H. Hwang, H. Kim, S. Kwon, Y. D. Suh* and J.-M. Nam*, Nature Nanotechnology, 6, 452-460, (2011).

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The development of a new synthesis method for Yb3+, Er3+, and Eu3+- codoped YVO4 and its applications

Chu Thi Bich Thao B.T.Huy 이용일*

창원대학교 화학과

Highly luminescent rare earth based materials is a fast growing area of materials research. Recently, much attention has been paid to develop upconversion materials due to this kind of materials have many promising characteristics, such as non-autobleaching, low auto-fluorescence, and high penetration depth in biological tissues.… It is ideal to use YVO4: Yb3+Er3+Eu3+ phosphors for bioimaging application being investigated. In this work, YVO4 (yttrium orthovanadate) nanoparticles were prepared for using melamine formaldehyde (MF) as a template. In this case, europium (Eu3+) and erbium (Er3+) were used as activators and ytterbium (Yb3+) as sensitizer, respectively. The results were characterized by X-ray diffraction (XRD), Fourier-transform IR spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM). In the present study, the material shows good emission intensity and upconversion properties when this material excitatied by UV and IR. YVO4: Yb3+Er3+Eu3+ material is design to apply for bio-imaging, photodynamic therapy, laser, and photovoltaics.

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Characterization and Sensing Application of Au attached Carbon Nanotubes

이명순 김 돈*

부경대학교 화학과

The Au nanoparticles(AuNPs) attached carbon nanotubes (Au-CNTs) were prepared and discussed their chemical, electrical properties, and sensing application. The crystallinity of the CNT phase was confirmed by analyzing the G and D bands in their Raman spectra. The electrical conductivity of the highly crystalline carbon phase of Au-CNTs (rAu-CNT = 250 nm) was ~10^4 S/cm. The field effect transistors (FETs) based on the Au-CNTs, which were assembled on a SiO_2/Si wafer using the dielectrophoresis technique, showed that the Au-CNTs would be a good functional electronic material for future electronic and sensing applications. The transconductance and hole mobility of the FETs are 3.6×10^{-4} A/V and 3.1×10^4 cm^2/Vs, respectively. Also, we have investigated AuNPs attached multiwall nanotubes(MWCNT)-FET sensors for non-enzymatic carbohydrates detection. This is a unique realization of a MWCNT based carbohydrates sensor, which does not rely on enzymes or electrochemical redox mediators to function, but rather on a combination of sensing affinity between the carbohydrate and the active part of the AuNPs-CNTs based FET.

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Realization of practical sheet-type biosensor based on multi wall carbon nanotubes and micro-pore filter paper for early detection of prostate cancer

지성경 이명순 김 돈*

부경대학교 화학과

The aim of this study is realization of an inexpensive, simple and sensitive biosensor to detect early stage of prostate cancer using bioactivated-multi wall carbon nanotubes (MWCNTs, diameter 20 nm, length 5 μm) and a micro-pore filter paper (pore size 0.45 μm). For the immunoassay of prostate specific antigen (PSA), which is a biomarker of prostate cancer, carboxylated MWCNTs were activated with PSA antibody (monoclonal antibody of the prostate specific antigen) by using N-(3-dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride (EDC) and N-hydroxysulfosuccinimide sodium salt (NHSS). The activated MWCNTs were deposited on micro-pore filter paper to use as a bio-sensisensor. The sensor can assay from 0 to 500 ng/mL of PSA level within 2 h with the detection limit of 1.18 ng/mL with an inexpensive bench top digital multimeter (5 1/2 digits). The detection range and sensitivity of the prepared sensor are good enough to diagnose the early stage of prostate cancer (> 4 ng/mL of PSA). This paper-based biosensor is 23 times cheaper (fabricated biosensor price: 2.4 $) and 12 times faster than enzyme-linked immunosorbent assay (ELISA), which is a general method for the detection of a specific protein in modernized hospitals. Furthermore, the maximum detection limit is about 50 times higher than ELISA

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Rietveld Quantitative Phase Analysis of Porcelain Materials

김재겸 박종현[1] 김종영[2] 김승주*

아주대학교 에너지시스템학부 [1]아주대학교 에너지시템화학과 [2]한국세라믹기술원 이천분원

Porcelain is widely used in diverse applications, ranging from stoneware and white ware, to structural and thermal wares. Typical porcelain bodies are made from materials collected from selected deposits using different mixing proportions of clay, feldspar and quartz, which are heat-treated to form a mixture of glass and crystalline phases. The phase determination and quantification of the mineral and amorphous phases are of special importance in the study of porcelain materials. On the basis of X-ray diffraction (XRD) data, the Rietveld refinement method was originally used for crystal structure analysis. Rietveld quantitative phase analysis is also a powerful method for determining the quantities of crystalline and amorphous components in multiphase mixtures. In this work, porcelain raw materials fired at different temperatures were characterized by powder XRD using the Rietveld method.

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Laser-Induced Patterning of ZnO Nanorod / Reduced Graphene Oxide Composites on Graphene Oxide Film

정재민 이민형*

경희대학교 응용화학과

Development of advanced materials and structures for supercapacitor and battery is critical to achieve energy storage devices with high performance. Metal oxide or hydroxide graphene hybrids can increase chemical and electrical coupling effects, and also high surface area and electrical conductance of graphene are attractive points of graphene as an advanced material for energy storage devices. In this work, we present the selective growth of ZnO nanorod/ reduced graphene oxide composites on graphene oxide film via laser-induced reaction. The patterned complexes could be used as hybrid-capacitor electrodes due to its pseudo capacitance (ZnO) and electric double layer capacitance (graphene). Optimized design of electrodes could be achieved by programming of laser scanning lines.

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Morphology-Dependent Catalytic Performance of MoO_3/MoS_2 Heterojunction Nanostructures for Hydrogen Evolution Reaction

배영은 이민형*

경희대학교 응용화학과

Core-shell nanostructures of $MoS_2@MoO_3$ with two different shapes were fabricated by simple routes: chemical vapor deposition (CVD) of MoO_3 followed by shallow sulfur doping. Our synthesis is very attractive, because the CVD processes performed at relatively low temperature. Interestingly, morphologies of MoO_3 core can be controlled from 2D-blade to 1D-nanorod structures depending on the distance from the solid precursors of MoO_3. MoO_3 core provides good electron transfer path, and MoS_2 shells are good hydrogen evolution reaction (HER) catalyst. MoS_2 shells also prevent degradation of MoO_3 in acidic condition. In this study, we focused on comparing HER-catalytic performance of $MoS_2@MoO_3$ core-shells depending on the morphologies based on several electrochemical analyses.

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Nanocomposites Containing Cationic and Anionic Clays for Improving Thermal Stability and Mechanical Strength of Polypropylene

류현주 양재훈 최진호*

이화여자대학교 화학.나노과학과

In order to improve the thermal stability and mechanical strength of polypropylene (PP), we prepared various PP nanocomposites with organoclay depending on the content of organo-clays. PP solution were mixed with cetyltrimethylammonium-fluorine mica (CTA-ME) and stearate-layered double hydroxide (SA-LDH) suspensions dispersed in xylene to form PP nanocomposites. According to the X-ray diffraction analysis, (00l) peaks corresponding to CTA-ME and SA-LDH were not observed, indicating that organoclays were well exfoliated and homogeneously dispersed in PP matrix. According to thermogravimetric analysis, the thermal stability of PP nanocomposites containing cationic and anionic clays were enhanced compared to intact PP. The mechanical strength of PP was improved after nanocomposition with CTA-ME and SA-LDH.

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Yttrium(III) incorporated layered double hydroxide for bio-application

엄새란 양재훈 최진호*

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Yttrium-90 (90Y) is one of the popular candidates as the radiotherapeutic species. A pure β-emitter 90Y has fewer environmental radiation restrictions, and it has a suitable for the irradiation of larger tumors because of its long residence time property. In the case of 90Y microspheres as radiotherapy agents, they are injected into an organ diseased with cancer. When they are trapped in a small blood vessel linked the cancer, they kill the cancer cells due to emit highly β-rays of 90Y and are remained inside a human body. Therefore it is necessary to develop the novel radiotherapeutic materials, which should be eliminated from body after radioactive of 90Y for a cancer treatment. Layered double hydroxide (LDH) incorporating Y is a good candiate material due to the bio-compatiblity, that is, LDH is non-toxic material and slowly dissolved in the body fluid condition. In the present study, the LDHs of Mg2Al1-xYx?(CO3)?nH2O (x = 0 ? 1) were successfully synthesized via coprecipitation and hydrothermal treatment. With increasing the Y3+ content, the particle size of prepared LDHs decreased and the hexagonal morphology was changed to thin round plate-like one. According to X-ray diffraction analysis, with increasing Y3+ content (x) from 0 to 0.4, a and c lattice parameters of MgAlY-LDHs were changed from 3.04 to 3.07 ? and from 22.7 to 24.0 ?, respectively, indicating that the increase of yttrium contents led to the expansion between the hydroxide layers. According to FT-IR analysis, a peak at 1357 cm-1 corresponding to the O-C-O symmetric vibration band of CO32- with D3h symmetry was observed for x =0. However, in case of Y3+ incorporated LDHs (x = 0.1 ? 0.4), peaks at 1510 cm-1 and 1385 cm-1 corresponding to asymmetric and symmetric vibration bands were observed. These differences are attributed to the lattice distortion by incorporating larger yttrium ions than Mg2+ and Al3+ into the LDH lattice.

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Metal-Organic-Framework Nanoparticles Anchored on Inorganic Nanosheets Applicable as Carbon Dioxide Absorbent

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Highly porous metal-organic-framework (MOF)—Inorganic nanosheet nanocomposites are synthesized by the crystal growth of MOF nanoparticles in the presence of the colloidal suspension of exfoliated inorganic nanosheet. The resulting materials are new type of nanocomposites consisting of MOF nanoparticles and layered metal oxide nanosheets, which can be used as CO_2 gas absorbents. The incorporation of layered inorganic nanosheet improves the structure stability and CO_2 adsorption capability of MOF, which is attributable to the stabilization by hybridized inorganic nanosheets and the increased amount of functional groups acting as binding sites for CO_2 molecules. The present study clearly demonstrates that the hybridization of inorganic nanosheets with the MOF can provide a powerful way to synthesize novel efficient materials for CO_2 absorbent.

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Enhanced electrocatalytic activity of Zn-Fe layered double hydroxides/RGO exfoliated nanosheets : Oxygen evolution reaction catalyst

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경희대학교 화학과 [1]경희대학교 응용화학과

Cost-effective and high efficiency electrocatalysts for water oxidation to evolve oxygen gas play a key role in water splitting and renewable energy system. Here, we report Zn-Fe layered double hydroxides(LDH) with intercalated carbonate were fabricated by co-precipitation synthesis. Besides, Zn-Fe LDH nanosheet with reduced graphene oxide enhance electrochemical activity. The method of sample preparation is solution based exfoliation synthesis. The exfoliated single-layer nanosheets exhibit higher oxygen evolution activity than the corresponding bulk LDHs. The structural properties of LDH electrocatalysts were characterized by Powder X-ray Diffraction (PXRD), SEM. The elctrocatalytic activity of the catalysts was studied by linear sweep voltammetry.

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Vanadium Oxide-Reduced Graphene Oxide Nanocomposites Applicable as Cathode Materials for Sodium-Ion Batteries

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Mesoporous nanocomposites of vanadium oxide nanosheets and reduced graphene oxide (rG-O) can be synthesized by the restacking of the colloidal mixture of rG-O and vanadium oxide nanosheets with sodium ions. The resulting vanadium oxide-rG-O nanocomposites show mesoporous morphology originating from the house-of-cards-type stacking structure of the nanosheets with the preservation of pentavalent oxidation state of vanadium ion. According to the electrochemical measurement, the hybridization with rG-O leads to the significant enhancement of the first discharge capacity of vanadium oxide from ~100 to ~150 mAh g^{-1} (at 80mA g^{-1}). The present study demonstrates the usefulness of exfoliation-hybridization scheme in exploring the efficient cathode material for sodium ion batteries.

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Effect of Sulfurization on the Electrode Performance of $Na_2Ti_3O_7$ for Sodium Ion Batteries

오승미 김인영 황성주*

이화여자대학교 화학·나노과학과

Sodium titanate ($Na_2Ti_3O_7$) is sulfurized by annealing in inert atmosphere with carbon disulfide (CS_2). The $Na_2Ti_3O_7$ structure remains unchanged upon the sulfurization at 400 ^oC. However, the reaction at higher than 400^oC induces the phase transition of $Na_2Ti_3O_7$. The sulfurization reaction induces the color change of $Na_2Ti_3O_7$ from dark gray to light gray, suggesting the change of the oxidation state of titanium ion. According to the galvanostatic charge-discharge measurements, an additional plateau appears at 1.6 V upon sulfurization process related to interaction between sulfur and sodium. The sulfurized materials deliver larger discharge than the pristine material, which is attributable to the generation of additional plateau. The present study demonstrates that the sulfurization with CS_2 provides an effective way to improve the electrode performance of $Na_2Ti_3O_7$ for sodium ion batteries.

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Increased Strength of 3DP Structures with Polysaccharides

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한국과학기술원(KAIST) 화학과

For the 3D printing industry, powder bed and inkjet 3d printing, known as 3D printing (3DP), brings a new level of considerable material flexibility to the manufacturing industry. Especially, binders are considered to be significant factors due to their transparency, adhesiveness, and reliability. However, the problems of using commercial binders is the post processing, but most of the cover adhesives are toxic and can induce eye and respiratory irritation.One of the solutions to not go through with post-treatment process is to combine powders and binders with stronger and biocompatible adhesives. One of which is derived from polysaccharides. Here, we propose a new 3DP systems for manufacturing the powder based structures. The powder, which is generally used, is composed of calcium sulfate hemihydrate which can be transformed to a ‘needle-shape’ when it adsorbs water based binder. It helps the powder to undergo physical crosslinking and the binders help to make more solid structures. By binding the powder with polysaccharides solution and stacking layer by layer, we demonstrate the sturdy structures are made. Solidification undergo at molecular level with powder and polysaccharide based binder solution. Chemically, calcium of the powder mediated coordination crosslinking gives strong mechanical property. The study suggests that biocompatible adhesives enhance mechanical properties of powder based 3DP structures by chelation.

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High-Yield Exfoliation of Metal Chalcogenide Nanosheets via Anion Doping

PIAO MEINA JINXIAOYAN[1] 김인영[1] AdpakpangKanyaporn[1] 황성주[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

High-yield preparation of two-dimensional nanosheets is of great importance for the further exploration of their unique properties. In this study, we develop an efficient way to improving the exfoliation yields of molybdenum disulfide via nitrogen-doping. The nitrogen was doped into the molybdenum disulfide nanosheets by heating the pristine molybdenum disulfide in the ammonia atmosphere at high temperature. Then use lithiation method expanse the crystal lattice and disperse the product in water. Analysis of the exfoliated nanosheets shows that the exfoliation yield was enlarged. This discovery may be a profitable approach to solve the problem of the limit of low yield. We believe that this work would benefit the application of molybdenum disulfide in nanomaterial field.

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Effective Control of the Crystal Growth and Photocatalyst Activity ofNoble Metal Nanoparticles Using Inorganic Nanosheets as Substrates

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Highly dispersed metal nanoparticles on the surface of layered titanate are synthesized by the crystal growth of Au and Pt nanoparticles at the terminal oxygen atoms exposed on the surface of trititanate ($Ti_3O_7^{2-}$). To confirm the beneficial role of terminal atoms in dispersing metal nanoparticles, layered lepidocrocite titanate ($Ti_{0.91}O_2^{0.36-}$) which possesses flat surface with only the terminal oxygen atoms are also used as reference. According to size characterization using SEM and TEM analysis, the Au-trititanate nanocomposite shows more monomodal distribution and smaller size of Au nanoparticles than Au-lepidocrocite titanate. In Pt-titanate nanosheet, the similar results were obtained. The change of the bonding aspect between titanium and metal ions was analyzed by using XANES, FT-IR, and Raman spectra. The photocatalytic property of these nanocomposites materials was measured by reduction of carbon oxide gas and artificial photosynthesis of hydrocarbon by splitting water. The lepidocrocite titanate-based nanocomposite shows the better activity for the H_2 generation than that of the trititanate-based nanocomposite, which is attributable to more effective electron transfer path of lepidocrocite titanate than that of trititanate. These researches demonstrate that the surface structure of metal oxide nanosheets controls the crystal growth of metal nanoparticles, and furthermore, regulates the photocatalytic effect.

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Facile morphological evolution of Cu_2O microcrystals using microwave-assisted method

여별이 조영식 허영덕*

단국대학교 화학과

We presented the facile method for morphological evolution of Cu_2O microcrystals. The Cu_2O microcrystals were prepared by using a commercial microwave oven. The Cu_2O products with various morphologies, such as 8-pod, 12-pod, (6×4)-pod, 6-pod, star-like, concave octahedron, and octahedron, were obtained by adjusting reactant concentrations. The open shaped crystals, such as 8-pod, 12-pod, (6×4)-pod, 6-pod, and star-like, were formed under the branching crystal growth mechanism for the lower reactant concentration. Whereas, the closed shaped crystals, such as concave octahedron and octahedron, were formed under the crystal habit formation for the higher reaction concentration. We also presented porous structures of Cu_2O products. The long and sharp branched nanowires in each arm provide effective building blocks for porous structures. These porous structures were obtained at the lowest reactant concentration with longer microwave irradiation time.

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Atomic Layer Deposition of Lanthanum Oxide with Thickness Scaling: Growth and Characterization

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경남대학교 교양기초교육원 [1]경남대학교 과학교육과

Lanthanum Oxide (La2O3) is the most promising insulator for the next-generation high-k gate insulators to achieve higher drivability as well as lower gate leakage. Characteristics such as high permittivity (κ=25~30), large band gap(Eg = 5.8ev), high band offset with respect to silicon are important in the miniaturization. In this work, we demonstrate determining the growth characterization and electrical property of a La2O3 thin film with a thickness down to 30 nm using thermal atomic layer deposition (T-ALD) process. La2O3 thin film was grown by T-ALD including La-precursor (alkylmides, cyclopentadienyls) and H2O as oxygen source, respectively. It was dependence of the film thickness and the growth rate on the deposition temperature. This study will be expected to contribute to additional scaling of gate oxide and improvement of efficiency of semiconductor.

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[발표취소] Ferroelectricity on a antiferromagnet triangular lattice, RbFe(MoO4)2

이창훈* 심지훈 이왕로[1]

포항공과대학교(POSTECH) 화학과 [1]전북대학교 기초교양교육원

발 표 취 소

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Fe(Ⅲ)-C-S co-doping in graphitic carbon nitride polymer for band gap tuning and photoreduction of CO_2 to methanol

MOHAMMAD KAMAL HUSSAIN 강영종[1,*]

서강대학교 화학과 [1]한양대학교 자연과학대학 화학과

Polymeric graphitic carbon nitride, g-C3N4 is a medium band gap indirect semiconductor of purely organic nature. Owing to its favorable band gap (Eg= 2.7eV) and its absorption within the visible range, it finds its utility in hydrogen production and water splitting at the same time. However, its conduction band edge position is variable depending upon synthesis route taken and the final condensation product formed. Our aim is to do fine tuning the reduction potential of g-C_3N_4 by the cumulative effect of simultaneous Fe(Ⅲ) ion doping, carbon self-doping and sulfur doping. As a result of these dopants, pi-electron delocalization estimated to be increased and a new electronic state below the conduction band should be formed. Hence we can also observe a red shift or decrease in the band gap. Facile electrons with lesser reductive energy from this new conduction band can effectively reduce CO_2 to methanol.

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Preparation of lanthanum and cerium oxide layers by electrodeposition with organic solution

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한림대학교 화학과

Layers of lanthanum and cerium oxide were prepared by electrodeposition performed with organic solutions above 30 V. Three concentrations for both lanthanum and cerium ions ranging from 0.05 to 2.0 mg/mL were employed for the electrodeposition. Depostion time varied from 30 minutes to 8 hours. Currents were monitored during the process and turned out to be below 0.8 mA at the highest concentration of both ions. Morphology and composition of lanthanum and cerium oxide layers were examined by scanning electron microscopy, X-ray diffraction and X-ray photoemission spectroscopy.

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Target preparation of lanthanum oxide on Ti by electrodeposition

최정희 정용희*

한림대학교 화학과

Targets of lanthanum oxide were prepared on Ti by electrodeposition at high voltages ranging from 200 to 1000 V. Each electrodeposition lasted 30 minutes. Mass gains of targets for each step of the process varied with the voltage and concentration employed for the electrodeposition. Currents were monitored during the process and they were below 3 mA regardless of lanthanum ion concentrations. Morphology of the targets were examined by scanning electron microscopy. Finer grains of lanthanum oxide were prevailing at the lower concentrations.

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Electrochromic devices based on porous V2O5 thin films for smart windows

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(주)마프로 기술연구소 [1]부경대학교 화학과

Electrochromic(EC) materials are able to the reversible optical change by redox reaction. Among a number of EC materials known so far, WO and Prussian blue are most practically used as cathodically and anodically coloring materials, respectively, because of the inorganic robustness. However, for building applications the blue color of WO3 and Prussian blue films in the colored state is not as favorable as brown or pale yellow colors for most building applications. For color tuning, we prepared V2O5 thin film which is a thermodynamically stable and shows multi colored electrochromism according to applied potential.V2O5 nanoparticles were synthesized by simple thermal-decomposition of vanadyl oxalate, which is prepared by mixing with a molar ratio of commercial micro-sized V2O5/oxalic acid 1:3 to 1:5. Nanoporous V2O5 thin films on conductive glass were prepared by wet coating and post heat treatment. The films showed a two-step electrochromism, yellow to blue, and then blue to khaki in two voltage ranges: -0.5V to 1.2V and -0.5V to -1.6V versus SCE, respectively. A electrochromic(EC) device fabricated with V2O5 and Prussian blue or V2O5 and WO3 films on ITO glass. V2O5/Prussian blue device exhibited 60% transmittance change at 660nm and long-term stability of more than 2,000cycles. The switching time of EC device was 3s from yellow to green color (+0.8 V), and 1.2 s from green to yellow color (-1.6V).

