일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PLEN-1**
발표분야: 기조강연
발표종류: 특별강연, 발표일시: 목 13:30, 좌장: 김병문

Computations To Explain and Predict: Cycloadditions for Organic Synthesis, Chemical Biology, and Organic Materials

K. N. Houk

Department of Chemistry and Biochemistry, University of California, Los Angeles (UCLA)

Cycloadditions have been known for nearly 100 years and have now been applied to synthesis, materials chemistry, and chemical biology. Examples of these will be described. My group continues to develop theories and models to understand the mechanisms, reactivities, and selectivities of these reactions. Applications of the distortion/interaction model to understand and predict bioorthogonal reactions will be discussed. Molecular dynamics studies of time-resolved imechanisms of cycloadditions give an intimate picture of how molecules react.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 신승훈

Enantioselective Cooperative Organocatalysis using a High-Performance Chiral Anion Generator

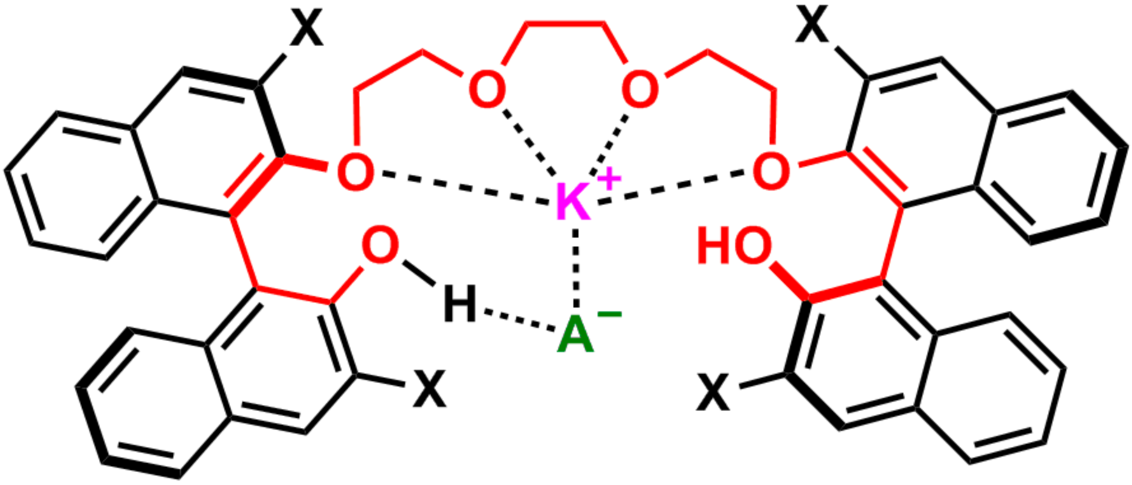
송충의

성균관대학교 화학과

Cooperative catalysis, the simultaneous binding and activation of reacting partners resulting in both the pre-organization of the substrates and stabilization of the transition state structures, is a fundamental principle in enzymatic catalysis. For cooperative catalysis using small organic molecules, we recently developed a new structural motif for multifunctional catalysts that can be used to generate a chiral anion from an inorganic salt in “one phase”. Using this chial anion generator as an organocatalyst, excellent catalytic activity and enantioselectivity have been achieved for a range of organic reactions. The single crystal X-ray structure of the complex of the catalyst and a potassium salt (e.g. KF) provides interesting insight into the origin of the catalytic activity and stereoselectivity.[1-3]

References:

1.*Angew. Chem. Int. Ed.* 2009, *48*, 7683-7686.
2.*Angew. Chem. Int. Ed.* 2010, *49*, 8915-8917.
3.*Nature Communications* 2012, *3*, 1212.



Chiral Bis-Hydroxy Polyether

Chiral Anion Generator

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **POLY1-1**

발표분야: Photoresponsive Materials

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 손해정

Conjugated polymers and conjugated polyelectrolytes for organic photovoltaic cells

우한영

부산대학교 나노과학기술대학 나노융합공학과

Recently, bulk-heterojunction (BHJ) polymer solar cells (PSCs) have been extensively studied as one of the attractive renewable energy sources due to low cost, light weight, solution processibility and potential applications in flexible large-area devices. Here, we report semi-crystalline planar donor-acceptor type (D-A) alternating copolymers as a photovoltaic material for polymeric solar cells. In addition, interfacial engineering between the inorganic metal oxide and organic active layers using the ionic conjugated polyelectrolytes (CPEs) layer has been developed for high efficiency inverted-type organic optoelectronic devices. Spontaneously oriented interfacial dipoles within the CPE layer lower the energy barrier for electron injection/transport and reduce the interfacial contact resistance and inherent incompatibility between the hydrophilic metal oxide and hydrophobic active layers. The amphiphilic CPE layer provides an excellent alternative to interfacial engineering of the metal oxide/organic semiconductor interface in optoelectronic devices, such as iPSCs and iPLEDs.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY1-2**
발표분야: Photoresponsive Materials
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 손해정

Effects of Solubilizing Group Modification in Fullerene Bis-adducts on Polymer Solar Cells

김범준

한국과학기술원(KAIST) 생명화학공학과

Structural control of solubilizing side groups in fullerene?based electron acceptors is critically important to optimize their performance in bulk heterojunction (BHJ)?type polymer solar cell (PSC) devices. The structural changes of fullerene derivatives affect not only their optical and electrochemical properties but also their solubility and miscibility with electron donor polymers. Herein, we synthesized a series of o?xylenyl C60 bis?adduct (OXCBA) derivatives with different solubilizing side groups to systematically investigate the effects of fullerenederivative structures on the photovoltaic properties of PSCs. End group modifications of OXCBA dramatically affect photovoltaic performance in blend films with poly(3?hexylthiophene) (P3HT), resulting in power conversion efficiencies (PCEs) ranging from 1.7 to 5.3%. We found that this large range in PCE values is mainly due to differences in the blend morphology and interfacial area of the P3HT:OXCBA derivative films caused by changes in the hydrophobicity of the OXCBA derivatives and their interfacial interaction with P3HT. The trend in photovoltaic performance of the different OXCBA derivatives agrees well with those of the interfacial tension, PL quenching, and exciton dissociation probability, which suggests that changes in the interfacial interaction with P3HT are largely responsible for their photovoltaic performances.

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장소: 일산KINTEX
발표코드: **POLY1-3**
발표분야: Photoresponsive Materials
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 손해정

Exceeding the Limit in Organic Solar Cells

Xiaoyang Zhu

Columbia University, USA

This lecture aims to explore key mechanistic issues in an emerging photovoltaic technology based on organic and polymeric molecules, i.e., plastic solar cells. While there have been various predictions on whether or when photovoltaic technologies, including plastic solar cells, can be cost-competitive with electric power generation based on fossil fuels, on sometimes neglects the most important outcomes of fundamental research: the serendipity, the unpredictable, and the ground breaking discoveries that can throw the foundation of old predictions out of the window. I will present two examples from recent research in my laboratory on organic photovoltaics. The first example is within the realm of conventional theories and we aim to understand a critical step in charge separation at donor/acceptor interfaces in organic photovoltaics, namely the formation and dissociation of interfacial charge transfer excitons [1]. In particular, we show the critical role of hot charge transfer excitons in setting the fundamental time limit for charge separation in organic photovoltaics [2]. The second example illustrates the serendipity and potentially groundbreaking nature of research. We show how an intriguing physical phenomenon, exciton fission in which a singlet exciton breaks up into two triplet excitons in organic semiconductor materials, may be used to build solar cells with power conversion efficiency exceeding the fundamental limit (the so-called Shockley-Queisser limit) of conventional solar cells. We show how singlet exciton fission can occur in organic semiconductors due to a many electron quantum coherent process [3-4], and how we can efficiently extract two electrons from the quantum superposition [5].[1] M. Muntwiler, Q. Yang, W. A. Tisdale, X.-Y. Zhu, Phys. Rev. Lett. 101 (2008) 196403.[2] A. Jailaubekov, A. P. Willard, J. Tritsch, W. L. Chan, N. Sai, L. Kaake, R. I. Gearba, K. Leung, P. J. Rossky, X.-Y. Zhu, Nature Mater. 12 (2013) 66-73.[3] W.-L. Chan, M. Ligges, A. Jailaubekov, L. Kaake, L. Miaja-Avila, X.-Y. Zhu, Science 334 (2011) 1541-1545.[4] W. L. Chan, M. Ligges, X.Y. Zhu, “The energy barrier in singlet fission can be overcome

through coherent coupling and entropic gain," Nature Chem. 4 (2012) 840-845.[5] W.-L. Chan, J. R. Tritsch, X.-Y. Zhu, J. Am. Chem. Soc. 134 (2012) 18295-18302.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY1-4**
발표분야: Photoresponsive Materials
발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 김범준