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Enhanced electrochromic stability of P3HT films modified by graphene oxide monolayer

김태호 나윤채*

한국기술교육대학교 에너지신소재화학공학부

Electrochromism is defined as reversible optical changes during the redox reactions induced by externally applied potential. Among various electrochromic materials, Poly (3-hexyl thiophene) (P3HT) shows optical modulations between red and pale blue in color during the redox reactions with a fast response speed. However, organic electrochromic materials including P3HT have poor stability during the reactions, even in the neutral electrolyte such as Li^+ based solutions. A graphene oxide (GO) has recently been reported to enhance the mechanical properties of polymer due to GO-polymer interactions. Herein, we investigated the improvement of P3HT stability induced by using a GO monolayer as a protective layer. The GO/P3HT films on ITO glass were prepared by spin-coating of P3HT solution and by transferring GO on P3HT film by a Langmuir Schaefer method. Electrochromic stability of the GO/P3HT films was studied by using cyclic voltammetry, chronoamperometry, and UV-Vis spectrophotometry etc. The results showed that compared to pristine P3HT films, the enhanced electrochemical and optical stabilities of the bilayer films were obtained. These findings indicate that GO monolayer play an important role to improve the stability of P3HT.

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Application of a conducting polymer nanocomposite on hydrogen peroxide sensors

김민영 심윤보[*]

부산대학교 화학과

Surface composition and condition of the electrode plays a significant role in improving the catalytic effect. The enhanced catalytic activity for a H2O2 sensor is proposed based on modified conducting polymer nanocomposites. Of these, the pTTBA nanocomposite film formed by electropolymerization of TTBA monomer and metal mixture solution shows the best catalytic activity. The characterization of sensor probe surface was done employing surface analysis and electrochemical experiments. The probe was examined for interfering substances to electrochemical reduction of H2O2. The sensor probe showed a dynamic range from 0.5 µM to 5.0 mM with the detection limit of 0.05 ± 0.01µM. Sensitivity retained 95% of initial sensitivity up to 31 days. The performance of the sensor was evaluated with normal and cancer cell cultures.

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Biosensor using a hemeprotein-biomaterial modified electrode

LIANG QIAN 심윤보[1,*]

부산대 화학과 [1]부산대학교 화학과

In the present work, the hybrid biomaterial structure was constructed by incubation of a hemeprotein with copper sulphate in PBS. Sensor probes were fabricated by polymerization of functionalized conducting polymer after Au nanoparticles deposition, then hemeprotein-biomaterial attached on the layer, which exhibited well defined redox peaks at 0.107V/-0.005 V in a 0.1M phosphate buffer solution (pH 7.4). The redox processes show quasi-reversible behavior and the electron transfer rate constants were calculated by Laviron's equation. Morphology and performance of the hemeprotein-biomaterial modified electrodes were investigated using surface characterization methods and voltammetry. Finally, sensor probes were examined to detect hydrogen peroxide released by cells.

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A Metal Complex Mediator Self-assembled on Au Nanoparticles and CNT-rGO for Glucose Sensor

김정인 심윤보*

부산대학교 화학과

A glucose sensor was constructed with metal complex self-assembled Au nanoparticles and multi-walled carbon nanotubes with reduced graphene oxide (MWCNT-rGO) on a screen printed carbon electrode (SPCE). A metal complex was applied as an electron mediator to a disposable glucose sensor using NAD-GDH. The sensor was characterized using SEM, TEM, XPS, and electrochemical techniques. The experimental parameters in terms of pH, temperature, and concentration of metal complex and CNT for the glucose sensing were optimized. Common interferences were completely avoided using the proposed sensor. A linear calibration was obtained for glucose between 3 mg/dL and 300 mg/dL and a detection limit of 2.22 ± 0.7 mg/dL was obtained.

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Highly selective and sensitive determination of nicotine with dye composited conductive polymer

민수진 심윤보*

부산대학교 화학과

A highly selective and sensitive nicotine (NIC) sensor was developed by incorporating a dye composite layer on to the conductive polymer layer. Electrocatalytic response was observed at 0.88 V through the strong electrostatic interaction between nicotine and the sensor surface. The sensor was effective for blocking interferences from various negatively charged species, which was attributed to the presence of sulfonate groups in the sensor surface. The experimental parameters were optimized in terms of pH, composite ratio, and applied potential. The sensor demonstrated the best performance in the amperometric detection of NIC in a dynamic range of 0.5μM~300μM with a detection limit of 420.0 ± 4.5nM.

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Effects of fluorine substituted $LiFeBO_3$ as a cathode material for lithium ion batteries

안지은 이영일* 이지원

울산대학교 화학과

$LiMBO_3$ (M=Fe, Mn and Co) is increasing to interest due to its strong boron-oxygen covalent bond, high theoretical specific capacity, environmental friendly benefit, and less expensive. The fluorine substituted $LiFe(BO_3)_{1-x}F_{3x}$ composites have been synthesized by solid-state reaction using planetary mill method without carbon coating. It was characterized by XRD, SEM and cycling test. The XRD results of composite indicate fluorine anions have been successfully substituted to BO_3^{3-} sites without structural modification. Electrochemical analysis has been also performed with various C-rates and cycleability.

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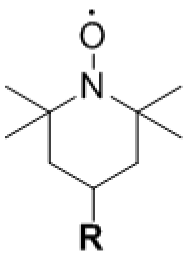
The Convenient Preparation of TEMPOL Derivatives as High Energy Density Organic Electrolyte: Application for Redox Flow Battery

함창한 성현준 안철진*

창원대학교 화학과

Redox flow battery (RFB) is a type of electrochemical energy storage devices. It is necessary to improve the energy density in RFB system. In this paper, we prepared 4-hydroxyl-TEMPO derivatives as high energy density electrolyte, which investigated the electric effects through the CV.



< R : -H, -OH, -N$_3$, -SO$_2$Me, -SO$_2$Ph >

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Facile Electrochemical Detection of Botulinum Neurotoxin Type E Using a Two-Step Proteolytic Cleavage

박선화 양해식*

부산대학교 화학과

Facile electrochemical methods for measuring protease concentration or protease activity are essential for point-of-care testing of toxic proteases. However, electrochemical detection of proteases, such as botulinum neurotoxin type E (BoNT/E), that cleave a peptide bond between two specific amino acid residues is challenging. This study reports a facile and sensitive electrochemical method for BoNT/E detection. The method is based on a two-step proteolytic cleavage using a target BoNT/E light chain (BoNT/E-LC) and an externally supplemented exopeptidase, L-leucine-aminopeptidase (LAP). BoNT/E-LC cleaves a peptide bond between arginine and isoleucine in IDTQNRQIDRI-4-amino-1-naphthol (oligopeptide-AN) to generate isoleucine-AN. Subsequently, LAP cleaves a bond between isoleucine and AN to liberate a free electroactive AN species. The liberated AN participates in electrochemical-chemical-chemical (ECC) redox cycling involving $Ru(NH_3)_6^{3+}$, AN, and a reducing agent, which allows a high signal amplification. Electrochemical detection is carried out without surface modification of indium-tin oxide electrodes. We show that dithiothreitol is beneficial for enhancing the enzymatic activity of BoNT/E-LC and also for achieving a fast ECC redox cycling. An incubation temperature of 37 ℃ and the use of phosphate buffered saline (PBS) buffer resulted in optimal signal-to-background ratios for efficient BoNT/E detection. BoNT/E-LC could be detected at concentrations of ca. 2.0 pg/mL, 0.2, and 3 ng/mL after 4 h, 2 h, and 15 min incubation in PBS buffer, respectively, and ca. 0.3 ng/mL after 2 h incubation in bottled water. The method developed could be applied in fast, sensitive, and selective detection of any protease that cleaves a peptide bond between two specific amino acid residues.

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Voltammetric determination of hexavalent chromium using a nanoporous gold modified electrode

최승민 박민욱 심윤보*

부산대학교 화학과

The determination of Cr (VI) ion is performed with nanoporous gold (NPG)-organic ligand plated glassy carbon electrode (GCE). The surface of the modified electrode was characterized by impedance spectroscopy, SEM, EDS, and XPS. Experimental variables that have an effect on the peak current, such as pH, supporting electrolytes, the ratio of gold to nickel, and the concentration of organic ligand were optimized. Interference effects of other metal ions were also tested at various electrolytes. Linear sweep voltammetry (LSV) was performed to analyze hexavalent chromium by scanning the potential between +0.8 and +0.3 V without any preconcentration time. Calibration plot using NPG-organic ligand modified GCE were obtained in the dynamic range from 10ppb to 10ppm. The detection limit for Cr (VI) ion was determined to be 5 ppb. This method was investigated to analyze the Cr (VI) in the real samples like tap water.

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Electrochemical Detection of Vaccinia Virus in a Solution Containing L-Ascorbic Acid

박선화 서정욱 양해식*

부산대학교 화학과

Washing processes cannot fully remove interfering species that remain on biosensing surfaces when a sample solution contains a high concentration of interfering species. This study reports an immunosensing scheme employing electroreduction-based electrochemical-chemical (EC) redox cycling that allows sensitive detection of Vaccinia virus (VV) in a solution containing a high concentration of L-ascorbic acid (AA). To obtain high signal amplification, an enzymatic reaction by β-D-galactosidase (Gal) is combined with electroreduction-based EC redox cycling by an oxidant. Among the four possible oxidants (KIO_3, NaClO, Ag_2O, and H_2O_2), KIO_3 shows the highest signal-to-background ratio and is chosen. During an incubation period of 10 min, Gal converts β-D-galactopyranoside into *p*-aminophenol (AP), which is oxidized to *p*-quinone imine (QI) by KIO_3. When -0.05 V vs. Ag/AgCl is applied to an immunosensing electrode, QI is reduced to AP, and the regenerated AP is then reoxidized by KIO_3. The electroreduction-based EC redox cycling is induced. An indium-tin oxide electrode modified with reduced graphene oxide and an applied potential of -0.05 V are used to achieve low and reproducible background currents, slow O_2 reduction, and fast electroreduction of QI. KIO_3 favorably converts AA into noninterfering species during the incubation period. The detection limit for VV in commercial 50 % mandarin juice (AA concentration = 0.7 mM) is 4×10^3 plaque-forming unit (PFU) per mL. The new EC redox cycling scheme is promising for sensitive detection of proteins, viruses, and bacteria in solutions containing high concentrations of AA.

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Synthesis and Catalytic Features of Au@SiO2@M (M = Au, Pd, AuPd) Core-Shell Nanoparticles for Fuel Cells

박성철 심준호[1,*]

대구대학교 화학과 [1]대구대학교 화학·응용화학과

In our research, we present the controlled synthesis of Au@SiO2@M (M = Au, Pd, AuPd) nanoparticles (NPs) and core-shell morphologies by modified sol-gel process with the assistance of tetraethylorthosilicate. The aim of this work is to explore the oxygen reduction reaction (ORR) properties of Au@SiO2@AuPd NPs, giving a systematic comparison between their electrocatalytic activities and those of bimetallic core-shell counterparts (Au@SiO2@Au and Au@SiO2@Pd). The size, morphology, elemental composition, and optical properties of the core-shell were characterized using field-emission scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction, and UV-vis spectroscopy. The electrocatalytic activity of the Au@SiO2@AuPd for ORR in alkaline media was investigated by rotating disk electrode (RDE) and cyclic voltammetry (CV). The porous Au@SiO2@AuPd NPs can be used as supportless electrocatalysts that exhibit comparable ORR catalytic activities to commercial carbon-supported Pt catalysts (20 wt% Pt on Vulcan XC-72, Pt-20/C).

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Silver Decorated Schiff base Functionalized Graphene for Enhanced Electrocatalytic Oxygen Reduction Reaction in alkaline fuel cells

박동철 Mohammad Shamsuddin 전승원*

전남대학교 화학과

Newly synthesized Schiff base [SB, 1,8-napthalenediamine, N^1,N^8-bis(2-pyridinylmethylene)] functionalized electrochemically reduced graphene with silver (Ag) nanoparticles (ERGO/SB-Ag) has been introduced in electrochemical oxygen reduction reaction (ORR) for alkaline fuel cells (FCs). The structural features of catalyst are characterized by several instrumental techniques. The transmission electron microscopy (TEM) images suggest a well dispersed AgNPs onto ERGO/SB surface. The ORR activity of ERGO/SB-Ag has been investigated via cyclic voltammetry and hydrodynamic voltammetry techniques in 0.1 M KOH aqueous solution. Comparative CV analysis suggests a general approach of intermolecular charge-transfer in between graphene sheet and AgNPs via SB which leads to the better AgNPs dispersion and subsequently superior ORR kinetics. The ERGO/SB-Ag has superior electrocatalytic activity towards ORR than that of state-of-the-art Pt/C in respect to the half-wave potential and current density. The Koutecky?Levich and Tafel analysis suggest that the proposed main path in the ORR mechanism has direct four-electron transfer process with faster transfer kinetic rate on the ERGO/SB-Ag.

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Preparation, electrochemical behavior and electrocatalytic activity of p-xylylenediamine functionalized graphene supported Pd nanoparticles as formaldehyde sensor

EJAZ AMMARA 전승원*

전남대학교 화학과

A novel electrochemical sensor based on p-xylylenediamine functionalized graphene supported Pd nanoparticles (G-PxDA-Pd) has developed and employed as an efficient electrocatalyst on formaldehyde oxidation reaction (FOR). The physical characterization of the sensor has studied using x-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). TEM study revealed good dispersion of Pd nanoparticles on the G-PxDA-Pd surface. The electrochemical activity has been studied by cyclic voltammetry, differential pulse voltametry and chronoamperometry for the determination of formaldehyde in 2M KOH. The proposed sensor has high sensitivity, good selectivity and fast response to formaldehyde. The oxidation peak current shows a linear relationship with the formaldehyde concentration in the range of 0.5 mM to 12 mM. The detection limit has calculated as 3.24 ?M (S/N = 3). The experimental data further reveals that the electrooxidation of formaldehyde inhibits the formation of the poisonous intermediate, such as CO.

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Electrochemical oxidation and determination of dopamine by reduced graphene oxide supported cobalt oxide catalyst

YASMIN SABINA Mohammad Shamsuddin 전승원*

전남대학교 화학과

Reduced graphene oxide supported cobalt oxide (rGO/Co3O4) has been prepared by hydrothermal method and applied for the electrochemical determination of dopamine (DA). The rGO/Co3O4 has been characterized via transmission electron microscopy (TEM) and X-ray photoelectron spectroscopic (XPS). The electrochemical detection of DA on rGO/Co3O4 has verified through the cyclic voltammetry, differential pulse voltammetry and amperometric techniques in a 0.1 M phosphate buffer solution (PBS) at optimized pH 7.4. The interference has also been investigated in presence of ascorbic acid (AA), glucose, serotonin, N2H4, and uric acid. The rGO/Co3O4 has shown a comparatively good analytical performance for DA with 220.80 ?A mM?1 cm?2 sensitivity, 0.027 ?M limit of detection (where S/N = 3). As a result, the rGO/Co3O4 catalyst can be employed to detect DA with a good linear range, high sensitivity and low detection limit.

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Redox cycling-amplified enzymatic Ag deposition and its application in the highly sensitive detection of creatine kinase-MB

Al-Monsur Jiaul Haque 양해식*

부산대학교 화학과

We report a novel enzymatic Ag-deposition scheme combined with chemical-chemical (CC) redox cycling of 4-aminophenol (AP) by reduced β-nicotinamide adenine dinucleotide (NADH). This novel scheme allows a higher Ag-deposition rate (i.e., higher signal amplification) than a scheme using only enzymatic Ag deposition. As a result, the immunosensor obtained using CC redox cycling-amplified enzymatic Ag deposition provides a much lower detection limit than the immunosensor using only enzymatic Ag deposition. Therefore, this can be applied for the highly sensitive detection of a cardiac biomarker, creatine kinase-MB (CK-MB).

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전기삼투펌프를 이용한 인슐린 펌프개발

이현수 신운섭[*] Enhua Zhu[1]

서강대학교 화학과 [1]서강대학교 바이오융합기술

인슐린 주입은 췌장의 기능이 전혀 없는 제 1 당뇨 환자에게는 필수적이고, 증상이 심한 제 2 형 당뇨환자에게도 당뇨 개선에 효과가 있음이 많이 보고되고 있다. 현재 인슐린은 인슐린펜을 이용한 주입이 가장 많지만, 자동적으로 지속적으로 주입될 수 있는 장점을 가진 펌프 활용이 지속적으로 늘어나고 있다. 기존의 인슐린펌프는 가격이 비싸고, 부피 및 무게가 큰 단점이 있는데, 본 연구실에서 패치형으로 개발하고 있는 인슐린펌프는 부피 및 무게를 작게 구현할 수 있어 2~3 일간 몸에 부착하여 스마트폰으로 콘트롤하여 활용할 수 있는 형태이다. 이는 저전력펌프로서 무선통신을 포함하더라도 작은 리튬전지, CR1220 (3.0 V, 40 mA·h) 1 개로 3 일 이상 충분히 구동 가능함을 확인하였고, 펌프시스템은 5 일 동안 안정되게 구동되었다.

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전기삼투펌프의 적용 - 체내 이식형 약물 주입기

전석민 신운섭[*] Enhua Zhu[1]

서강대학교 화학과 [1]서강대학교 바이오융합기술

체내 이식형 약물전달 펌프는 체내 특정 부위의 약물 주입에 많이 활용되고 있는데, 극심한 통 증이 수반되는 암환자 및 만성통증환자의 경우에는 척수강에 0.5~4 mL/day 속도로 모르핀을 지속적으로 주입하여 통증을 완화시킨다. 척수강 내에 약물을 직접 투여하게 되면 경구 투여의 300 배, 정맥 투여의 100 배 이상의 효과를 나타내며, 다른 부위로 약물이 순환되지 않기 때문에 부작용이 적고, 이식형으로 되어 있으므로 샤워 등 환자의 일상 생활에 불편을 주지 않는 장점이 있다. 현재 이러한 펌프는 전량 고가로 수입되어 활용되고 있는데, 본 연구실에서 개발된 전기삼투펌프는 초소형, 초경량이며 저전력 구동이 가능하고, 최근 오랜 기간 안정되게 작동될 수 있는 방법을 개발하였기 때문에 이를 대체하기 위한 펌프로 개발 가능했다. μL 단위의 유량 컨트롤, 초저전력 구동 등을 구현하여 전기삼투펌프가 체내 이식형 펌프로서 적합함을 확인하였다.

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Iodine substitution effect of monoclinic structured $LiFeBO_3$ as cathode materials for Li-ion batteries

이한솔 이영일* 이형동 박재영

울산대학교 화학과

There are intensive research activities into alternative electrode materials for the next generation of Li-ion batteries, particularly for use in hybrid electric vehicles and grid scale battery. Monoclinic structured lithium metal borate, $LiMBO_3$ (M = Mn, Fe and Co) for cathode material of Li-ion battery have attracted great interest due to their high theoretical capacity (220mAh/g), excellent safety for nature, and high energy density with small polyanion volume. However, lithium transition metal borates are considered to have intrinsically low ionic and electronic conductivity, which is believed to be the cause of the poor electrochemical performance. Iodine substituted $LiM(BO_3)_{1-x}I_x$ (M=Fe) have been proposed as alternatives to the conventional cathode material. It is characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), and electrochemical test.

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Electrochemical properties of Carbon quantum dots and B,N doped Carbon quantum dots

오성훈 장병용*

부경대학교 화학과

Carbon quantum dots are recently discovered when SWNTs derived from arc-discharge soot is purified by Electrophoretic Analysis. Carbon quantum dots is expected to replace heavy metal based quantum dots (ex. CdSe, CdTe, CdS..) in biosensing and optoelectric devise because of its chemical inertness, a lack of optical blinking, low photobleaching, low cytotoxicity, and excellent biocompatibility. In this, we synthesize Carbon quantum dots and doped with B,N Carbon quantum dots for investigation of electrochemical properties. We also expect to apply this Carbon quantum dots in Electrochemiluminescence.

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Characteristics for electrodeposition of Mg-doped CdSe

정재구 노영철 채원석*

대진대학교 화학과

Electrodeposition of a Cadmium selenide(CdSe) thin film was studied to find the optimum conditions under which the deposition temperature could be lowered. CdSe films were electrochemically deposited on ITO using Chrono amperometry in an aqueous solution. A simple and novel deposition cell was designed to allow simultaneous thermostating and polychromic illumination. X-ray diffraction (XRD) analysis have confirmed that these films were indexed as cubic symmetric structured pure CdSe (JCPDS: 19-0191), and UV-visible absorption spectra measurements have shown an optical band-gap energy. Band-gap energy of mg-doped CdSe is shifted.