Photonic crystal geometry for organic solar cells

고두현

한국과학기술연구원(KIST) 광전융합시스템연구단

Photonic crystal solar cells have the potential for addressing the disparate length scales in polymer photovoltaic materials, thereby confronting the major challenge in solar cell technology: efficiency. One must achieve simultaneously an efficient absorption of photons with effective carrier extraction. Unfortunately the two processes have opposing requirements. Efficient absorption of light calls for thicker PV active layers whereas carrier transport always benefits from thinner ones, and this dichotomy is at the heart of an efficiency/cost conundrum that has kept solar energy expensive relative to fossil fuels.This dichotomy persists over the entire solar spectrum but increasingly so near a semiconductor's band edge where absorption is weak. We report a 2-D, photonic crystal morphology that enhances the efficiency of organic photovoltaic cells relative to conventional planar cells. The morphology is developed by patterning an organic photoactive bulk heterojunction blend of Poly(3-(2-methyl-2-hexylcarboxylate) thiophene-co-thiophene) and PCBM via PRINT, a nano-embossing method that lends itself to large area fabrication of nanostructures. The photonic crystal cell morphology increases photocurrents generally, and particularly through the excitation of resonant modes near the band edge of the organic PV material. The device performance of the photonic crystal cell showed a nearly doubled increase in efficiency relative to conventional planar cell designs.

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발표코드: **POLY1-5**
발표분야: Photoresponsive Materials
발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 김범준

Highly Efficient Polymer Optoelectronic Devices by Plasmonic Silver Nanoparticles

김진영

울산과학기술대학교(UNIST) 친환경에너지공학부

Surface plasmons are waves associated with strongly enhanced electromagnetic fields occurring on the surface because of their interaction with the free electrons of the certain metals. The coupling of surface plasmons and excitons in organic materials can improve the performance of organic optoelectronic devices. ITO-free polymeric electronic devices (PEDs) are successfully demonstrated by replacement of the ITO electrode with a solution-processed PEDOT:PSS electrode containing Ag nanoparticles (NPs). Enhanced optical and electrical properties of PEDOT:PSS electrode with Ag NPs have resulted in efficiency increases of 124% for polymer light-emitting diodes (PLEDs) and 32% for polymer solar cells (PSCs) compared to devices without the Ag NPs. Furthermore, we have demonstrated highly efficient PEDs using carbon dot-supported silver nanoparticles (CD-Ag NPs) and high-performance PSCs using plasmonic effect of multi-positional silica-coated silver nanoparticles. The achievements of our PEDs are a major step toward high efficiency PLEDs and PSCs that can be fabricated in large areas using low cost printing and coating technologies.

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장소: 일산KINTEX
발표코드: **POLY1-6**
발표분야: Photoresponsive Materials
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 김범준

Conjugated polymers for visible to near IR photon harvesting

김은경

연세대학교 화학공학과

Conjugated polymers (CPs) have been collected strong interests for their tunability of colors, and low cost of preparation for organic devices. Herein we report preparation of CPs for visible and near IR photon harvesting. For a maximum conversion efficiency, we optimized monomer structure and doping states of the CPs to facilitate charge transport process. In addition, light harvesting structures were prepared to give high photo conversion efficiency from CP based cells.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY2-1**
발표분야: Synthesis and Application of Microporous Polymer Networks
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 홍창섭

Carbon Dioxide Capture with Porous Coordination Polymers and Organic Polymers

백명현

서울대학교 화학부

Carbon dioxide capture from the industrial flue gas has become one of the most important issues in recent scientific community, since increase in carbon dioxide concentration is implicated in global warming. Industry flue gas contains not only carbon dioxide but also other gases, and its composition is dependent on the combustion methods. Porous coordination polymers (PCPs) and porous organic polymers (POPs) have great potentials to be applied in carbon dioxide capture. To apply them in capturing CO2 from the industry flue gas, they should have high carbon dioxide adsorption capacity and high adsorption selectivity over other gases. In this lecture, various synthetic strategies of PCPs and POPs as well as their pore modification methods, which have been developed in our laboratory for carbon dioxide capture application, will be discussed.