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Direct electron transfer from bacteria to the electrode using modified carbon nanoparticles

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Direct electron transfer from bacterial cells to the electrode is essential in microbial fuel cells for achieving high current density. Here we show carbon nanoparticles can act as a bridge connecting microbes and the electrode. They are small enough to penetrate bacterial cell membrane to reach the electron transfer system in a cytoplasmic membrane. Carbon nanoparticles however are agglomerated in aqueous solution making them impenetrable to the membrane because of their hydrophobicity. We used Ketjen black (KB), a high area carbon nanoparticle whose diameter is about several tens of nanometers and modified them with 4-aminobenzoic acid to impart charges on the surface so that individual carbon particles are dispersed in water. Thus modified particles were added into the microbial culture and mixed well. After centrifugation, collected bacteria-KB composite was applied on the graphite surface. Upon addition of glucose, we observed catalytic oxidation current. Current was linearly increased with glucose concentration up to 25 mM. This result indicates that carbon nanoparticles can be used as a wire to directly transferring electrons from the bacteria to the electrode. Microbial fuel cells based on the direct electron transfer are expected to generate higher power density than conventional cells.

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A New Class Electroactive Fe and P-Functionalized Graphene for Oxygen Reduction

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While metal and electronegative N-containing carbon has aroused great interest as an efficient catalysttowards the oxygen reduction reaction (ORR), no combination of metal with other heteroatomcontainingcarbon has received considerable attention. This has motivated us to explore theperformance of carbon functionalized with metal and electropositive phosphorous. Herein, we presentthe first report on the synthesis of a new class of electroactive Fe- and P-functionalized graphene (GPFe)and its electrocatalytic properties in alkaline and acidic media. The introduction of Fe causes remarkablesynergistic effects on P-doped reduced graphene oxide by increasing surface area, enhancing the Pdoping level due to the interaction between Fe and P and generating electrochemically active Fe?Pspecies. N-oxides are known to be in-active for ORR in Fe?N systems, whereas in present Fe?P systems,oxides of Fe and P are found to be beneficial for ORR. Interestingly, after the introduction of Fe, mostlyinactive P-doped carbon becomes active in acidic medium. We propose that this study will surelyprovide renewed insights into active sites for ORR in metal and heteroatom-doped carbon systems.

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Iodine-treated heteroatom-doped carbon : conductivity driven electrocatalytic activity

SINGHKIRANPAL 유종성[1,*]

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A high conductivity and surface area are the most highly desired properties of an electrocatalyst. Herein, wereport a novel technique to synthesize highly conductive and microporous N and S-doped carbon frompolyaniline (PANI) via a simple, template-free hydrothermal method followed by carbonization in thepresence of iodine. The iodine treatment removes a large amount of the attached oxygen atoms andother heteroatoms and, as a consequence, increases the carbon content. Thus, the iodine treatmentdecreases the doping of catalytically active heteroatoms, which is unfavourable for the ORR, but at thesame time, significantly increases the electrical conductivity, which is beneficial for the ORR. Inparticular, iodine-treated carbonized PANI (CPANI) shows an exceptionally high conductivity i.e., about 3times that of untreated CPANI. Iodine treatment is also found to enhance the micropore surface area ofthe PANI during carbonization without using a harmful activating agent or a hard template. Anelectrocatalytic study indicates that the activity of the iodine-treated sample is considerably higher thanthat of an untreated sample. This remarkable upsurge in activity is mainly attributed to the large increasein the conductivity and surface area of the iodine-treated sample. The ORR activity is discussed in termsof the heteroatom content, surface area and conductivity of the carbon. This convenient, innovativeapproach can offer new possibilities for the design of future highly efficient fuel cell electrocatalysts.

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Improved process of graphene oxide fabrication and its application to glucose sensor

전원용 이보희[1] 이현선[1] 오유정[1] 최영봉[1] 김혁한[1,*]

단국대학교 나노바이오의과학과 [1]단국대학교 화학과

Graphene oxide (GO), easily fabricated by microwave, was changed to reduced graphene oxide (RGO) by cyclic voltammetry (CV) on the screen printed carbon electrodes (SPCEs) before glucose oxidase (GOx) dried for determination of glucose level without mediator. GO was prepared by microwave for 20 min at 210 OC under nitric acid solution. And oxygen of GO was investigated by FT-IR. To form the RGO on the SPCEs, CV was applied from -1.5 to 0 volt with scan rate of 100mV/sec. GOx was dried on the SPCEs for 24 h at ambient condition. Nafion of 0.5 wt% was casted on the GOx/SPCEs to make stable electrode. Morphologies of all electrodes were investigated by scanning electron microscopy (SEM). Various glucose concentrations were measured by CV and amperometry. Also, interference species such as ascorbic acid (AA) and uric acid (UA) were showed for no effect on the Nafion/GOx/GO-SPCEs. Our study has advantages that easy and fast fabrication process, non expensive, good sensitivity, and wide detection range of glucose.

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Porous Manganese Oxide Nanorods Dispersed on Reduced Graphene Oxides as a Binder-free Anode Paper for Lithium-Ion Batteries

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서울대학교 융합과학기술대학원 융합과학부

A porous and binder-free Mn_3O_4 nanorod/reduced graphene oxide (pMn_3O_4 NR/rGO) paper is mainly fabricated by a simple two-step process: vacuum filtration and thermal treatment. A MnOOH NR/GO paper prepared by a filtration technique is reduced to a pMn_3O_4 NR/rGO paper through heat treatment with N_2 atmosphere. The pMn_3O_4 NR/rGO paper consists of porous Mn_3O_4 nanorods distributed on the surface of rGO layers and a combination of stacked rGO layers and pMn_3O_4 NRs. In the hybrid structure, rGO nanosheets provide a conductive pathway for electrons and function as buffer layers to alleviate the pulverization of pMn_3O_4 NRs during the electrochemical reaction. Therefore, when this paper is directly used as an electrode in lithium-ion batteries, it presents a high discharge capacity during the first cycle, which quickly stabilizes in the following cycles and maintains a high reversible capacity even after many charge-discharge cycles, which is much higher than that of the corresponding rGO paper.

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The Effect of Redox Mediators in Slurry Electrodes on the Performance of an Electrochemical Flow Capacitor

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충남대학교 화학과 [1]한국에너지기술연구원 에너지저장연구실

The electrochemical flow capacitor (EFC) is a new electrochemical energy storage technology. The EFCs use a flow battery system design and are based on the charge storage mechanism of electrochemical capacitors. Since the architecture of the EFCs enables power and energy density capacity to be decoupled and optimized for the desired application, they can offer several advantages such as fast charging/discharging, long cycle life, and scalable energy capacity. Development of high-performance slurry electrodes is an essential technology in the EFCs. Numerous approaches have been explored to improve energy density in electrochemical capacitors. Among them, the use of organic redox molecules has shown significant potential to enhance the performance of electrodes. In this study, we demonstrate redox flow capacitors by using slurry electrodes including organic redox mediators. The effect of the redox molecules in slurry electrodes on the performance of the EFCs is also investigated.(Acknowldegement) This work was conducted under the framework of Research and Development Program of the Korea Institute of Energy Research (KIER) (B5-2414, B5-2502). This research was supported by Nano·Material Technology Development Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and Future Planning.(2009-0082580).

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Study on enhanced electrochemical properties and Li ion diffusion kinetics of Zr^{4+}-doped $Li_2FeP_2O_7/C$ as cathode material for lithium ion batteries

류다정 류광선*

울산대학교 화학과

Iron-based cathode materials are ideal for future lithium ion batteries in terms of low cost and environmental friendliness. In particular, they are very suitable as cathode electrode for large scale LIBs in applications related to electric vehicles(EVs), hybrid electric vehicles(HEVs), and stationary storage batteries. Here, one such example of opening a new family of polyanionic cathode systems is the bilithium metal pyrophosphates. Among them, lithium iron pyrophosphate compound offers the possibility of a two-electron reaction and the existence of a two-dimensional Li-ion channel. But they suffered from redox voltage drop owing to the rearrangement of constituent atoms for the first charging/discharging cycle.In this research, we prepared $Li_2Fe_{1-x}Zr_xP_2O_7/C$ (x=0, 0.01, 0.02, 0.03, 0.04, and 0.05) to increase redox voltage and reversible capacity by splash combustion synthesis with the theoretical capacity of 110mAh/g for a one-electrode reaction. In the electrochemical measurements, the doped materials show further decrease in polarization, upshifting redox voltage and stabilized atomic arrangement. Also, we investigated the ionic conductivity to compare with $Li_2FeP_2O_7/C$ and doped $Li_2Fe_{1-x}Zr_xP_2O_7/C$ with optimized content by using different electrochemical methods, including GITT, PITT, EIS, and CV, which are powerful techniques to investigate the kinetic behaviors. The diffusion coefficient of doped material exhibits the improved ionic conductivity than that of undoped material.

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Electrochemical deposition of palladium using anode catalyst for hydrazine catalysis in alkaline media

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전남대학교 화학과

Palladium (Pd) was directly electrodeposited onto glassy carbon electrode (GCE) by cyclic voltammetry (CV) from a bulk Pd2+ solution and applied for the electrochemical catalysis of hydrazine in an alkaline solution. The electrodeposited Pd (e-Pd) was evaluated by scanning electron microscope and transmission electron microscopy. The electrochemical deposition conditions of the e-Pd were verified and 6 cycles at 50 mV/s was the optimized. The electrochemical performances, kinetics and stability of e-Pd/GCE towards hydrazine oxidation reaction (HOR) have been evaluated using CV in 0.1 M KOH electrolyte. The HOR at e-Pd/GCE demonstrated an irreversible diffusion-controlled electrode process and a four-electron transfer involved reaction. With regard to cycle number, with increased cycling, the size and shape of the e-Pd changed but the HOR catalytic property decreased. As the conditions of electrochemical deposition were varied, the particle size and catalytic activity for formic acid were also changed.

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The electrochemical properties of VO_2/silica composite thin films with different polymorphs

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부경대학교 화학과 [1](주)마프로 기술연구소

VO_2 has several different polymorphs such as VO_2(A), VO_2(B), VO_2(C), VO_2(M) and VO_2(R), etc. Among them VO_2(M/R) has been most widely studied because of their reversible phase transformation. Since its temperature-dependent phase transition give rise to semiconductor-to-metal transition in its electrical property and concomitantly changes its optical property, VO_2(M) has been most interested ad a thermochromic material applicable for smart window. However, VO_2 has not been attracted for electrochemical property although it is electroactive material. Only VO_2(B) has been studied as electrode material for lithium ion batteries because of inorganic electroactive nanoparticles by utilizing silica precursors. The method provides highly transparent and uniform thin films of inorganic electroactive nanoparticles. In this study we have prepared nanoparticles of three different polymorphs of VO_2 and their silica composite thin films and studied their electrochemical properties in aqueous and nonaqueous electrolyte solutions.

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Determination of trace heavy metal ions by differential pulse anodic stripping voltammetry using an electrochemically deposited graphene/bismuth nano composite film modified glassy carbon electrode

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The present study, a highly enhanced sensing platform based on the direct electrochemical reduction of graphene oxide (GO) colloidal solution at glassy carbon electrodes was developed for the determination of zinc, cadmium and lead by differential pulse anodic stripping voltammetry (DPASV). The object of this work is to improve the analytical performance and to fabricate a sensitive and mercury-free electrochemical platform combining the advantages of electrochemically deposited graphene (EG) together with the in situ plating bismuth (Bi) nano composite film coated glassy carbon electrode. The as-synthesized EG/Bi nanocomposite was characterized by Raman spectroscopy, transmission electron microsopy (TEM), scanning electron microscopy (SEM) and cyclic voltammetry. The experimental conditions regarding the effects of different operational variables such as pre-concentration potential, bismuth deposition time, bismuth concentration, and pH were studied to find optimized conditions for the purpose of determining trace metals. Liner calibration curves ranged from 10 μg/L to 100 μg/L for zinc, cadmium and lead. The composite film integrating the advantages of electrochemically deposited graphene, Nafion and bismuth enhanced the sensitivity of trace metal ion. The limit of detection was 0.09 μg/L for lead, 0.16 μg/L for cadmium and 1.93 μg/L for zinc (S/N = 3). The EG/Bi composite film electrodes were successfully applied to analysis of trace metals in real sample. This method offers several advantages over other graphene sheet fabrication techniques, such as simple, fast, free of chemical-reduction reagents. Also, the green preparation method greatly expands the scope of graphene based electrochemical sensing device and holds promise for its wide application in the analysis of various real samples.

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A Dip-coating Method for Fabrication of Multilayered Graphene-Mn_3O_4 Hybrid Nanostructures as High Rate Lithium-Ion Battery Electrodes

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High-performance lithium ion battery (LIB) with good cycling and rate is required in many application fields. To meet the increasing demand, new designed electrode structure is very desirable. In this study, we have fabricated a multilayered graphene-Mn_3O_4 hybrid nanostructure using a dip-coating approach. In the electrode, a nickel foam with high porosity is used both as a template and current collector for the fabrication of porous structured electrodes. Also, the alternatively stacked graphene nanosheets provide electron pathways for high electron transfer rate. Because of their unique structure, the electrodes show excellent electrochemical performances (~ 1000 mA h g-1 after 50 cycles at a current density of 200 mA g-1). The improvement of the electrochemical performances could be contributed to the 3D multilayered structure and synergic effect between graphene and Mn_3O_4 nanoparticles.

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Synthesis and characterization of copper sulfide dendrite

김원빈 조미숙 이영관*

성균관대학교 화학공학과

Here we demonstrate a novel strategy for the preparation of copper sulfide dendrite. Copper dendrite as a template was electrodeposited on nickel foam by hydrogen gas bubbling. The surface of copper dendrite was homogenously sulfidized by vaporization of hydrogen sulfide from thiourea. The surface sulfidizing was controlled by the concentration of thiourea and reaction temperature and time. The composition and structure of copper sulfide and copper dendrite were investigated by scanning electron microscope, X-ray diffraction analysis, and X-ray photoelectron spectroscopy. Electrochemical properties of copper sulfide were confirmed by cyclic voltammetry. The performance of nickel sulfide as the electrode materials was determined by non-enzymatic glucose detection.

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Preparation and characterization of various morphology of nickel sulfide

김수찬 조미숙 이영관*

성균관대학교 화학공학과

Various morphology of nickel sulfide grown on Ni foam was prepared via a hydrothermal method in mix solvent of ethanol and water. The morphology of nickel sulfide was verified by the ratio of ethanol and water. When the ratio of water was increased, nickel sulfide was grown like dendrite. While the ratio of ethanol was increased, nickel sulfide was grown like flake-wall. The morphology and composition of various nickel sulfide were investigated by scanning electron microscope, X-ray diffraction analysis, and energy dispersive spectrometer. Electrochemical properties of nickel sulfide as a function of morphology were charaterized by cyclic voltammetry and electrochemical impedance spectroscopy. Accroding to the morphology of nickel sulfide, its surface area was changed and affected the electric conductivity and ion/electron transfer. The performance of nickel sulfide as the electrode materials was determined by non-enzymatic glucose detection. It is concluded that various morphology of nickel sulfide was well controlled by the kinds of solvent and affected the electrochemical properties.

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One-step electrochemical synthesis of PANI/rGO composite on paper substrate

오성훈 장병용*

부경대학교 화학과

we synthesis PANI/GO composite on paper substrate by in situ electro-polymerization and electrochemical reduction of graphene oxide. Polyaniline is a well-studied conducting polymer with its ease of synthesis and conductivity. And graphene was used to supplement the disadvantages of PANI. In this, the cellulosic paper was coated with the PANI/rGO composites by two-electrode cell in the sulfuric acid solution. This PANI/rGO composite coated paper can be applied to the supercapacitor for wearable device due to its flexibility.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

FeF_3 Nanoparticles Embedded in Activated Carbon Foam (ACF) as a Cathode Material with Enhanced Electrochemical Performance for Lithium Ion Batteries

김한아 김종식*

동아대학교 화학과

FeF_3 has been actively studied as an alternative cathode material because it has a high theoretical capacity of 237 $mAhg^{-1}$ (2.0-4.5 V) for the storage of one lithium ion. In addition, it has low toxicity and is cost effective compared with Co, Mn, and Ni-based electrode materials. In spite of these advantages, FeF_3 has serious shortcomings of poor electronic conductivity and slow diffusion rate of lithium ions, leading to a lower reversible specific capacity than its theoretical capacity. In this work, we prepared FeF_3/activated carbon foam (ACF) nanocomposites by impregnating FeF_3 nanoparticles in the mesoporous ACF. These nanocomposites show enhanced electrochemical properties as a cathode compared with those of bulk FeF_3. For example, the FeF_3/ACF has a discharge capacity of 195 $mAhg^{-1}$ during the first cycle. It is worth noting that during the 4th cycle, due to a slow activation process, FeF_3/ACF achieves a reversible capacity as high as about 221 $mAhg^{-1}$ (at rate of 0.1 C in the voltage range 2.0-4.5 V). The cycling stability is also improved, discharging a capacity of about 199 $mAhg^{-1}$ at the 50th cycle (0.2% fading per cycle).

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Electrochemical characterization of antibiotic transfer reaction at ITIES

한혜연 이혜진[1,*]

경북대학교 화학 [1]경북대학교 화학과

본 포스터는 항생제가 서로 섞이지 않는 두 전해질 (수용성 액체/유기성 액체) 계면에서 이동하는 반응에 따라 전류값의 변화를 측정하여 항생제의 약리학적 성질을 조사한 연구 결과를 나타냈다. 수용성 액체와 유기성 액체 사이에 계면을 형성하고 물의 pH 를 변화시킬 때 항생제 이온의 전하가 달라져서 편극화 된 계면에서 전이하는 정도 차이가 나고 이에 따라 전류의 변화가 일어나는 것을 전기화학적 방법으로 조사하였다.

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Minimization of non-specific interactions of proteins using mixed monolayer surface modification

김은미 이혜진*

경북대학교 화학과

본포스터에서는 바이오센서 표면에 단백질의 비특이적반응을 최소화하기위해 다양한 종류의 모노레이어를 혼합하여 센서의 표면을 처리하였다.
비특이적 반응 정도 및 유무를 확인하기 위해 모노레이어의 조성 및 비율을 변화시켰으며 센서표면에서의 전기화학적 활성을 갖는 효소반응을 이용하였고, 이들 반응에 의한 전압전류법 신호를 측정함으로써 그 비특이적 반응 효과를 정량적으로 분석하고자 하였다.

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Effect of blocking agents on reducing non-specific adsorption onto biosensor surface

DIBAFARHANASHARMIN 이혜진*

경북대학교 화학과

We have previously demonstrated a bioaffinity mediated biosensing strategy through the attachment of selective capture biomolecules onto gold nanoparticle modified carbon chip surfaces [1]. Configuring such sensors, one of the challenging issues is to effectively removing non specific adsorption from undesired biomolecules. In this poster, electrochemical analysis of various blocking agents assembled on sensor surfaces were investigated and the effect of non-specific adsorption behavior on gold modified sensor chips were optimized, in particular for protein detection. References:1.F. S. Diba, S. Kim, H. J. Lee, Biosensors and Bioelectronics 72 (2015) 355-361.

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Integrated paper-based microfluidic device with electrochemical sensor using digital craft cutter and conductive pen

Veasna Soum 채희도[1] 백승휘[1] 조애리 권오선[*] 신관우[2,*]

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

Development of paper-based microfluidic analytical devices and sensors for diagnosis and environment monitoring has been very attractive since a decade, because paper, a ubiquitous and familiar organic polymer in Earth, is a good base substrate to analyze various chemical and biological specimens due to flexible, hydrophilic, printable, disposable by fire and low cost, although glass and plastics are commonly and massively used as rigid substrate for assays. Very recently active paper analytical device to manipulate digital microfluidic drops by applying the electric potential has developed becomes more and more as an advanced and integrated device so that it refers to an active paper-based microfluidic chip, simply active paper chip. However, it required many complicate processes for fabrication of not only a chip base, which is mostly actuated by electrowetting technique, but also sensors, which mostly detects electrochemically. In this report, new simpler fabrication of active paper chip with electrochemical sensor by using a computer-controlled digital craft cutter (Cricut, USA) equipped with a knife cutter and two conductive pens (Fig. 1a,b). Two conductive pens were prepared with filling very high dispersive ink made of silver nanoparticle and CNTs suspension. After printing the specific patterned electrode on paper for active paper chip, two cut-layers of Scotch tape film were attached on paper and thus the integrated microfluidic channel with electrochemical sensors were simple achieved by the digital cutter and the conductive pens (Fig. 1c,d). This manufacturing process was performed entirely on one PC consumed in a few minutes. This simple manufacturing procure of paper chip is the first time ever. Conductivity of printed Ag-pen on paper has been investigated as a function of curing temperature, showing the high printing quality. Our microfluidic device can absorb in very fast 1 cm/s and very accuracy sample volume (Fig. 1e). We demonstrated that the μPEDs are capable of quantifying the concentration of various analyses such as glucose, urine acid, triglyceride, and LDL in whole blood sample. Because it is simple, accurate, and low-cost, this technique should be useful in health care at point-of-care device. References1.P. K. Yuen and V. N. Goral, Lab Chip, 2010, 10, 384.2.Z. Nie, F. Deiss, X. Liu, O. Akbulut and G. M. Whitesides, Lab Chip, 2010, 10, 3163?3169. 3.……..

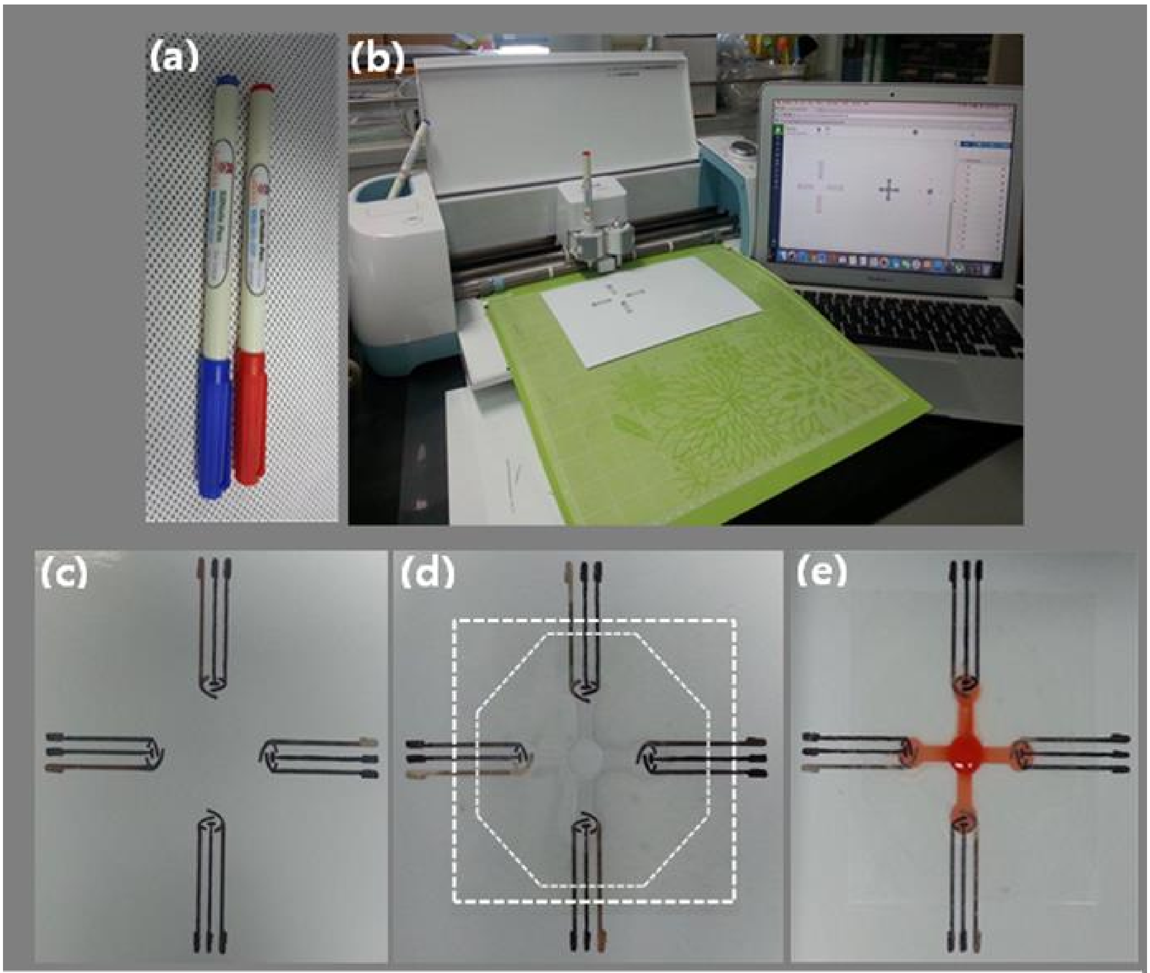

Fig. 1. (**a**) Silver (blue) and CNTs (red) conductive pen. (**b**) Co-working of digital craft cutter and conductive pen. (**c**) Multi-electrochemical sensor. (**d**) Integrated microfluidic channel with electrochemical sensors. (**e**) Sample transportation to each detecting sites.

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Superior electrocatalytic oxygen reduction in alkaline media by silver and cobalt alloyed nanoparticles grafted on sulfonated graphene

주유리 Mohammad Shamsuddin 전승원*

전남대학교 화학과

The sulfonated graphene oxide-supported silver and cobalt alloyed catalyst has been synthesized by an electrochemical reduction method (denoted as ERGO-S-AgCo) for electrocatalytic oxygen reduction reaction (ORR). The sulfur has been used as anchoring site via π-π interaction for AgCo nanoparticles (NPs). This material has been characterized by various instrumental methods. The morphological analysis shows the AgCo alloyed NPs are well set on to the thiolated graphene with better dispersion. The X-ray photoelectron spectroscopy (XPS) shows electrochemical reduction has been done successfully with the increasing of C/O ratio. Also, the X-ray diffraction (XRD) data reveals that the Co is presents with the oxidized form into AgCo alloyed NPs. The electrocatalytic activities have been verified using cyclic voltammetry (CV) and hydrodynamic voltammetry techniques in 0.1 M KOH electrolyte. The as prepared catalyst, ERGO-S-AgCo, has shown better ORR onset potential with superior mass activity which is higher than that of ERGO-AgCo. The reaction kinetics has confirmed that the ORR at ERGO-S-AgCo catalyst follows a four electron transfer reaction process.

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Direct carbonization of multiwall carbon nanotube grafted polyimide on carbon cloth for supercapacitor application

김대겸 성광동 박원철*

서울대학교 융합과학기술대학원 융합과학부

Polyimides (PIs) are widely used in the fields of microelectronics or mechanical industry due to their unique properties such as high mechanical strength, high thermal stabilities, and low dielectrics. Also as a carbon source, carbonized PIs are often used as electrode materials for electrochemical energy storage due to their high carbon yield and simple carbonization process. Carbon nanofibers produced by electro spinning PIs and further hear treatment have been studied as electrode material for supercapacitor. In this work, multiwall carbon nanotubes (MWNT) are well dispersed in polyamic acid (PAA) solution by in situ polymerization synthesis technique to form grafted structure. The MWNT grafted PAA were coated on carbon cloth surface and carbonized at various temperature conditions under inert atmosphere. Cyclic voltammetry, chronopotentiometry, and electrochemical impedance spectroscopy were measured to study the electrochemical energy storage performances for supercapacitor application.

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Simple solvothermal synthesis of $CuFe_2O_4$-graphene composite as electrode material for supercapacitor application

ZHANGWANG Jin xuanzhen 박원철*

서울대학교 융합과학기술대학원 융합과학부

In this work, we reported a facile approach to prepare a uniform copper ferrite nanoparticle-attached graphene nanosheet ($CuFe_2O_4$-GN). A one-step solvothermal method featuring the reduction of graphene oxide and formation of $CuFe_2O_4$ nanoparticles was efficient, scalable, green, and controllable. The composite nanosheet was fully characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS), which demonstrated that $CuFe_2O_4$ nanoparticles with a diameter of approximately 100 nm were densely and compactly deposited on GN. To investigate the formation mechanism of $CuFe_2O_4$-GN, we discussed in detail the effects of a series of experimental parameters, including the concentrations of the precursor, precipitation agent, stabilizer agent, and Graphene oxide on the size and morphology of the resulting products. Furthermore, the electrochemical properties of $CuFe_2O_4$-GN composite were studied by cyclic voltammetry and galvanostatic charge-discharge measurements. The composite showed high electrochemical capacitance (576.6 F/g at 1 A/g), good rate performance and cycling stability. These results demonstrated that the composite as a kind of electrode materials had a high specific capacitance and good retention. The versatile $CuFe_2O_4$-GN held great promise for application in a wide range of electrochemical fields because of the remarkable synergistic effects between $CuFe_2O_4$ nanoparticles and graphene.

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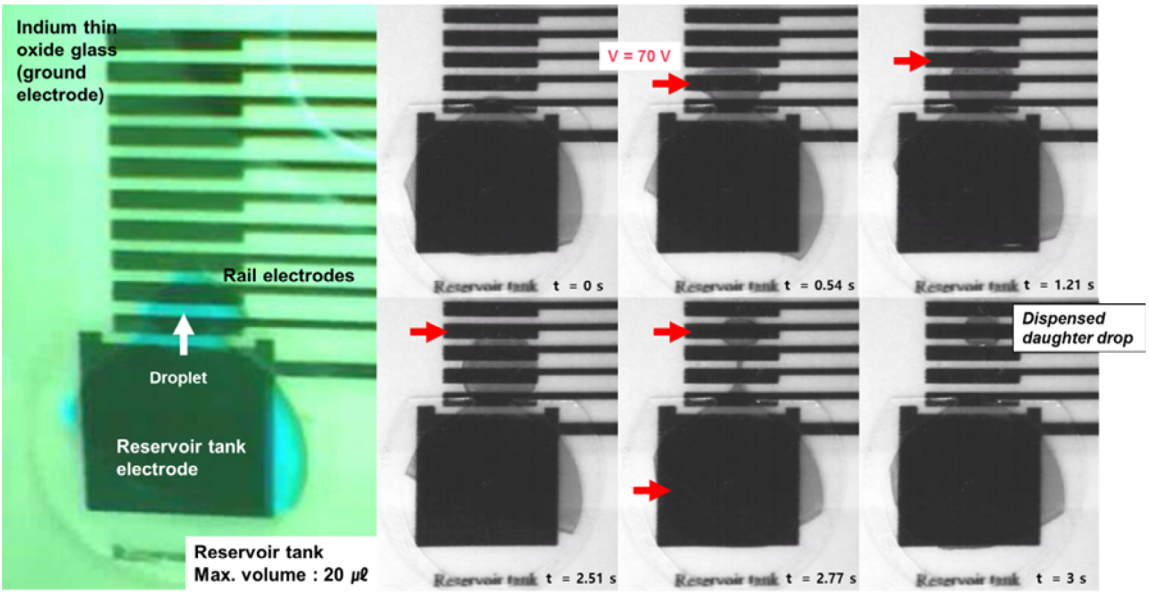
Automated on closed paper chip droplet separation and dispensing with volume control by electro-wetting actuation

백승휘 채희도 Veasna Soum[1] 유수련[2] 조애리[1] 최재학[3] 권오선[1,*] 신관우[4,*]

서강대학교 화학과 대학원 [1]서강대학교 화학과 [2]서강대학교 화학과,바이오계면연구소 [3]충남대학교 고분자공학과 [4]서강대학교 화학과 및 바이오융합과정

Controlling on-chip droplet two different types of active paper-based micro fluidic chips, open and closed, in which the drop was actively actuated by using an electrowetting phenomenon has been explored. Closed paper chip systems based on parallel-plate devices, and open paper chip systems based on single-plate devices. In case of open paper chip systems, it is possible to droplet transporting, merging and reaction that is already studied. Among the manipulations of droplet, droplet separation and dispensing phenomenon is possible only closed chip systems. It is possible to separated and dispensed droplet that can be operated in the open chip systems in continuously. In this research was the study of the materials that consist of the closed paper chip system and study for the droplet separation and dispensing phenomenon in morphologically.


Indium thin oxide glass (ground electrode)
Rail electrodes
Droplet
Reservoir tank electrode
Reservoir tank Max. volume : 20 μℓ
V = 70 V
Reservoir tank t = 0 s
Reservoir tank t = 0.54 s
Reservoir tank t = 1.21 s
Dispensed daughter drop
Reservoir tank t = 2.51 s
Reservoir tank t = 2.77 s
Reservoir tank t = 3 s

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Real-time detection of nitric oxide generated from plasma using a perfluorinated xerogel-derived amperometric microsensor

신소민 이진선 최경훈[1] 양현희 박민지 박봉주[2] 신재호*

광운대학교 화학과 [1]광운대학교 플라즈마바이오과학센터 [2]광운대학교 전자바이오물리학과

A contact dielectric barrier discharges (DBD) plasma has recently been employed in emerging novel biomedical applications, including bacterial decontamination and chronic wound treatment. Such antimicrobial and healing efficacies may be related to the formation of reactive oxygen and nitrogen species (ROS and RNS; e.g., OH·, O2·?, NO, ONOO·?, and H2O2) by plasma exposure. Among several reactive species, nitric oxide (NO) has been extensively studied due to its phagocytic and antithrombotic activities, and angiogenic property. In order to treat the plasma to the skin for the purpose of chronic wound treatment, Rather than direct treatment of plasma, it is necessary indirect treatment. For these reasons, after it has been placed on the wound by introducing the hydrogel, it was treated with plasma. However, studies on NO generation via plasma treatment in biological milieu have been hindered due to no appropriate method for the measurement of NO. Herein we employ an electrochemical NO sensor to measure NO concentration generated by a contact DBD plasma in hydrogel. The working Pt electrode is modified with perfluorinated xerogel membrane to improve sensor's selectivities over readily oxidizable interfering species and other ROS and RNS produced during plasma radiation. Furthermore, direct, real-time detection of NO generated in hydrogel by plasma treatment will be performed by using an NO-sensing microelectrode (a conical tip size =

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Perfluorooctyltriethoxysilane Functionalized Graphene Oxide as a Corrosion Inhibitor Coating on AZ-31 Magnesium Alloy

IKHE AMOL BHAIRUBA 표명호*

순천대학교 인쇄전자공학과

AZ-31 magnesium alloy is one of the lightest materials which has attracted considerable interest in applications to aerospace and electronics for its excellent properties, such as low density, high ductility, and high specific strength. However, AZ-31 Mg alloy is vulnerable to corrosion under ambient conditions, limiting its widespread usage. Various methods gave been exploited to protect the Mg surface from corrosion. Organic coating which is a very simple and effective method, has also been extensively studied to reach this goal. In some examples, noticeable results by polymer coating have been reported, but there still remains a wide room for further improvement, when compared with commercially utilized chromate coating. In this work, we report the synthesis and corrosion protection of perfluorooctyltriethoxysilane (PFOTS) functionalized GO (PFOTS/GO). A simple one step method was used for the synthesis of PFOTS/GO, which was then chemically reduced to produce PFOTS/reduced GO (PFOTS/rGO). The PFOTS/rGO was coated on the Mg alloy by spin-coating or dip-coating with a dispersion of the same in a suitable organic solvent. The high surface area of rGO provides superior coverage, allowing minimal consumption of PFOTS/rGO for effective coating. The hydrophobic property of the PFOTS/rGO promotes the corrosion inhibition property greatly. In contrast to bare AZ-31 Mg alloy, the PFOTS/rGO-coated AZ-31 Mg alloy exhibited a significant increase of the impedance in the electrochemical impedance spectroscopy and a substantial positive shift of the Ecorr (in 3.5 wt% NaCl solution) in potentiodynamic polarization measurements. Preliminary studies showed that thermally reduced GO-coated AZ-31 Mg alloy to exhibit reasonably good corrosion inhibition behavior. We believe that the synergy between the hydrophobic nature of PFOTS and corrosion inhibition property of rGO can enhance the corrosion inhibition phenomenon. The hydrophobic PFOTS/rGO and simplicity in coating present a

practically cost-effective procedure for the efficient corrosion inhibition of AZ-31 Mg alloy in 3.5 wt% NaCl solution.

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Graphene oxide with intercalated Cationic fullerene for supercapacitors applications

<u>KRISHNAN SENTHILKUMAR</u> S.J. Richard Prabakar 표명호*

순천대학교 인쇄전자공학과

Supercapacitors, with promising high power densities and long cycle life, have attracted considerable attention due to their widespread applications in electric vehicles and high power appliances. Currently, carbon based porous materials such as activated carbon, activated carbon fibers, carbon aerogels, graphene, etc., are popularly used as electrode materials for supercapacitor applications. Graphene oxide (GO), an intermediate in the graphene synthesis from graphite, laden with oxygen functionalities behaves much like the quinone/hydroquinone redox switching process and has been exploited as a pseudocapacitor [1]. However, the inevitable partial stacking occurring in GO, reduce surface area exposure to the electrolyte, thus substantially affecting the pseudocapacitive response.In the present work, we present a new strategy to prepare a cationic fullerene (CFU) intercalated graphene oxide (GO-CFU) composite. In an aqueous solution, positively charged CFU was electrostatically aligned with oppositely charged GO. The CFU behaving as a spacer between GO layers, suppress the GO stacking and expose basal plane oxygen functionalities with electrolyte more effectively. XRD analysis of GO-CFU shows that the (001) and (002) plane of GO is shifted negatively (by 2Θ of 1 and 1.2°, respectively) which validates the intercalation of CFU into GO layers. Preliminary studies with the GO-CFU composite as a supercapacitor electrode material revealed a noticeable 5 fold increase in capacitance in contrast to GO. Further study is underway to optimize the ratio of GO/CFU to arrive at the best response. Reference[1]B. Xu, S. Yue, Z. Sui, X. Zhang, S. Hou, G. Cao, and Y. Yang, “What is the choice for supercapacitors: graphene or graphene oxide?,” Energy Environ. Sci., vol. 4, no. 8, p. 2826, Aug. 2011.

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Rational Syntheses of Pt Nanoparticles Supported on Titanium Carbide and Their Electrocatalytic Performance

박현욱 이은직[1] 김근오 권영욱*

성균관대학교 화학과 [1]성균관대학교 나노과학기술협동학부

In this study, we report the ultrasound-assisted polyol synthesis (UPS) of well-dispersed Pt nanoparticles (NPs) on Titanium Carbide (TiC) and their electrochemical performance for Methanol Oxidation Reaction (MOR) and Oxygen Reduction Reaction (ORR). In order to prepare Pt/TiC samples, metal precursors and TiC were dispersed in ethylene glycol and irradiated by ultrasound for 3 h. Through the structural analyses of Pt/TiC, we found that samples have uniform particle size (4~5 nm) and well-dispersed Pt NPs on TiC. Electrochemical performance of samples was investigated by rotating disk electrode (RDE) measurement. Compared with commercial Pt/C and Pt/TiC showed the enhanced ORR and MOR activity in acid media. In conclusion, we demonstrated that the strong metal-support interaction (SMSI) effect between Pt and TiC leads the enhanced electrocatalytic performance and durability.

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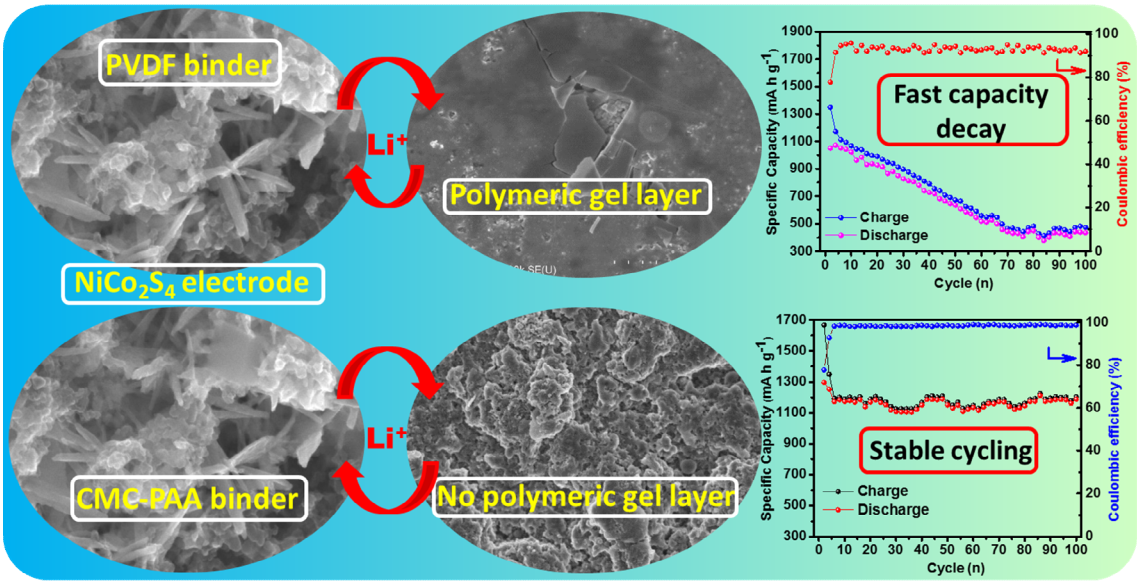
High Capacity and Outstanding Cycling Stability of Ternary $NiCo_2S_4$ Nanorods as Li ion Battery Anode

dhrubajyoti bhattach **SINHAMAHAPATRA APURBA**[1] **유종성**[2,*]

고려대학교 화학 [1]*대구경북과학기술원(DGIST) 에너지시스템공학전공* [2]*대구경북과학기술원(DGIST) 에너지시스템공학과*

Formation of polymeric gel passivation layer over electrode surface has a lethal effect on the rate and cycling performance of metal sulfide-based Li ion battery anode. Herein, it is demonstrated that a composite binder consisting carboxymethyl cellulose and polyacrylamide can substantially suppress or restrict the formation of this insulating layer. Ternary spinel $NiCo_2S_4$ nanorods are tested for the first time as anode electrode for Li ion battery using this novel composite binder and found to show not only high specific capacity but also extraordinary rate performance and cyclic stability with almost no capacity decay upt0 100 charge-discharge cycles because of restriction in the formation of polymeric passivation layer.


PVDF binder
Li+
Polymeric gel layer
$NiCo_2S_4$ electrode
Fast capacity decay
Specific Capacity (mA h g-1)
Coulombic efficiency (%)
Charge
Discharge
Cycle (n)
CMC-PAA binder
Li+
No polymeric gel layer
Stable cycling
Specific Capacity (mA h g-1)
Coulombic efficiency (%)
Charge
Discharge
Cycle (n)

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Effect of 4-biphenylacetonitrile as electrolyte additive in high voltage Lithium ion battery

송지겸 이경구*

군산대학교 화학과

4-biphenylacetonitrile is used as an electrolyte additive to improve the cycling performance of high voltage (~4.9V) lithium-ion battery. The electrochemical behaviors and surface chemistry of LiNi0.5Mn1.5O4 are investigated via Linear Sweep Voltammetry (LSV), Cyclic Voltammetry (CV), charge?discharge test, X-ray photoelectron spectroscopy (XPS), field emission selective electro measurement (SEM), transmission electron microscopy (TEM) and electro impedance spectroscopy (EIS). It is found that the cycling performance of the cell Li/LiNi0.5Mn1.5O4, using an electrolyte of 1.0 M LiPF6 in ethylene carbonate(EC) / dimethyl carbonate (DMC) / ethylmethyl carbonate (EMC) (1/1/1, in volume), can be improved by adding 4-biphenylacetonitrile into the electrolyte. Electrochemical measurements and SEM, TEM, XPS analyses show that a protective film is formed on LiNi0.5Mn1.5O4 when 4-biphenylacetonitrile is used, which contributes to the cycling performance improvement of the cell.

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Iron-polypyrrole electrocatalyst with high activity and stability for the oxygen reduction reaction in both alkaline and acidic conditions

TRAN THANH NHAN **송민영[1] SINGHKIRANPAL[2] 양대수[1] 유종성[1,*]**

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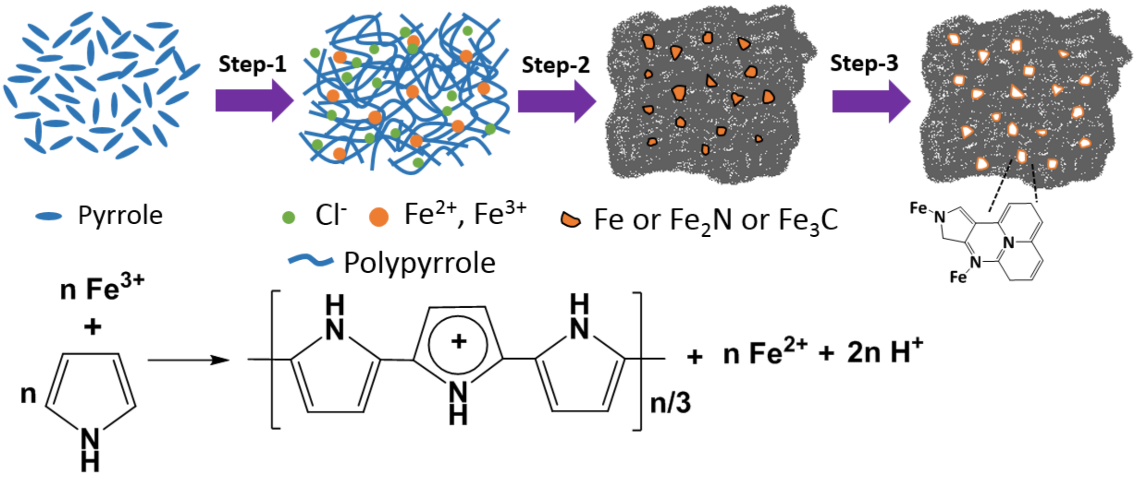
Herein we present a facile template-free method to synthesize a new non-noble metal carbon catalyst for oxygen reduction reaction (ORR) by pyrolizing polypyrrole in presence of ferric source, which interestingly serves dual purpose of an oxidant for pyrrole polymerization and an iron source. It is found that as-prepared catalyst exhibits high catalytic activity for ORR in both alkaline and acidic conditions. The catalyst prepared at pyrolysis temperature of 900 °C (FePPy-900) shows exceptionally high ORR activity with onset potential of -14 mV, which is similar to that of Pt/C, whereas the half-wave potential ($E_{1/2}$) of FePPy-900 is -98 mV, which is more positive than that of Pt/C at the same catalyst loading amount in alkaline condition. Furthermore, the FePPy-900 catalyst also illustrates exceptionally high ORR activity in acidic condition with onset potential and haft wave potential of 606 mV and 523 mV, respectively, which are almost comparable with those (610 mV and 503mV) of state of the art Pt/C catalyst, demonstrating remarkable high ORR activity in both alkaline and acid media despite relatively low surface area. In addition, the FePPy-900 catalyst displays much better stability and methanol tolerance than Pt/C and exhibits four electron transfer pathway in both alkaline and acidic conditions.


Step-1
Step-2
Step-3
Pyrrole
Cl-
Fe2+, Fe3+
Polypyrrole
Fe or Fe2N or Fe3C
Fe
N
N
Fe
N
n Fe3+
+
n
N
H
H
N
+
N
H
H
N
n/3
+ n Fe2+ + 2n H+

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Development of a large scale microbial electrolysis cell using copper oxide coated with MoS_2 photocathode

전용원 구경민[1] 김성현[2,*]

건국대학교 생명공학과 [1]건국대학교 생명특성화대학 특성화학부 [2]건국대학교 특성화학부생명공학과

A microbial electrolysis cell (MEC) is promising green energy technology for producing hydrogen because of its sustainability. By the application of small external voltage, hydrogen can be produced at the cathode from the oxidation of organic substances by bacteria at the anode. A lot of efforts have been poured to effectively produce hydrogen minimizing methane production as small as possible. Here we show that p-type semiconductor copper oxide is able to effectively reduce protons to hydrogen molecules under visible light irradiation. A major problem is that copper oxide is easily corroded when operated long time. To solve this problem, we developed a simple method which was to coat the copper oxide surface with MoS_2 particles that can serve as a protecting layer and proton reduction catalyst. We constructed a 550 mL MEC cell and tested it for more than 1000 h. We observed a constant H_2 production at rate of 1.29 m^3 H_2 /m^3/day with an energy efficiency of 118.3 % when 0.8 V was applied under visible light irradiation from LED whose intensity was 17 mW/cm^2. Virtually no methane with H_2 purity of 99.5 % was produced when operated in a continuous batch mode at 30 °C. COD removal was ca. 91.5 % at the end of operation.

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Joint Effects of Photoactive TiO2 and Fluoride-Doping on SnO2 Inverse Opal Nanoarchitecture for Solar Water Splitting

윤건 강순형*

전남대학교 화학교육과

Nowadays, the exploration of new photoelectrode architectures to improve the light-harvesting and charge-collection properties of photoelectrochemical cells and related devices have been regarded as a challenging work. Here, we synthesized the inverse opal SnO2 for photoelectrochemical water splitting by the spin-coating method exploring the polystyrene beads with a size of approximately 350 nm. The SnO2 inverse opal structure shows the photonic crystal effect with a well-ordered hexagonal structure packing. Upon this film, the photoactive TiO2 layer with various thicknesses from 10 nm to 40 nm was deposited by atomic layer deposition. Herein, it is expected that an optimal TiO2 layer takes part in a role as a photoactive material. Adding to these results, the F doping on the SnO2 inverse opal film was also examined with the TiO2 layers. These results were confirmed using Field-emission scanning electron microscopy, X-ray diffraction and ultraviolet-visible spectrophotometer. Detail results and discussion would be presented.

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Visible Light Absorbing TiO2 Nanotube Arrays by Sulfur Treatment for Photoelectrochemical Water Splitting

윤건 강순형*

전남대학교 화학교육과

Herein, we report the preparation and characterizations of the sulfur (S)-doped TiO2 nanotube (TONT) arrays prepared by a sulfurization process of TONT arrays via electrochemical anodization on a Ti substrate with a pure TONT arrays The S-doped TONT arrays were prepared with the annealing temperature from 450 ºC to 550 ºC under H2S gas for 10 min, and these reaction conditions corresponded to no modification of the morphological features relative to that of the TONT arrays. Furthermore, the 500 ºC annealed S-doped TONT arrays showed enhanced visible light absorption and high electric conductivity, thus resulting in the most improved photocurrent density (2.92 mA cm-2 at 1.0 V vs sat. Ag/AgCl) in the 0.1 M KOH solution as compared with that (0.965 mA cm-2 at 1.0 V vs sat. Ag/AgCl) of TONT arrays. Furthermore, the incident photon-to-electron conversion efficiency (IPCE) of the S-doped TONT arrays exhibited approximately 43% in the UV region whereas the TONT arrays had 32% IPCE in the UV region. In addition, the small photoactivity in the visible light region for the S-doped TONT arrays was observed up to a 600-nm wavelength, where the IPCE value of 2.4% at 500 nm was achieved in the S-doped TONT arrays, in contrast to the negligible IPCE values for the TONT arrays. However, the relatively reduced photocurrent density (2.04 mA cm-2 at 1.0 V vs sat.Ag/AgCl) was achieved at further sulfurization temperature at 550 °C for the S-doped TONT arrays; this value is attributed to the rough tube shape and atomic level defects in the edge region for the excessively S-doped TONT array, which indicated a role as the light scattering centers and the electron-hole trap sites.

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Synthesis and Characterization of bio-compatible semi-IPNs PANI/PAAM hydrogel for electrochemical capacitor

문미미 조보배 유국현*

동국대학교 화학과

Mostly, Electrolyte was liquid phase, but it has problem such as the water leak. To overcome this obstacle, solid state electrolyte which has highly stability and safety is currently being studied.In this study, a Semi-interpenetrating networks (Semi-IPNs) hydrogel was synthesized with Polyaniline(PANI) having a high electric conductivity and Polyacrylamide(PAAM) for usage as electrolyte and electrode material.The hydrogel has elastic and bio-compatible properties.Semi-IPNs hydrogel are composited of PANI entrapped within the network of PAAM. The structure and morphological properties was characterized by SEM, IR, Swelling ratio analysis. Semi-IPNs PANI/PAAM hydrogel is expected to apply a biocompatible electric capacitor because PAAM is biomaterial.

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Synthesis and Electrochemical Characterization of Silver Ion Treated Electrospun Cobalt Nanotubes

유아름 김명화[1] 이종목 이영미[*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

Recently much attention has been paid to one-dimensional (1D) nanostructures. One of the most promising method to prepare 1D nanostructures is electrospinning. Electrospinning has gained much attention due to not only its diversity of the electrospinning materials but also its simplicity. In this study, we prepare Co nanotubes by electrospinning, followed by calcination and reduction. AgCo nanotubes are synthesized through the galvanic replacement reactions (GRR) between Co nanotubes and Ag precursor in aqueous solution and characterized electrochemically. In order to optimize the synthetic condition for AgCo nanotubes, we control the reduction time of Co_3O_4 nanotubes and the GRR time between Co nanotubes and Ag precursor.The morphologies and compositions of the prepared AgCo nanotubes are characterized by field-emission scanning electron microscopy, transmission electron microscopy, X-ray diffraction and X-ray photoelectron spectroscopy. For the electrochemical characterization, three-electrode cell is used with a glassy carbon electrode loaded with the synthesized AgCo nanotubes as the working electrode and a saturated calomel electrode (SCE) as the reference electrode, and a coiled platinum wire as the counter electrode. Electrochemical activities of these nanomaterials for oxygen reduction reaction (ORR) are characterized with rotating disk electrode (RDE) voltammetry in 0.1 M NaOH aqueous solution. The ORR catalytic activity of AgCo nanotubes is compared with the ones of Ag nanowires and Co nanotubes.This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (2014R1A2A2A05003769).

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Synthesis and Characterization of Electrospun Cobalt-Nickel Nanotube and Studies of its Electrochemical Properties

이혜림 유아름 김명화[1] 이영미 이종목*

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

Electrospinning technique recently has been attracted because it is simple, versatile and low cost method to construct variety of nanostructures. In this study, we prepared Co-Ni nanotubes by electrospinning followed by calcination. We synthesized Co-Ni nanotubes with various ratio of Co precursor and Ni precursor to compare morphologies and electrochemical properties.The morphologies and compositions were characterized by field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD). For electrochemical measurements, three-electrodes were used with a glassy carbon electrode loaded with the synthesized nanotubes as a working electrode, a Pt wire as a counter electrode, and saturated calomel electrode as a reference electrode. To estimate the catalytic activities toward oxygen reduction and capacitive behaviors of Co-Ni nanotubes, we used cyclic voltammetry, rotating disk electrode voltammetry, and electrochemical impedance spectroscopy.

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Amperometric Dual Microsensor for Simultaneous Measurements of Glucose and Oxygen

박근아 이종목[1] 이영미[1,*]

이화여자대학교 화학나노과학 [1]이화여자대학교 화학나노과학과

Glucose is primary energy source of physiological metabolism and oxygen (O_2) is also consumed in this process. Therefore, real-time simultaneous detection of these materials in vitro/vivo is valuable in medical and biological sciences. In this study, we demonstrate the development of an amperometric glucose/O_2 dual microsensor which can measure these materials simultaneously, and the analytical performances of this dual sensor, such as selectivity, sensitivity, response time, are characterized. The sensor is made of dual platinum (Pt) disk working electrodes (each dia. = 25 μm), SCE as the reference electrode, and Pt wire as the counter electrode. The dual working electrode is fabricated using simple Pt microwire and etched/sharp Pt microwire. Both Pt microdisks are electrochemically etched to form a recessed micropore for O_2 sensing and a truncated cone-shaped micropore for glucose sensing. Both micropores are filled with porous Pt layers via electrodeposition of Pt from Pt precursor solution. The surface of O_2 sensing electrode is silanized for selectivity to O_2. On the other hand, the truncated cone-shaped Pt electrode is used as a non-enzymatic glucose sensor to measure the glucose levels with high spatial and temporal resolution. This unique tapered pore shaped structure provides sufficient selectivity to glucose over typical interfering species such as AA and AP without any additional membrane. The sensitivity and selectivity of the dual sensor show the feasibility and suitability 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 Science, ICT& Future Planning (2014R1A2A2A05003769).

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An Effective Method to Synthesize a Metal oxide-Graphene Nanocomposite for Supercapacitor Application

장우리 이연식 구혜영[1,*]

전북대학교 화학공학부 [1]한국과학기술연구원(KIST) 전북분원 복합소재기술연구소

With increasing demand for sustainable and renewable power sources in modern electronic industries,supercapacitors have attracted tremendous attention because of their high power density, excellent pulse charge-discharge characteristics, long cycling life and safe operation. Up to now, various materials, including carbonaceous materials, conducting polymers, transition metal oxides/hydroxides, and hybrid composite, have been widely investigated as electrodes for supercapacitors. Graphene is an excellent substrate to host active nanomaterials for energy applications due to its high conductivity, large surface area, flexibility, and chemical stability.Among the transition metal oxides, manganese oxides is regarded as a promising electrode material for supercapacitors due to its environmental compatibility, low cost and abundant availability. Therefore, the combination of Manganese oxide and graphene seems to be a promising attempt to achieve a possible synergic effect to improve the performances of graphene-based supercapacitors.Herein, we simply synthesized reduced Graphene oxide/ manganese oxide nanocomposite by a controlled thermal decomposition of metal oxalates with regular morphologies for high-power supercapacitor electrodes.The electrochemical properties of the composites as potential electrode materials for supercapacitors were investigated using different electrochemical techniques including cyclic voltammetry (CV), galvanostatic charge?discharge. The reduced Graphene oxide/ manganese oxide nanocomposite were used as a supercapacitor electrode. The specific capacitance in a three-electrode system was 2460 F/g at a current density of 1 A/g with capacitance retention of 95% after 3000 cycles.

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Electrochemical detection of Hydrogen Peroxide using an improved nanobiointerface with catalase/CdTe quantum dots

최인녕 이용일*

창원대학교 화학과

Hydrogen peroxide detection is immense value in various fields including food, pharmaceuticals, bleaching and sterilization industries. Hence significant amount of efforts are put in towards its sensitive and selective identification. Though various methods namely ESR, chemiluminescence, spectrophotometry, chromatography, fluorescence and titrimetry are used widely but they possess several demerits. To rectify these deficits and provide available platform the rescue came in the form of electrochemical methods. Researchers put their valuable efforts initially without any interface and later with bulk interfaces. Compared to these materials the nanointerfaces play a predominant role for improving the selectivity and sensitivity. In the similar platform we have attempted the electrochemical detection of hydrogen peroxide using catalase enzyme and quantum dots as a nanointerface. Primarily quantum dots are characterized using Fourier transform infrared spectroscopy(FT-IR), Field Emission Scanning Electron Microscopy(FE-SEM) and photoluminescence(PL) for the evaluation of their characterization and morphology. Then electrochemical studies were carried out using cyclic voltammetry technique. Typical sensor parameters namely the linearity, response time, sensitivity, interference effect, reproducibility and stability were analyzed. The experimental results are found to be satisfactory with the earlier reports. This can be quite useful in the determination of hydrogen peroxide in blood serum samples which can serve as a biomarker for many of the oxidative stress related diseases.Key words: CdTe quantum dots; catalase; hydrogen peroxide; electrochemical; cyclic voltammetry.

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Electrodeposition of Iridium on Glassy Carbon for Nonenzymatic Ascorbic Acid Detection

김현영 조아라 이영미* 이종목*

이화여자대학교 화학나노과학과

In this presentation, we demonstrated the electrodeposition of iridium nanoparticles (Ir NPs) and its electrochemical properties. The Ir NPs were prepared by simple electrodeposition method via a reduction of iridium(Ⅲ) on a glass carbon (GC) electrode. The structure of Ir NPs was characterized by field emission scanning electron microscopy (FE-SEM) and energy dispersive X-ray spectroscopy (EDS). The SEM images showed the Ir NPs have reverse micelle structure with 100 nm scale. The electrochemical activity of the Ir NPs was measured by CHI-750D and the experiments were all conducted in 0.1 M phosphate buffer solution (PBS, pH 7.4). The Ir NPs exhibited the possibility of an amperometric biosensor for ascorbic acid (AA) with selectivity against possible interferents, acetamidophenol (AP), uric acid (UA), dopamine (DA), and glucose. The applied potential for AA oxidation was determined by linear sweep voltammetry (LSV).

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In-situ growth of Prussian blue nanocubes and RGO/Prussian blue/Pt nanocomposite as an active electrocatalyst for methanol oxidation

강인학 **Shanmugam Manivannan*** 김규원*

인천대학교 화학과

Herein, we report a facile synthetic strategy for the in-situ growth of high-quality Prussian blue nanocubes (PBNCs) onto the amine functionalized silicate sol-gel matrix (TPDT)-RGO films through the electrostatic interaction. Subsequently, Pt nanostructures are electrodeposited onto the preformed ITO/TPDT-RGO-PB electrode to prepare the RGO/PB/Pt nanocomposite electrode. The importance of this method is that the PBNCs could be in-situ grown on the surface of the RGO. The modified electrodes are characterized by FE-SEM, EDAX, XRD, XPS and electrochemical techniques. The RGO/PB/Pt nanocomposite exhibits the synergistic electrocatalytic activity and high stability towards the methanol oxidation. The porous nature of the TPDT matrix and unique electron transfer mediating behavior of PBNCs integrated with RGO in the presence of Pt nanostructures facilitated synergistic electrocatalytic activity for methanol oxidation.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Optimization of pulling condition of M13 phage for use as sensor platform

서예지 김규원*

인천대학교 화학과

M13 phage composed of five coat proteins like pVIII, pIII, pVI, pIX and pVII proteins. Using amine functional group of M13 phage coat protein as linker, we try to fabricate the sensor. In order to know how many expose amine functional group of M13 phage coat protein on electrode according to pulling rate and M13 phage solution concentration, gold electrode modified M13 phage using pulling method. After, conjugate the electrochemical active molecule to amine functional group of M13 phage coat proteins. Then confirm to exposure amount of the amine group of the M13 phage coat protein through the electrochemical detection.In this contribution, we present optimized condition of the M13 phage pulling, and investigated whether the primary amine of M13 phage coat protein can use for the sensor.

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장소: 대구 EXCO
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발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synergistic electrochemical biosensor utilizing supramolecular association of enzyme on sol-gel matrix embedded gold nanoparticles supported reduced graphene oxide-cyclodextrin nanocomposite

Shanmugam Manivannan 김규원*

인천대학교 화학과

Herein we present β-cyclodextrin (CD) attached reduced graphene oxide (RGO) nanosheets supported on the silicate sol-gel matrix embedded gold nanoparticles (Au NPs) modified electrode surface as a new affinity binding nanocomposite. Modified electrode is fabricated through the layer-by-layer drop casting followed by the immobilization of the chemically modified enzyme (HRP-ADA). This affinity system is based on the supramolecular association between the CDs and HRP-ADA is mimicking the biological avidin-biotin interactions. The cavity of the CD attached at the RGO surface (RGO-CD) functions as a macro cyclic host to form stable supramolecular inclusion complexes with enzyme conjugate. The silicate sol-gel matrix embedded Au NPs has improved the interfacial interaction with the RGO-CD nanosheets at the electrode surface and thus exhibits the synergistic electrocatalytic effect towards the H2O2 in the presence of 1 mM Hydroquinone when compared to the individual electrocatalytic effects of Au NPs and RGO-CD nanosheets, respectively.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Surface attached β-cyclodextrins controlled growth of 3D gold dendrites on reduced graphene oxide sheets and its electrocatalytic studies

Shanmugam Manivannan 김규원*

인천대학교 화학과

In this study, 3D gold dendritic nanostructures (Au-DNs) with multi-branched architectures are grown by electrodeposition at the reduced graphene oxide (RGO) nanosheets functionalized with β-cyclodextrins (CD). The structural features of the Au-DNs and their interfacing mechanism with RGO are characterized by UV-Visible, FESEM, EDX, XPS, XRD and Raman analysis. The study revealed that the morphology of the Au-DNs strongly depends on the CD functionalized on RGO CD (RGO-CD) and experimental parameter such as electrodeposition time and ad layer of ammine functionalized silicate sol-gel matrix (TPDT) used for RGO attachment at the ITO electrode surface. CDs functionalized on the RGO surface played unique role to obtain the Au dendrites growth at the RGO surface by electrodeposition. The electrochemical studies showed that the Au-DNs exhibited synergistic catalytic activity towards the nitrite and glucose electrooxidation.

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발표분야: 전기화학
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Cobalt Sulfide Nanocages from Prussian Blue Analogues as a Platinum Alternative Electrocatalyst for Dye-Sensitized Solar Cells

김민수 방진호[1,*]

한양대학교 바이오나노학과 [1]한양대학교 바이오나노학과, 응용화학과

As a next-generation solar cell, dye-sensitized solar cells (DSSCs) have received great attention for decades. One of the issues to be addressed is the use of high-cost Pt electrocatalyst for counter electrode. In this work, we devise a novel approach to prepare cobalt sulfides with exotic compositions and a nanostructure using Prussian blue analogues. Electrocatalytic activity of cobalt sulfides is governed by compositions and crystal structures. In particular, a hollow cobalt sulphide nanocage with mixed compositions (CoS1.097/Co3S4) exhibits a high catalytic activity when used as a counter electrode. We are capable of obtaining a higher efficiency of 8.49% as compared to Pt CE (7.40%), and in-depth electrochemical investigation reveals the origin of the electrocatalytic activity of this new electrocatalyst.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High-Performance Water Electrolysis by Cobalt Disulfide on Carbon Fiber Paper Substrate

김지연 방진호[1,*]

한양대학교 바이오나노학과 [1]한양대학교 바이오나노학과, 응용화학과

Dihydrogen holds great promise as an alternative energy carrier in the near future. Water electrolysis has been considered to be one of the main routes to produce dihydrogen without fossil fuels. There are several hurdles to be overcome, one of which is the use of platinum (Pt) as an electrocatalyst. Extensive effort has been devoted to replacing Pt catalyst with earth-abundant materials in recent years. In this work, cobalt disulfide on carbon fiber paper (CFP) is prepared and evaluated as an alternative electrocatalyst. Our study reveals that cobalt disulfide and CFP work together to provide a high catalytic activity for hydrogen evolution reaction. In-depth characterization combined with electrochemical study provide new insights into this interesting synergistic effect, which is attributed to a gradual activation by defects on carbon surface.

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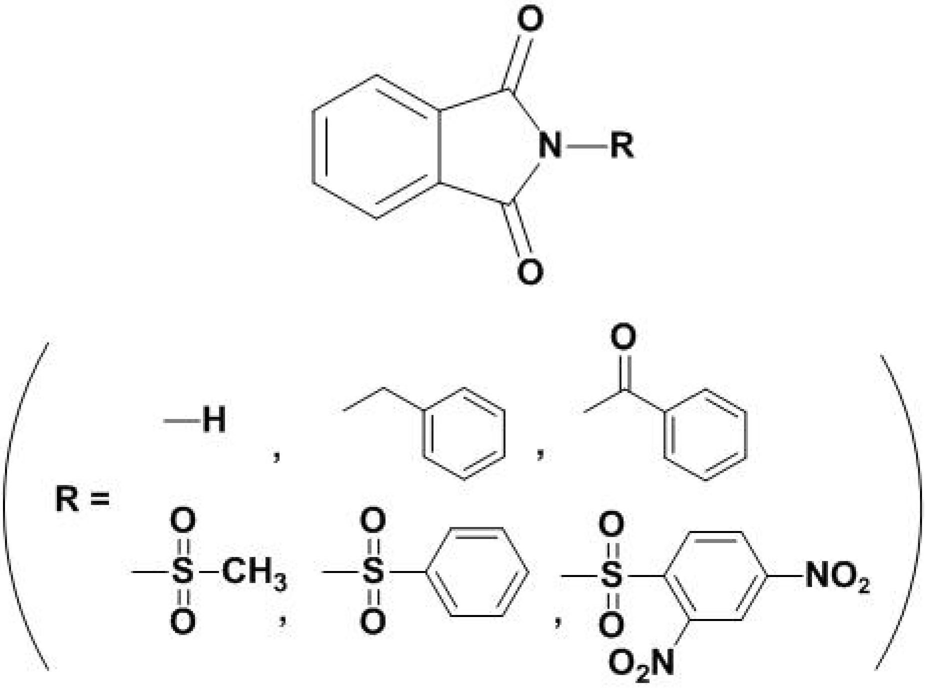
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The Convenient Preparation of Phthalimide Derivatives as High Energy Density Organic Electrolyte: Application for Redox Flow Battery

곽현주 팽다슬 안철진*

창원대학교 화학과

Redox flow battery (RFB) represents a type of electrochemical energy storage devices. It is necessary to improve the energy density in RFB system. In this paper, We prepared Phthalimide derivatives as high energy density electrolyte, which investigated the electric effects through the CV.



대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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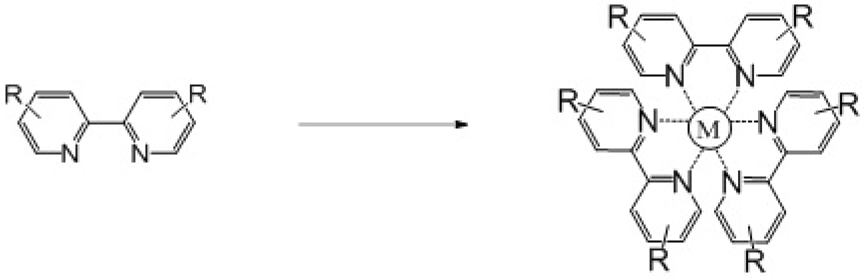
발표코드: **ELEC.P-560**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The Preparation of Bipyridine Ligand and 1,4-Benzoquinone Derivatives as High Density Electrolyte: Application of Redox Flow Battery

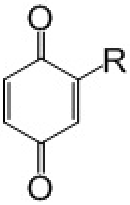
김은선 김지연 안철진*

창원대학교 화학과

Redox flow battery is a type of electrochemical energy storage device. It is necessary to prepare the high density of electrolyte to improve the voltage. To improve the energy density, we prepared bipyridine ligand and 1,4-benzoquinone derivatives as organic electrolyte. In this paper, we will present the preparation of bipyridine ligand and 1,4-benzoquinone derivatives and the tendency of CV(Cyclic Voltammetry) depending on various functional group.



[R= COOH, COOEt, NO_2, NH_2]



[R= H, CH_3, Cl, N_3]

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **ELEC.P-561**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

WO3/FeOOH Compostie for Photoelectrochemical Water Oxidation

남기민* 서종혁 장규연[1] 박기상

목포대학교 화학과 [1]목포대학교 화학화

Collecting and storing solar energy in chemical bonds, as nature accomplishes through photosynthesis, is a highly desirable approach to solving the energy challenge. The most popular strategy is photoelectrochemical (PEC) water splitting to produce hydrogen sustainably. A composite structure was prepared using WO3 (2.8 eV band gap) and FeOOH nanorod. The composite shows enhanced photocurrent under full UV-visible illumination. The hole generation at the WO3 easily transfer to FeOOH which is an important role in the enhancement of the photocurrent.

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발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Preparation BiVO4/FeOOH Composite for Photoelectrochemical Water Oxidation

남기민* 주은진 박기상

목포대학교 화학과

Photocatalysis is a light-driven chemical process over the surface of a semiconductor that can produce hydrogen from water. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary co-catalyst that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through catalysts. To investigate the effect of catalyst on BiVO4 (band gap: 2.4 eV), a layered structure was prepared using FeOOH catalysts. The synthesis and characterization of the semiconductor electrodes and the effect of co-catalyst layers on the photoelectrochemical performance are discussed in detail.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **ELEC.P-563**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Solar water splitting with organic metal halide perovskite photoanode

<u>Hoang minh tam</u> 한지훈 오일환*

금오공과대학교 응용화학과

In the race of using solar energy, perovskite solar cells have attracted interests by dint of its breakthrough improvement in power conversion efficiency to nearly 20% within several years. However, application of organic metal halide (OMH) perovskites in photoelectrolysis of water for energy storage has not been placed in proper care due to their low stability. Herein, we report a photoelectrochemical water oxidation using OMH perovskite materials as both the light absorber and energy converter. Perovskite-based photoanodes not only yielded a high photovoltage and current output but also exhibited a substantial stability for as long as hundreds of seconds, which is a very positive sign in applications of perovskites. Furthermore, we are developing new perovskite-like materials with higher stability and more suitable band gap for water splitting. This will pave the way for perovskites to find more application in the solar energy.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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장소: 대구 EXCO
발표코드: **ELEC.P-564**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Photoelectrochemical Hydrogen Production using Inverted Perovskite Solar Cell

한지훈 **Hoang minh tam** 오일환*

금오공과대학교 응용화학과

Solar water splitting based on organic metal halide (OMG) perovskite materials is reported. Conventional perovskite solar cell structure consists of electron transport material (ETM)/perovskite/ hole transport material (HTM)/ metal electrode. In this configuration, the perovskite electrode functions as photoanode and can be oxidized and easily damaged in harsh oxidative environment. On the other hand, the inverted configuration functions as photocathode and provide more benign reductive environment. Here, we fabricate perovskite-based photocathode consisting of HTM/ perovskite/ ETM/ catalyst, which provides highly stable photoelectrode for solar water splitting.

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장소: 대구 EXCO
발표코드: **EDEC.P-522**
발표분야: 초중등교사·화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

'분자운동과 상태변화' 단원에 나타난 시각자료 효과성 연구- 2009 개정 교육과정 7학년 과학교과서를 대상으로 -Effectiveness of Visual Resources Illustrated in the Unit 'Molecular Motion and Change of State'- Focused on 7th Grade Science Textbooks -

한옥희 박종근[1,*]

경상대학교 화학교육 [1]경상대학교 화학교육과

본 연구는 2009 개정 교육과정 7 학년의 화학 단원에 제시된 시각자료가 학습에 적절한 효과성을 나타내는지 확인해보고자 9 종 과학 교과서를 분석하고, 학생의 시각자료에 대한 이해정도를 조사하였다. 이를 위해 첫째, 각 교과서별로 시각자료의 개수, 종류, 역할 및 시각자료 역할에 따른 세부 요소 분포를 분석하였으며, 둘째, 일부 단원을 지정하여 학생들의 동기유발, 자로제공, 실험방법 안내, 실험결과 정리에 있어, 설문조사를 통하여 어떤 종류의 시각자료가 개념 이해에 대한 효과성 여부를 학업성취도별로 분석하였다. 이러한 연구결과는 학습자의 입장에서 학습효과성이 높은 시각자료가 무엇인지 확인하고, 학습활동에 있어 이를 수준별로 활용할 수 있으며, 앞으로 화학단원에서 교과서의 개정방향을 제시하는데 그 목적이 있다.

일시: 2015년 10월 14~16일(수~금) 3일간
장소: 대구 EXCO
발표코드: **EDEC.P-523**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

물질의 확산에서 시각과 청각을 동시에 활용한 실험이 과학 실험 수업의 학습 성취에 미치는 영향

정경화 박용섭 권혁규[1] 정범식 방경곤 이우붕[*]

경북대학교 화학교육과 [1]경북대학교 디지털미디어아트학과

이 연구는 물질의 확산 실험에서 일반적인 시각적 효과를 주는 실험과 일반적인 실험에 음향 효과를 주어 시각뿐만 아니라 청각적 효과를 동시에 주는 것을 통하여 학생들이 학업의 성취에 미치는 영향을 비교하였다. 액체의 확산인 물에 잉크방울을 떨어뜨렸을 때의 확산의 모습과 향을 피워 기체가 확산되는 모습으로 실험을 실시하였다. 실험은 일반적으로 실시하는 실험의 확산되는 모습을 영상으로 담아 영상 시그널을 음향으로 바꾸어 청각으로도 확인할 수 있도록 하였다. 고등학생을 대상자로 하여 남학생 70 명으로 실시하였으며, 1 차 일반적 물질의 확산 실험을 실시한 후 2 차 시각과 청각을 동시에 이용한 실험을 실시하여 학습효과를 알아보았다. 그 결과 1 차 실험결과보다 2 차 실험결과에서 실험에 대한 흥미도와 집중도가 높게 나타났으며, 공간 추론 능력이 향상되는 것을 발견할 수 있었다. 확산 실험을 시각적으로 확인하는 것보다 시청각이 동시에 사용하였을 때 그 결과에 대한 학생들의 반응이 더 우세하게 나타나는 것이 확인되었다.

대한화학회 제116회 총회 및 학술발표회 (The 116th General Meeting of the Korean Chemical Society)

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발표코드: **EDEC.P-524**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

스마트기기를 활용한 소집단 과학 수업

강석진

전주교육대학교 과학교육과

이 연구에서는 초등학교 과학 수업에서 스마트기기를 활용한 소집단 수업의 효과를 인지적, 정의적 측면에서 조사하였다. 1 개 초등학교의 5 학년 학생 38 명을 학급 단위로 처치 집단과 통제 집단으로 배치하였다. 사전 검사로 자기주도적 학습 능력 검사, 조 활동 기술 검사, 지식 공유 수준 검사를 실시하였다. 스마트기기를 활용한 소집단 수업을 실시한 처치 집단의 경우, 학생들이 새로운 수업 전략에 익숙해질 수 있도록 연습 수업을 1 회 실시하였다. 수업 처치는 4 개의 주제에 대하여 총 8 차시 동안 실시하였다. 처치 집단의 수업에서는 4~5 명씩으로 소집단을 구성한 뒤, 학생들 사이의 활발한 상호작용을 유발하기 위하여 소집단별로 완수해야 하는 과제를 제시하였다. 이 과제를 완수하기 위해서는 스마트기기를 이용하여 동영상에서 정보를 수집하고 소집단 구성원의 협동이 필요하도록 과제를 구성하였다. 스마트기기는 소집단별로 제공하였다. 과제 해결에 필요한 정보를 제공하는 동영상은 EBS 의 EDRB 와 유투브의 동영상에서 적절한 것을 선정하여, 학생용 활동지에 각 동영상의 접속 URL 을 QR 코드로 제시하였다. 또한 소집단 과제는 학생들의 동기를 유발할 수 있도록 흥미로운 상황으로 제시하였고, 모든 구성원들이 과제의 수행 과정과 결과물 제작에 참여하도록 구성하였다. 통제 집단은 교과서와 지도서에 기초하여 전통적인 방식의 과학 수업을 실시하였다. 통제 집단과 처치 집단의 수업은 동일한 교사가 실시하였다. 사후 검사로 학업 성취도 검사, 조 활동 기술 검사, 지식 공유 수준 검사를 실시하였다. 학업 성취도 검사 점수는 이전 과학 성적을 공변인으로 하고 자기주도적 학습 능력 수준을 구획 변인으로 하는 이원 공변량 분석을 실시하였다. 조 활동 기술 검사와 지식 공유 수준 검사 점수는 각각의 사전 검사 점수를 공변인으로 하고 자기주도적 학습 능력 수준을 구획 변인으로 하는 이원 공변량 분석을 실시하였다. 연구 결과, 학업 성취도에서는 수업 처치와 자기주도적 학습 능력 수준 사이에 유의미한 상호작용 효과가

나타났다. 그러나 조 활동 기술 검사와 지식 공유 수준 검사에서는 유의미한 효과가 나타나지 않았다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

중등 과학교사의 과학 평가 실태와 지향

노태희 이재원 강석진[1] 강훈식[2,*]

서울대학교 화학교육과 [1]전주교육대학교 과학교육과 [2]춘천교육대학교 과학교육과

이 연구에서는 중등 과학교사들이 실시하는 과학 평가와 교사들이 지향하는 평가의 사례를 목적과 방법의 측면에서 조사하였다. 연구 대상은 중등 과학교사 92 명으로, 학교에서 교사가 실시했던 평가 사례와 구성주의적 평가를 실시할 수 있는 전형적인 가상 상황에 대하여 교사가 지향하는 평가 사례를 조사하기 위한 검사지를 개발하였다. 교사의 경력, 평가 관련 교육 경험의 유무, 구성주의적 과학 평가관 수준 등 교사의 특성 변인도 조사하였다. 교사들이 실시하는 과학 평가 사례를 분석한 결과, 대부분의 교사는 총괄평가와 같은 전통적인 목적의 평가를 실시하는 경향이 있었고, 선다형 평가와 실험, 보고서, 논술형 평가가 가장 많이 사용되는 평가 방법이었다. 전형적인 평가 상황에서 과학교사들은 다양한 유형의 구성주의적 평가 방법을 지향한 반면, 여전히 전통적 평가 목적에서는 벗어나지 못하였다. 이때, 구성주의적 과학 평가관 수준이 높은 교사가 형성평가를 지향하는 비율은 구성주의적 과학 평가관 수준이 낮은 교사들에 비해 유의미하게 높았다.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

남한과 북한 과학 교과서의 물질영역 탐구 활동 비교

김건희* 박현주

조선대학교 과학교육학부

이 연구는 남한과 북한 과학 교과서의 물질 영역에 있는 탐구 활동을 비교?분석한 것이다. 연구대상은 남한의 과학과 교육과정의 물질 영역의 탐구활동과 그와 동일한 내용의 북한 과학 및 화학 교과서의 탐구활동이다. 탐구 활동은 탐구 유형, 탐구 내용, 탐구 상황, 실험 재료 등 에서 분석하였다. 연구 결과에 따르면 첫째, 탐구 유형의 경우, 북한 과학 교과서는 주로 간단한 실험 재료를 사용하여 과학 현상을 확인하는 해보기 유형이 많았다. 반면남한 과학교과서에서는 제한된 실험 도구와 재료이지만 실험을 설계하고 실험을 수행하고, 사고 과정을 통해 탐구를 수행하는 생각하기 유형이 많은 것으로 나타났다. 둘째, 탐구 내용의 경우, 전체적으로 남한 교과서가 과학탐구의 반영 정도가 높았으며, 북한 교과서는 기초 탐구에서 활동을 주로 제시하여 관찰을 주로 하는 반면 남한 교과서에서는 주어진 자료를 해석하거나, 가설을 설정하여 결론을 도출하는 통합 탐구의 반영이 더 높았다. 셋째, 탐구 상황의 경우, 북한 과학 교과서는 주로 기본 과학 개념의 이해와 형성에 작용하는 교과 내의 탐구적 상황이 압도적으로 많은 비율을 차지하였으나 이와 달리 남한 교과서는 과학 개념과 자연과 환경, 우리 주변의 일상적인 상황 및 기술/사회적인 부분을 다루고 있는 것으로 나타났다.

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중등 과학교사의 융합인재교육(STEAM) 수업 실행에 대한 문화역사적 활동이론(CHAT) 측면에서의 이해

최숙영 김민환 노태희*

서울대학교 화학교육과

이 연구에서는 문화역사적 활동이론(CHAT)을 분석 도구로 한 사례연구를 통해 중등 과학교사의 STEAM 수업 실행에 대해 조사하였다. 서울특별시에 소재한 고등학교에서 근무하고 있는 2 명의 과학교사가 연구에 참여하였다. STEAM 수업을 실행하기 전에 모든 교수학습 자료를 수집하였고, 수업을 관찰하고 녹화하였으며, 각 교사가 근무하는 학교의 교무실, 학급 분위기 등을 관찰하였다. STEAM 수업의 전, 중, 후에 걸쳐 여러 차례 면담을 실시하였다. 교사들의 STEAM 수업 실행을 CHAT 을 통해 분석하기 위해 지속적 비교 방법을 사용하였다. 활동체계의 다양한 요소들이 교사들의 STEAM 수업 실행에 미치는 영향과 활동체계 요소들 간의 상호작용을 중심으로 분석하였다.

연구 결과, 교사들의 STEAM 수업 실행에서 특징적인 공통점과 차이점이 있었다. STEAM 수업 실행에서 두 교사 모두 학생 중심의 자기주도적 활동에 대한 고려가 부족하였는데, 이에 대해 교사들은 이러한 수업 활동이 교과 내 STEAM 수업에 적합하지 않다는 이유를 들었다. 두 교사의 STEAM 수업 실행에서 나타난 차이점은 STEAM 수업에 대한 교사의 전문성과 관련된 주체 요소였고, 이에 따라 교사들의 STEAM 수업 실행 양상도 다르게 나타났다. 교사들의 STEAM 수업 실행에 긍정적 영향을 미친 활동체계의 요소들은 도구 요소인 학교의 환경적 특성, 규칙 요소인 STEAM 과 관련된 정책 등이 있었다. 반면, 부정적 영향을 미친 것은 규칙 요소의 측면에서 STEAM 수업을 실행하기에는 충분하지 않은 과학 교과의 수업 시수였다. 활동체계 요소들 간의 상호작용에는 부정적인 것과 긍정적인 것이 모두 있었다. A 의 경우 학생활동 지도의 어려움, B 의 경우 수업 준비의 어려움이 부정적 상호작용으로 나타났고, 두 교사 모두에게서 STEAM 수업에 대한 성공적 경험이 긍정적

상호작용으로 나타났다. 활동체계 요소들 간의 상호작용은 교사들의 활동체계에 다양한 변화를 가져왔는데, 이는 학생들의 수업 참여 태도 변화나 관리자의 인식 변화와 같은 학교 현장의 변화, STEAM 수업에 대한 교사의 인식과 실행 의지의 변화, STEAM 교원연수에 대한 요구 등으로 나타났다.

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Korea Science Academy of KAIST Organic Chemistry Program for Science-gifted High School Students

오진호* 천만석[1]

한국과학영재학교 화학생물학부 [1]한국과학영재학교 화학

KAIST 부설 한국과학영재학교는 한국 최초의 과학영재학교로서 2003 년부터 선택형 맞춤씩 교육과정을 바탕으로 미래 인류에 공헌할 수학 및 과학 고등학교 과학영재학생들을 교육해 오고 있다. 한국과학영재학교는 수학과 과학교과의 교원의 전문성을 바탕으로 과학영재학생들에게 대학과 연계된 Advanced Placement(AP) 속진 교육 프로그램과 심화 교육 프로그램을 제공하고 있다.고등학교 과학영재학생들의 과학에 대한 흥미와 관심을 고취시키기 위해서는 대학과 연계된 AP 프로그램 뿐만 아니라 심화교육 프로그램의 개발이 필요한 실정이다.한국과학영재학교에서는 화학심화 교과목으로 최근 개정된 4 차 교육과정에서 “기초유기화학”, “기초분석화학”, “분광학입문”, “나노화학의 입문” 및 “화학과 에너지”를 제공하고 있다.본 연구에서는 화학 심화교육 프로그램으로서 한국과학영재학교의 유기화학 수업을 소개함으로써 고등학교 과학영재학생들을 위한 유기화학 교육 프로그램 개발에 대해 논의하고자 한다. 한국과학영재학교 유기화학 수업은 자기주도적인 학습능력과 팀 협동력 향상을 위한 “팀 협동 문제 해결활동”에 기반을 두고 “문제 해결 및 발표 수업”과 “유기합성 프로젝트 활동”으로 구성하여 운영해 오고 있다.2015 학년도 1 학기 한국과학영재학교 기초유기화학 수업을 바탕으로 소개하고자 한다.

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발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cyanide oxidation using hematite nanocomposite for heterogeneous Fenton reaction

오세영 장준원*

(재)포항금속소재산업진흥원 융합산업연구팀

Hematite nanocomposite(HN) were fabricated via anodization of iron layer in 1M Na_2SO_4 containing 0.5 wt% NH_4F electrolyte, holding the potential at 20, 40 and 60 V for 20 min, respectively. Cyanide dissolved in water was degraded through the Fenton-like reaction using HN film with H_2O_2. In case of HN-40V in the presence of H_2O_2 3 %, the first-order rate constant was found to be 1.7×10^{-2} min^{-1}, and indicated to be 1.2×10^{-2} min^{-1} on hematite powder. Degradation of cyanide was much less with only H_2O_2. Therefore, this process proposed in this work can be an excellent alternative to traditional catalysts for Fenton-like reaction.

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CO_2 absorption properties of $NaNO_3$-MgO absorbent with NaCl additive

곽진수 권영욱* 김강영 조승익 안영인

성균관대학교 화학과

The primary purpose of carbon capture and storage (CCS) is reducing CO_2 emission from fossil fuel. There are three types of available CO_2 absorbent depending on the operating temperature; low-(below 200 ℃), intermediate-(between 200~500 ℃), and high- (above 500 ℃) temperature absorbents. Presently, MgO, with the help of a promoter $NaNO_3$, is the only known intermediate-temperature absorbent that satisfies the thermodynamic requirements. In this study, we have investigated the effect of NaCl additive on the CO_2 absorption properties of $NaNO_3$-MgO absorbent. Five absorbents with different NaCl (NaCl/($NaNO_3$+NaCl) : 0, 0.035, 0.2, 0.4, 0.6) molar fraction were synthesized. From temperature swing and isothermal CO_2 absorption data, absorbents with NaCl additive show lower CO_2 absorption capacity and kinetics than commercial $NaNO_3$-MgO absorbent. However, some interesting results are obtained from CO_2 absorption and desorption cycle data. Generally, $NaNO_3$-MgO absorbents show bad cycle durability and kinetics. But absorbent with NaCl additive (0.6 molar fractions) shows enhanced cycle durability and kinetics gradually.

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Study of CO_2 absorption mecahnism of MgO promoted by $NaNO_3$ and $NaNO_2$

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MgO is well known as an intermediate-temperature CO_2 absorbent because its carbonate decomposition temperature is lower than other alkaline metal oxide. Its CO_2 absorption efficiency is very low because its lattice enthalpy is so high. $NaNO_3$ is used as a promoter in order to enhance CO_2 absorption capacity of MgO. MgO can absorb about 75% of CO_2 with $NaNO_3$. But $NaNO_3$ has several problems to use a promoter of CO_2 absorption. It can be decomposed into noxious material and the velocity of CO_2 absorption of MgO promoted $NaNO_3$ is not fast enough. MgO promoted $NaNO_3$ has long induction period about 30minutes. So we wanted to find another promoter which can compensate a defect of $NaNO_3$ and has similar efficiency for CO_2 absorption promoter with $NaNO_3$. We chose $NaNO_2$ because it has similar chemical and physical properties with $NaNO_3$. Using only $NaNO_2$ for promoter, the efficiency is not good enough. However, MgO showed high performance for CO_2 absorption with $NaNO_2$&$NaNO_3$ mixture and the absorption velocity of MgO is higher than using only $NaNO_3$. $NaNO_2$ decompose at 400. MgO promoted $NaNO_2$&$NaNO_3$ mixture needs high temperure to desorb CO_2 from Mg_2CO_3. so we try to complement on this point. We could reduce the CO_2 desorption temperature by adding $LiNO_3$. We expect $NaNO_2$&$NaNO_3$ mixture can be a good promoter for CO_2 absorption

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Effect of Alkaline?earth Metal Carbonate Salts on CO_2 absorption kinetics on $NaNO_3$?MgO Absorbent

김강영 조승익 곽진수 안영인 권영욱*

성균관대학교 화학과

MgO-based CO2 absorbents have been investigated for the operation in the intermediate temperature of 300~500℃. Typically, these absorbents are composed of MgO and a promoter. NaNO3 or other alkali nitrates have been explored as the promoter. Although the overall reaction mechanisms have been clarified by previous studies as that the promoter is the medium for the reaction between CO2 and MgO, many details are not yet clear. We believe that clear elucidation of the details reaction mechanism is the first step for the improvement of the performance of the MgO-based absorbents. The absorption isotherms of NaNO3?promoted MgO absorbents in the literature and our own data shows sigmoidal curves. We interpret this as a signature of autocatalyzed kinetics of CO2 absorption. We further conjectured that this behaviour may arise from the growth kinetics of MgCO3, which involves nucleation and growth steps. In order to verify this idea, we have prepared various NaNO3-MgO absorbent samples with different alkaline?earth metal carbonates added. The carbonate salts did not affect the CO2 absorption capacity of MgO, but they appeared to enhance the CO2 absorption kinetics. However, the facilitation effects of the added carbonate disappears from the second cycle of the absorption-desorption cycles. These observations are consistent with the proposed mechanism of nucleation and growth of MgCO3 crystals. Further, our observations indicate that the growth of MgCO3 is the rate-determining steps. Details of experimental data and their implications to the CO2 absorption kinetics by MgO-based absorbents will be presented.

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Effect of Promoter on Desorption of CO_2 of MgO Absorbent

조승익 권영욱* 김강영 곽진수 안영인

성균관대학교 화학과

Nitrate-promoted MgO is a representative intermediate-temperature (at 300~500℃) CO_2 absorbent. Many researchers have explored the behavior of MgO-based CO_2 absorbent but the role of promoter and the exact operating mechanism of MgO absorbent are still unclear. In order to improve its performance, it is imperative that we understand CO_2 absorption/desorption process of MgO absorbents and the role of promoter. According to the recent reports, it has been established that a nitrate promoter increases the CO_2 absorption capacity and accelerates the CO_2 absorption rate of MgO. On the other hand, the mechanism of desorption of CO_2 from $MgCO_3$, the product of CO_2 absorption by MgO, has attracted far less attention. However, we believe that lowering the desorption temperature and facilitating the desorption kinetics are also important aspects to be taken into consideration in designing CO_2 absorbents. The input energy and cost of operation can be lowered by reducing the gap between absorption and desorption temperatures. Also, the durability of MgO absorbent may be increased by lowering the desorption temperature. In this study, we demonstrate that the promoter $NaNO_3$ encourages CO_2 desorption as well. We found that the presence of Li ions in the promoter further lowers the desorption temperature by about 20°C. The effects of the promoter on the desorption of CO_2 can be explained in terms of the changes of relative thermodynamics between MgO and $MgCO_3$ by having contacts with the promoter. Details of our experiments and their analyses will be presented in our presentation.

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Prediction about thermal property changes of ammonium perchlorate according to the purity

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Usually energetic materials are exposed to the thermal environment like seasonal change. So thermal property and stability of energetic materials are very important to management and safety. Ammonium Perchlorate (AP) is widely used in the composite propellants and composite explosives as an oxidant. By the way, Self-Accelerationg Decomposition Temperature (SADT) test is one the most important test for energetic materials. Using AKTS program, this SADT result can be simulated with simple DSC data. In this study, we investigated influence of AP purity to SADT result by simulation using AKTS thermokinetic program. DSC data was collected from different AP samples which have different purities.

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Synthesis and Characterization of DNAM(4,6-Dinitroamino-1,3,5-Triazine-2(1H)-one) for a new insensitive high explosives

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둔감화약의 필요성이 크게 대두되고 있지만, 일반적으로 안정하고 충격에 둔감한 화약들은 화약 성능이 떨어지는 반면, 높은 에너지를 가지는 대부분의 화약들은 민감한 경향을 가진다. 따라서, 폭발에너지가 높으면서 예기치 못한 자극이나, 동조폭발에 반응하지 않는 화약이 끊임없이 요구되고 있다. DNAM(4,6-Dinitroamino-1,3,5-Triazine-2(1H)-one)은 분자 내에 질소를 도입하여 성능과 밀도(1.95g/cm3)가 높으면서도 충격과 마찰에 매우 둔감한 특성을 갖는 분자화약으로, 폭발반응 시 대기 중에 안정하고 환경 친화적인 질소를 방출하는 특성을 가지고 있다. 공업용 원료로서 매우 값싼 멜라민을 출발물질로 사용하여 1 단계의 합성공정을 통해 반응이 완료되는 장점 또한 가진다. 재결정에 의한 입도나 형상 조절이 어려운 물질이나, 충전밀도가 높고 연소특성이 좋아 추진제의 성분으로도 응용이 가능하다.

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Shewanella oneidensis requires electron shuttles for efficient inorganic Hg(II) reduction

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SShewanella oneidensis MR-1 is a dissimilatory metal reducing bacterium that can reduce inorganic divalent mercury [Hg(II)] at low Hg(II) concentrations (< 0.3 μM). MR-1 is also known to secrete extracellular dissolved organic compounds like flavin mononucleotide (FMN) and riboflavin. The role of extracellular dissolved organic compounds for Hg(II) reduction by MR-1 was investigated by comparing the inorganic Hg(II) reduction rates by wild type and Δbfe (mutant lacking the ability to secrete FMN). Results showed that wild type strain reduced up to 39±2% of the spiked Hg(II) (20 nM) whereas the mutant, Δbfe, reduced up to 21±1%. Further investigation revealed that Hg(II) reduction rate by wild type is higher than that of Δbfe (2.8 × 10-6 vs 1.9 × 10-6 M-1s-1). Increased Hg(II) reduction rate by wild type strain than Δbfe is attributed to electron shuttling of flavin. Moreover in cell suspension media the presence of 1 μM FMN, riboflavin and Anthraquinone-2,6-disulfonate (AQDS) reduced 23, 21 and 21% Hg(II), respectively, within 180 minutes, whereas in the absence of electron shuttles MR-1 reduced only 2% Hg(II). This electron shuttling could be an important process of mercury detoxification in subsurface environments where dissolution of humic substances is limited.

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The kinetics of the photodemethylation of methylmercury in seawater: the role of dissolved organic matter

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Methylmercury (MeHg) is a neurotoxin that bio-accumulates in aquatic food chains. Photodemethylation is the major cause of MeHg reduction in surface seawaters, thereby limiting MeHg uptake by aquatic biota. Dissolved organic matter (DOM) plays an important role in the photodemethylation of MeHg because DOM can produce free radicals, including reactive oxygen species (ROS) and MeHg?DOM complexes. There are four potential pathways to MeHg photodemethylation: (1) direct photodemethylation of MeHg, (2) photodemethylation of MeHg by free radicals including ROS [$^1O_2$, $^3DOM^*$, e?aq, ·OH], (3) photodemethylation of MeHg?DOM complexes by free radicals (including ROS), and (4) direct photodemethylation of MeHg?DOM complexes via an intramolecular charge transfer. In order to investigate the effect of DOM on the photodemethylation of MeHg and its major pathway in seawater, we tested the demethylation rate of MeHg in artificial seawater under UV-A, in the presence or absence of DOM (humic acid and fulvic acid) and specific scavengers. The fluorescence quenching was measured by excitation-emission matrix fluorescence to confirm the complexation of MeHg by DOM during the photodemethylation experiment. The photodemethylation of MeHg followed a pseudo-first order kinetics, and the concentration of MeHg decreased as the UV-exposure time increased. The photodemethylation kinetics under various types and concentrations of DOM and scavengers are currently under investigation.

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Adsorption/desorption of uranium on iron-bearing soil mineral surface by column test and quantum calculation

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In this study, we evaluated the adsorption/desorption of uranium (U) in pure soil environment using continuous column reactor. We additionally investigated the adsorption/desorption mechanism of U on vivianite surface in molecular scale using quantum calculation. We observed that below 0.1 μM of U was detected after 20 d from U injection (1 μM) in adsorption test. However, all of absorbed U was detached from vivianite surface in 24 h by injection of CARB solution (1.44×10^{-2} M $NaHCO_3$ and 2.8×10^{-3} M Na_2CO_3). Based on exchange energy calculation, we found that $UO_2(CO_3)_2^{\ 2-}$ and $UO_2(CO_3)_3^{\ 4-}$ species have higher repulsive energy than $UO_2(OH)_2$ species. The results obtained from this study could be applied to predict the behavior of uranium in contaminated and remediation sites.

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국내·외 녹색화학 현황 및 대체물질 검색 프로그램

신충근

티오이십일 위해성연구팀

유해화학물질의 무분별한 사용으로 인해 지구 환경 및 인체에 화학물질의 중독, 암 유발 등 여러 가지 피해를 발생시켰다. 이에 주요 선진국을 중심으로 원료 물질로 이용되는 화학물질의 유해성저감, 제거를 목표로 하는 '녹색화학' 이론이 확산되고 있다. 특히, 미국, 덴마크 등 주요 선진국에서는 오래 전부터 산·학·연이 공동으로 대체 화학물질 개발에 대한 노력을 수행하여 유해화학물질을 대체할 수 있는 신뢰성 있는 화학물질 정보를 제공하기 위한 프로그램을 개발하여 배포, 운영하고 있다. 이에 국제적 변화에 부합하기 위해 우리나라는 2011 년부터 대체 화학물질 검색 프로그램 개발 사업을 진행하고 있으며, 국내·외에서 발표되는 유관 논문, 특허 등을 통해 약 380 종에 대한 대체 화학물질 정보를 수집, 가공 및 데이터베이스화 하여 대체물질을 쉽게 검색할 수 있도록 프로그램을 개발하였다. 본 프로그램에서는 화학물질 사용 용도별로 대체 화학물질과 기업사례 정보를 확인할 수 있고 국내·외 규제물질 목록 및 규제내용 제공을 통해 사용자가 쉽게 규제현황을 파악할 수 있으며, 전 세계 화학물질 규제동향 뉴스와 '1:1 문의' 기능을 통해 화학물질 정보 및 간단한 컨설팅을 받을 수 있다. 본 프로그램은 국내 논문, 유관 학회 전시와 포스터 발표 및 홈페이지 배너 운영 등 지속적인 홍보와 업데이트를 통해 약 250 여 사업장에 대체물질 검색 프로그램을 제공 하였으며, 환경부와 한국환경정책·평가연구원(KEI)의 정책활용에 사용되어 후속 연구가 진행 중이다. 본 프로그램은 중소기업에게 화학물질 정보 및 규제동향을 쉽게 접할 수 있도록 하여 유해 화학물질 사용저감 및 관리체계가 구축되며, 우리나라 녹색화학 기반구축에 도움이 될 것으로 기대된다.

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Effect of Pt and pH for Photocatalytic Oxidation on g-C3N4 under Visible Light

임종훈 최원용*

포항공과대학교(POSTECH) 환경공학부

Graphitic carbon nitride (g-C3N4) is a metal-free polymeric photocatalyst, with N-bridged tris-s-triazine moieties stacked in a graphitic structure. This material is successfully activated under visible light because of its narrow band gap (2.7 eV) and widely used for photocatalytic water splitting and degradation of organic pollutants. For enhanced photocatalysis of semiconductor, platinum is commonly used in many cases as a cocatalyst to retard fast recombination of photoinduced charge pairs. Therefore, platinized semiconductor photocatalysts exhibit enhanced photocatalytic activities for not only reduction (e.g., H2 generation) but also oxidation (e.g., degradation of pollutatnts) compared to bare semiconductor photocatalysts. Although Pt-C3N4 has been successfully used for photocatalytic reduction, its applications in photocatalytic oxidation are few. In this study, we confirmed that different reactive oxygen species (ROS) were generated depending on pH. At pH 3, OH radical was dominantly generated through the reductive decomposition of H2O2 that was produced from the reduction of O2, whereas singlet oxygen was generated at pH 7 on C3N4. However, the generation of OH radical and singlet oxygen was markedly decreased in the presence of Pt. Contrary to the result of photocatalytic H2 generation, the photocatalytic degradation of 4-CP and FFA with Pt-C3N4 was lower than that with bare-C3N4. The Pt effect of carbon nitride on the photocatalytic oxidation is clearly different from that on metal oxide photocatalysts.

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Resorcinol Formaldehyde-based Sensitizer for Charge-Transfer Complex with Hollow TiO_2 Working under Visible Light

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Titanium dioxide has been widely investigated for solar energy conversion, but its wide bandgap (3.2 eV) does not allow the utilization of visible light for better performance. To overcome this problem, many approaches have been tried. In this work, a titania-polymer hybrid catalyst was synthesized by an in-situ hydrothermal process that utilized a block copolymer (Pluronic F127) as a surfactant, resorcinol as a polymer precursor, titanium salt as a metal oxide precursor, and hexamethylenetetramine (HMTA). The material formed by this synthesis method has a hollow composite nanostructure consisting of TiO_2 nanoparticles covered with a resorcinol formaldehyde (RF) polymer shell. Photocatalytic reduction of Cr(VI) to Cr(III) in aqueous medium under visible light using RF polymer and Hollow TiO_2@RF polymer was investigated. RF polymer itself showed a moderate photoactivity under visible light for the reduction of Cr(VI). However, RF resin suffers from oxidation in alkaline media. Therefore, the conversion of chromate significantly decreased under alkaline condition with RF polymer alone. However, this drawback can be overcome by Hollow TiO_2@RF. With this, the reductive removal of Cr(VI) was enhanced and could be maintained under alkaline condition and during the repeated tests. Using a redox couple, photocurrent was successfully collected in the suspension of Hollow TiO_2@RF under visible light. The enhanced photocatalytic activity is ascribed to the fact that the photoinduced electrons in RF polymer are efficiently transferred to hollow TiO_2 under visible light through ligand-to-metal charge transfer (LMCT).

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Fe_2O_3/Nb_2O_5 composite photoanodes for Photoelectrochemical Solar Water Splitting

전태화 최원용*

포항공과대학교(POSTECH) 환경공학부

Solar water oxidation in photocatalysts is mainly initiated by holes transfer from the surface states to the electrolyte. However, surface states can also act as recombination center, so it may hinder hole transfer for water oxidation. So, herein, we employed Nb_2O_5 layer on the surface of hematite (α-Fe_2O_3) electrodes to investigate the charge separation and transfer process at the interface between semiconductor and electrolyte. Nb_2O_5/hematite composite electrodes were prepared via simple drop-casting of niobium (Nb^{5+}) precursor solution onto the as-annealed hematite electrode, and Nb^{5+}-ion treated hematite electrodes are further annealed to form Nb_2O_5 layer. Nb^{5+}-ion treated hematite electrode showed 3 times higher photocurrent than that of bare hematite (from 0.17 mA cm^{-2} to 0.51 mA cm^{-2}) at 1.23 V (vs. RHE) under A.M 1.5 solar simulated light condition. The addition of Co^{2+} ions as a co-catalyst for water oxidation in Nb_2O_5/hematite composite electrodes showed a further enhanced photocurrent performance by a factor of 3.2 (from 0.51 mA cm^{2+} to 1.63 mA cm^{2+}), and it also exhibited a cathodic shift of onset potential (~ 250 mV). Furthermore, photoelectrochemical (PEC) performances with hole scavenger indicate that the injection efficiency for water oxidation is highly enhanced by applying Nb_2O_5 layer on hematite (from 20% to 60 % at 1.23 V (vs. RHE)). This result shows that main role of Nb_2O_5 layer in hematite for water oxidation is to suppress the back reaction of photo-generated holes and enhance water oxidation process.

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Photoelectrochemical Degradation of Organic Compounds with Blue-TNTs

구민석 윤제용[1] 최원용*

포항공과대학교(POSTECH) 환경공학부 [1]서울대학교 화학생물공학부

The use of TiO_2 nanotube arrays as a photoanode material has suffered from rapid recombination of excited electron-hole pairs in aqueous solution. So, through the cathodic polarization method (electrochromism), we tried to overcome this drawback of titanate nanotube arrays. Since cathodic polarization causes electrons to accumulate in the conduction band, the conductivity of TNTs should be enhanced and also the recombination of electron-hole pairs could be retarded under irradiation. In a few papers, electrochromic titania nanotube arrays (as a denoted blue-TNTs) have been used for photocatalytic reactions, but it has not been studied for the photoelectrochemical oxidation processes. In this study, blue-TNTs were utilized as an anode material for photoelectrochemical degradation of organic compounds (*e.g.* 4-chlorophenol (4-CP), humic acid, and fulvic acid) under UV light irradiation. Titanate nanotube arrays showed significant electrochromic characteristics under cathodic polarization, and its color turned dark blue. This phenomenon arises from the change of surface charge states of TNTs caused by intercalation of protons ($Ti^{4+} + e^- + H^+ \rightarrow Ti^{3+}H^+$). By this phenomenon, the photo-generated electrons could be easily separated from hole which generate hydroxyl radicals from water, and the conductivity of blue-TNTs electrode was higher than that of bare-TNTs electrode. Furthermore, the blue-TNTs electrode showed highly enhanced photocurrent as well as superior efficiency of hydroxyl radical generation compared to bare-TNTs electrode. The photoelectrochemical oxidation of organic compounds using the blue-TNTs was more efficient than the photocatalytic (PC) and electrochemical (EC) oxidation.

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Green synthesis of diisocyanate from bio-based materials

이건욱 정민석* 김훈식*

경희대학교 화학과

Recently, the utilization of bio-based materials is of great interest, due to depletion of fossil fuel and need of environmental protection. In this research, 1,4-diisocyanatobutane (BDI) was synthesized from the thermolysis of 1,4-dicarbamatobutane (BDC), which was prepared from the methoxycarbonylation of 1,4-diaminobutane (BDA), a bio-based material.

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Synthesis of glycerol carbonate by transesterification of dimethyl carbonate with glycerol

황준혁 김훈식[*]

경희대학교 화학과

Glycerol carbonate as a highly valuable product is synthesized by the reaction of glycerol which is by-product of biomass production with dimethyl carbonate. This transesterification of glycerol reaction has been studied as an alternative process of conventional phosgenation. 4-alkyl pyridine showed remarkable catalytic performances.

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Study of CO2 absorption and desorption using Sterically hindered alkanolamines

이지우 김훈식*

경희대학교 화학과

In this study, the CO2-adducts of sterically hindered amines (SHA) such as 2-[(1,1-dimethylethyl)amino]ethanol (TBAE) and 2-(n-butylamino)ethanol (BAE) were investigated by computational and spectroscopic studies. TBAE were found to reversibly interact with CO2 in a 1:1 molar ratio exclusively through the hydroxyl group, producing zwitterionic carbonate species, which lose CO2 at considerably lower temperatures than the CO2-adducts of other alkanolamines including monoethanolamine and diethanmolamine.

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Enhanced reduction of aquous nitrate by nanocrystalline zeolite supported bimetallic catalyst

HAMIDSHANAWAR 이우진[1,*]

한국과학기술원(KAIST) 건설및환경공학과 [1]한국과학기술원(KAIST) 건설 및 환경공학과

Nitrate pollution to groundwater and surface water bodies has increased around the globe due to enormous inputs from industry and agriculture. This situation has raised serious threats to ecological cycle and human health. Recently developed catalytic nitrate reduction has shown promising results in terms of nitrate removal, process kinetics, safe end products' selectivity and reaction stability. However, exclusive efforts are still required to further improve the reactivity, selectivity, stability and environmental sustainability of bimetallic catalysts. In this work, a novel and eco-friendly bimetallic catalyst supported by nano ZSM-5 zeolite was developed keeping in view above mentioned challenges. Nano ZSM-5 zeolite was selected as a support because it is a stable and environmentally benign material. Catalyst formulation was selected by optimizing promoter metals, noble metals, and calcination temperatures. Complete nitrate reduction (100%), high N_2 selectivity (85%) and elevated nitrate reduction kinetics (kinetic rate constant $k = 15.79 \times 10^{-2}$ min^{-1}; normalized kinetic rate constant $K' = 60 \times 10^{-2}$ min^{-1} $gcatalyst^{-1}$) were achieved at optimized conditions (i.e. Sn, Pd and 350 ^{o}C).

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Complete recovery and/or removal mixed heavy metals from wastewaters by coupling microbial fuel cells

최찬수

대전대학교 응용화학과

To remove and/or recover mixed heavy metals from the wastewaters two microbial systems were coupled; a microbial fuel cell (MFC) with heavy metals with high reduction potentials and a microbial electrolysis cell (MEC) with heavy metals with lower reduction potentials. The voltages generated by the MFC array were supplied to the MEC array. Two groups of heavy metals were removed and/or recovered simultaneously. The mixture of heavy metals imitating a plating solution contained 20 ppm Cr(VI), 5 ppm Cu(II), 5 ppm Ni(II), and 5 ppm Zn(II). All heavy metals were removed and/or recovered 99% within 10 minutes.

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Synthesis of Phosphate modified magnetic mesoporous carbon for removal of Uranium

이충섭 장윤석*

포항공과대학교(POSTECH) 환경공학부

Ordered mesoporous carbon functionalized with phosphates groups and magnetic nanoparticles has been successfully synthesized by modifying the mesoporous carbon with amino trismethylenephosphonic acid (ATMP). Through the in-situ reduction of Fe^{3+}, magnetic nanoparticles were successfully incorporated into the mesopores, resulting in the multifunctional mesoporous carbon, Fe-PCMK-3. The obtained composite carbon material possesses mesoporous structure, high Brunauer-Emmett-Teller (BET) surface area, large pore volume, phosphate ligand on the surface, and excellent magnetic property. The functionalized hybrid inorganic-organic adsorbent also showed high efficiency for the removal of aqueous uranium from waste solutions.

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Air-stable nanosized zero-valent iron modified with aromatic antioxidant compounds

이충섭 장윤석*

포항공과대학교(POSTECH) 환경공학부

Antioxidant attached nanosized zero-valent iron (nZVI) particles were synthesized to reduce depassivated layer in oxygen-rich conditions. nZVI particles were modified with antioxidants such as N-phenylglycine, phenoxyacetic acid, 2-anilinoethanol, and phenoxyethanol which have phenolic or aromatic amine structures that can scavenge hydroxyl radicals very well. The modified nZVI particles showed lower removal efficiency of TCE than bare nZVI right after synthesized. However, TCE removal efficiency of the modified particles was evidently higher than bare nZVI particle for cases of 1 week, 2 weeks and 1 month of aging. Some characterizations were conducted including XPS, FT-IR, SEM and TEM to investigate the surface conditions. These indicated that the modified nZVI using N-phenylglycine and phenoxyacetic acid can make a stable structure with nZVI. The result of a dissolution test implied that hydroxyl radicals prefer attacking N or O sites of the antioxidants rather than producing an iron oxide layer, which can decrease reactivity. These materials are more applicable for *in-situ* remediation compared with the bare nZVI to maintain reduction reactivity longer.

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Controlled-release Permanganate by Using Alginate Beads for the Effective Removal of Trichloroethylene and Its Application in Groundwater Remediation

이충섭 장윤석*

포항공과대학교(POSTECH) 환경공학부

Due to the relative insolubility of permanganate in trichloroethylene (TCE) contaminated zone and competitive pollutants in natural aqueous solutions, in order to completely remove TCE, an excessive amount of permanganate has to be used leading to the problems of a secondary pollutant (MnO_2) which is needed to be eliminated by filtering and the possible unpleasant color of water after remediation process. In this study, permanganate was effectively encapsulated in alginate beads with well-controlled releasing efficiency. Different ratios in weight between sodium alginate and permanganate were investigated, and the releasing experiments were also conducted in different pH conditions and different concentration of cross-linking cation. In TCE degradation experiments, the complete removal of TCE 15 mg/L was achieved after only 4 hours which was more effectively than using the same amount of free permanganate. Interestingly, approximately 20% of TCE can be adsorbed by using alginate beads only. The SEM images showed that alginate beads were well formed with the concentric layer-by-layer structure. When being immersed in aqueous solution, MnO_4^- distributed at the interfacial layers of the beads was firstly released into environment creating pores which could be the pathway facilitating either the further transportation of inside MnO_4^- or the intrusion of TCE from outside into the beads. Moreover, it was observed that no MnO_2 remained in solution which might be adsorbed onto the beads, and water with perfect transparent property was collected after experiment. For all these reasons, permanganate releasing alginate beads can be considered as a potential technique for *in-situ* remediation of groundwater.

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Novel H:ZnO Nanorods based Photoanode Sensitized by CdS and Carbon Quantum Dots for Photoelectrochemical Water Splitting

Nguyen Minh Vuong Logan Reynolds[1] Eric Conte[1] 이용일[*]

창원대학교 화학과 [1]Western Kentucky University

We report a promising simple strategy to improve the performance of photoanode for photoelectrochemical (PEC) water splitting. ZnO nanorods on ITO glass substrate were synthesized by hydrothermal method following calcinations in air at 500 ?C for 2 hours and pure hydrogen ambient at atmosphere pressure at 400 ?C for 30 min. Hydrogenated ZnO (H:ZnO) sample shows enhanced photocurrent in comparison to ZnO nanorods. To enhance the absorption in the visible light and near-IR regions, H:ZnO nanorods were sensitized by cadmium sulfide (CdS) nanoparticles and carbon quantum dots (CQDs). The CdS and CQDs sensitized H:ZnO nanorod film exhibited significantly improved PEC property after treatment in nitrogen ambient at 400 ℃ for 30 min. The optimized CdS and CQDs sensitized H:ZnO nanorod sample yields a photocurrent density of ~12.82 mA/cm2 at 0 V (vs. SCE) in 0.25 M Na2S and 0.35 Na2SO3 solution under the illumination of simulated solar light (100 mW/cm2 from 150 W xenon Arc lamp source). The optimal structure shows a solar-to-hydrogen (STH) conversion efficiency of ~3.85 % (at -0.67 V vs. SCE). The H2 gas generation using this optimal CdS and CQDs sensitized H:ZnO nanorods structure was obtained with 7.04 ml/cm2 in 1 hour. The morphology and property of samples were examined by SEM, XRD, TEM, UV-vis absorption and electrical measurement.

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Photocatalytic conversion of CO_2 to hydrocarbon fuel using carbon and nitrogen co-doped sodium titanate nanotubes

Abdul Razzaq 인수일[1,*]

대구경북과학기술원(DGIST) 에너지시스템공학 [1] 대구경북과학기술원(DGIST) 에너지 시스템 공학 전공

The excessive release of CO_2 into atmosphere is considered as a major cause of challenging issues of global warming, climate changes and environmental pollution. One effective approach to normalize atmospheric CO_2 is its conversion to hydrocarbon fuels via solar-spectrum photocatalysis. Among photocatalysts, Titania (TiO_2) or Ti-based materials have been intensively studied due to their abundant availability, nontoxicity, corrosion resistance, and chemical stability.However the relatively wide bandgap of TiO_2, approximately 3.2 eV, which is responsible for its excellent corrosion stability but with limitation of its absorption to UV wavelengths, some 4% of the terrestrial solar-spectrum energy. Numerous approaches have been used for reducing the TiO_2 bandgap as a means of absorbing, and utilizing, a greater portion of the solar spectrum energy, including metal ion implantation, non-metal doping and synthesis of low bandgap hybrid nanomaterials etc. Among the variety of available nanostructures layered-titanate nanotubes (TNTs), innovated by Kasuga et al, with advantages of the material architecture include large surface areas, improved adsorption capacity, moderate photocatalytic activity, and improved thermal and chemical stability. Motivated by the unique qualities of the layered-TNTs and the potential for simultaneous co-doping of the materials as a means to obtain improved photocatalytic properties we have investigated herein different samples of C,N-TNT with varied dopant concentrations their application under simulated solar light investigated for the photocatalytic conversion of CO_2 and water vapors to CH_4. The C,N-TNT sample with an intermediate doping concentration yields the maximum methane yield of 9.75 ?mol /g h. We concluded the key factors contributing in the improvement of photocatalyst performance includes light absorption, surface area and protonation effects in TNT influencing CO_2 adsorption sites and photogenerated electrons recombination centers.

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Recent Progress of Nanostructure Modified Anodes in Microbial Fuel Cells

이경석

대구경북과학기술원(DGIST) 에너지시스템공학전공

Microbial fuel cell (MFC) is a bio-electrochemical system which converts chemical energy into electrical energy by catalytic activity of microorganisms. Electrons produced by microbial oxidation from substrates such as organic matter, complex or renewable biomass are transferred to the anode. Protons produced at the anode migrate to the cathode via the wire and combine with oxygen to form water. Therefore MFC technologies are promising approach for generating electricity or hydrogen gas and wastewater treatment. Electrode materials are one of the keys to increase the power output of MFCs. To improve the cost effective performance of MFCs, various electrodes materials, modifications and configurations have been developed. In this paper, among other recent advances of nanostructured electrodes, especially carbon based anodes, are highlighted. The properties of these electrodes, in terms of surface characteristics, conductivity, modifications, and options were reviewed. The applications, challenges and perspectives of the current MFCs electrode for future development in bio or medical field are briefly discussed.

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Hexabromocyclododecane (HBCD) Diastereoisomers in meat from Korean markets

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

Hexabromocyclododecane (HBCD) is a brominated flame retardant used in polystyrene foams in thermal solution and electrical equipment. The HBCD commercial mixture consists mainly of γ-HBCD (70%) and two other diastereoisomers in lower amounts: β- and α-HBCD 16% and 13% respectively. HBCD has recently been adopted for addition to Annex A of Stockholm convention. The presence of HBCD in wide range of matrices, its suspected toxic effects and continuous massive use may indicate a public health concern. One of the many sources of human exposure to HBCD is through diet. Similar to other POPs it is expected that consumption of fish and meat are two important pathways of human oral exposure. However, in this research the HBCD concentration in meat samples were investigated due to higher consumption in Korean population in comparison with fish product. Little information is available regarding HBCD level in meat and to our knowledge this is the first study to determine the HBCD diastereoisomers in meat samples in Korea. In this study, a total of 59 meat samples were collected from local market and department stores of 5 cities in Korea. Concentrations of HBCD diastereoisomers were determined by liquid chromatography?tandem mass spectrometry (LC?ESI-MS/MS). α-HBCD was the predominant diastereoisomer in 90% of the meat samples. It has to be noted that the diastromeric distribution of HBCD can change due to bioisomerization and biotransformation in biological materials. The concentration was higher in pork (139 pg/g ww) than beef (110 pg/g ww), however, the difference was not significant. Levels of HBCD diastereoisomers found in Korean meat samples were relatively low in comparison with food samples from other countries.

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Occurrence and Trophic Magnification of PCNs, HBCDs, and DPs in the Ecosystem of King George Island, Maritime Antarctica

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

We investigated occurrence and trophic magnification of emerging persistent organic pollutants (POPs), including Polychlorinated naphthalenes (PCNs), Hexabromocyclododecanes (HBCDs), and Dehchlorane plus (DPs) and their related compounds, in the maritime ecosystem in Antarctica. The samples included Antarctic cod, icefish, limpet, amphipods, leopard seal, Gentoo penguin, Chinstrap penguin, kelp gull, and south polar skua. And the samples were collected in Baton peninsular of King George Island, Antarctica, from December 2013 to February 2014. The concentrations in the samples were lower or comparable to those from the aquatic and terrestrial ecosystem in the other regions. To our knowledge, this was the first or second study to report occurrence of the chemicals in the Antarctic biota, providing evidence of long range transport of these chemicals. We also calculated trophic magnification factor (TMF) of each congeners, based on the ratio of stable isotope nitrogen and the log-transformed POP concentrations. Some of the compounds, including HBCDs and PCNs, showed significantly positive correlations, suggesting biomagnification of the chemicals. And the TMF values were varied with different food-web models under consideration of different food web structures and treatment of non-detected data. This study suggested the long range transport and bioaccumulation of the emerging POPs, which are the POPs criteria of Stockholm Convention.

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Diastereoisomer-specific distribution of Hexabromocyclododecane (HBCD) in fish and marine invertebrates

신은수 장윤석*

포항공과대학교(POSTECH) 환경공학부

The levels and distributional characteristics of hexabromocyclododecane (HBCD) diastereoisomers have been largely reported for various fish and select shellfish. In this study, we reclassified a number and variety of marine invertebrates, including shellfish, to further contribute to the comprehensive understanding of the effects and assessment of human exposure to HBCD. Overall, 30 marine invertebrate species (n = 188) were investigated and the following order of ∑2HBCD (α- and γ-HBCD) was observed: fish > chordata > cephalopoda > echinodermata > bivalvia > crustacea. The marine invertebrates that were reclassified into nektonic and benthic organisms showed similar concentration of ∑2HBCD. The feeding habits and modes of the marine organisms were considered to compare the degree of bioaccumulation and diastereoisomer-specific distribution of HBCD due to the effects of the environment in and around pollution sources, as well as the organisms' metabolic capacities. To the best of our knowledge, this is the first study to examine the species-specific distribution patterns of HBCD for both fish and marine invertebrates. We expect to significantly expand the understanding of the environmental fate of HBCD for marine organisms.

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Formation of Titania-Silica Mixed Oxides in Solvent Mixtures and their Influences for the Photocatalytic CO_2 conversion to Hydrocarbon

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TiO_2-SiO_2 mixed oxide photocatalyst materials responsive to simulated solar light illumination have been synthesized by sol-gel method in various polar and nonpolar organic solvent mixtures. The photocatalysts were characterized by numerous experimental techniques and investigated for the photocatalytic conversion of CO_2 to CH_4. The TiO_2-SiO_2 mixed oxide photocatalyst prepared in benzene along with ethanol yield 21.0 ppm g^{-1} h^{-1} of methane production; however the material synthesized in hexane shows negligible amount of methane production under simulated solar light irradiation. These results indicate that aromatic nonpolar solvents can tune the textural and photocatalytic properties of photocatalysts compared to non-polar aliphatic solvents.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

The exposure assessment of new POPs in multimedia and development of monitoring technology for POPs alternatives

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포항공과대학교(POSTECH) 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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Risk Assessment of PCDD/Fs and DL-PCBs in Animal Food

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Polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs) and polychlorinated biphenyls (PCBs) are concerned compounds among 12 persistence organic pollutants of the Stockholm convention. These compounds can increase the risk of cancer and cause damage to immune system. The number of 17 PCDD/Fs has TEF (toxic equivalence factor) for calculation of TEQ value. Among the total 209 PCBs, only 12 PCBs congeners which have dioxin-like toxicity are classified as DL-PCBs. The amount of intake and exposure from animal food groups has simultaneously increased through economic development. Animal food samples (78 food, total 502 samples) collected in six cities have been analyzed for a range of dioxins (29 congeners; PCDD/Fs 17 congeners and dioxin-like PCBs 12 congeners) using the isotope dilution method in HRGC/HRMS. For the test method validation, certified reference materials were analyzed. Based on the measured dioxins levels, average daily dietary intake estimates of dioxins were calculated. For risk assessment of PCDD/Fs and DL-PCBs, the data of daily intake from Korea National Health and Nutrition Examination Survey (2008~2010) are considered. The range of detected PCDD/Fs and DL-PCBs (the total sum of PCDD/Fs and DL-PCBs) levels were 0.0000 ? 0.5050 pg WHO05-TEQ/g weight, low fat milk and duck egg, respectively. PCDFs, penta-PCBs and hexa-PCBs in congeners were mainly detected when converted into TEQ (toxicity equivalents). As a result of estimated daily intake and TEQ value, total amount of PCDD/Fs and DL-PCBs exposure to Korea general population was 0.05 pg-TEQ/kg bw/day. On account of Korean TDI (tolerable daily intake) is 4 pg-TEQ/kg bw/day, compared to TDI, daily intake of dioxins via fish ingestion was 1.3%.

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Photocatalytic Water-Splitting with Layer-by-Layer Assembled Photoelectrodes for in situ Regeneration of NAD(P)H

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It has long been a dream of scientists and engineers to realize industrial application of biocatalysts due to their prominent advantages over man-made catalysts. In principle, enzymatic catalysis can be used to synthesize virtually any kinds of chemicals including complex chiral molecules with a high selectivity and yield under mild conditions (e.g. ambient temperature and pressure, neutral pH, aqueous solution). Despite the tremendous benefits of biocatalysts, their practical application has been very limited especially because many useful enzymes consumes expensive cofactors to drive a catalytic reaction. To address such a problem, a huge amount of effort has been made to efficiently recycle cofactors. Among a lot of different methods reported to date, photochemical regeneration method has drawn great attentions from researchers due to its environmental friendliness. We have also previously reported that it is possible to biocatalytically synthesize chiral amino acids such as L-Glu by in situ photochemical regeneration of NAD(P)H cofactors with light-harvesting photosensitizers and electron mediators, the so-called biocatalytic artificial photosynthesis. To date, however, biocatalytic artificial photosynthesis is still at its infancy because sacrificial electron donors are still required for regeneration of cofactors.To address such a problem, a novel method have been introduced to fabricate photoelectrodes in the recent study. Photoelectrodes can split water and produce electrons, provide them to electron mediators, and eventually enable regeneration of cofactors. We found that multiple components for photocatalytic water-splitting can be readily assembled on substrate by a simple layer-by-layer assembly technique. Also, water-splitting activity is shown by the prepared electrode under visible light irradiation. Based on these findings, further integrate biocatalytic assemblies are tried on the photoelectrode to take a step closer into realization of biocatalytic artificial photosynthesis.

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Raman spectral characteristics of toxic chemicals analyzed by a Raman Agent Monitoring System

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A Raman Agent Monitoring System (RAMS) is a technique which exploits Raman scattering to provide stand-off detection and identification of toxic chemicals such as chemical warfare agents and toxic industrial chemicals deposited on the ground surfaces. The RAMS developed by Edgewood Chemical and Biological Center and ITT Corporation collects counts on photons emitted by an agent on a surface through a telescope and displays the result on a spectrograph. Raman scattering occurs when light interacts with a molecule. The molecule vibrates and scatters wavelength shifted light. The wavelength shifts and their associated intensities are dependent on the size, shape, and bond strength of the molecule creating, thus, a distinct spectral signature for the associated chemical. In this research, we measured toxic chemicals with a RAMS and analyzed Raman spectral signatures of Raman signals of that chemicals. These results can assist in selecting unique molecular markers for each chemicals to allow detection and identification of them in ground environments in moving.