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장소: 일산KINTEX

발표코드: **POLY2-2**

발표분야: Synthesis and Application of Microporous Polymer Networks

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 홍창섭

Computational Approach to the Design of Porous Materials for Gas Capture and Separation

정유성

한국과학기술원(KAIST) EEWS 대학원

In addressing the carbon emission problem, amine solutions such as monoethanolamine (MEA) are widely used in industry, yet their recovery costs are very high and notably corrosive. Porous solids that capture through physical adsorption rather than chemical absorption can have many advantages compared liquid based sorbents, including low recovery costs. Often, however, a big challenge in the design of new porous materials with high carbon uptakes is to introduce functional groups with high binding affinity towards CO2 but with low affinity for other gases such as N2. In this talk, I will present a few general aspects of carbon dioxide adsorption on to various porous solids, including how to tune binding affinities of various gases towards the building blocks of metal-organic framework (MOF), zeolite-imidazole framework (ZIF), and covalent-organic polymer (COP). Energy decomposition analysis can help understand the underlying adsorption mechanism which can then further inspire experimental design. Another point of discussion in this talk will be the magnetism in MOFs induced by gas adsorption. The origin of the latter novel magnetic phenomenon in porous crystal materials will be discussed.

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발표코드: **POLY2-3**
발표분야: Synthesis and Application of Microporous Polymer Networks
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 정유성

Metal-Organic Frameworks: Gas Adsorption and Other Intriguing Properties

홍창섭

고려대학교 화학과

Metal-organic frameworks (MOFs) are a class of porous, crystalline adsorbents that have recently attracted much attention for use in gas separations. The high tunability of their design may enable greater functionality with reduced adsorbent mass and volume compared to traditional solid adsorbents. Among the most interesting features of some MOFs is the presence of coordinatively-unsaturated metal centers (open metal sites) along the pore surfaces. These five-coordinate metal cations, known to behave as Lewis acids that strongly polarize gas adsorbents, are further amenable to post-synthetic functionalization. This talk will present the sorption and other physical properties of 3D networks with open metal sites. Sorption properties combined with other properties will be demonstrated in a single MOF. Also, extended version of MOF-74 featuring ~20 ?-wide channels with high-density open metal sites will be introduced and its exceptional CO2 adsorption properties will be discussed before and after functionalization with amines.

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장소: 일산KINTEX
발표코드: **POLY2-4**
발표분야: Synthesis and Application of Microporous Polymer Networks
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 정유성

The CO_2 Caves: Effective Carbon Capture by Nanoporous Covalent Organic Polymers

YAVUZCAFERTAYYAR

한국과학기술원(KAIST) EEWS대학원

Carbon dioxide capture and separation is an unresolved challenge tampering the feasibility of fossil fuels for energy production. Porous materials have long been evaluated for next generation CO_2 adsorbents. Crystallinity, however, is not needed for trapping gases as periodicity or order is not required in the sorbent solids. A good analogy would be that gases are like animals and simple caves would suffice to house them; crystal palaces are not necessary. Porous polymers - robust, inexpensive and amorphous - show promise as feasible materials for the capture of CO_2 from warm exhaust fumes. We report the syntheses of porous covalent organic polymers (COPs) with CO_2 adsorption capacities of up to 5616 mg/g (a world record - measured at high pressures, i.e. 200 bar) and industrially relevant temperatures (as warm as 65 ^{o}C). COPs are stable in boiling water for at least one week, in air up to 400 ^{o}C and theoretical calculations refer to an amorphous extended framework as density is likely the main reason for exceptional CO_2 capacities. COPs also show near infinite CO_2/H_2 selectivity and the highest CO_2/N_2 selectivity (288) to date. The latter is found to be due to a new concept of N_2-phobicity. Post combustion carbon capture from fossil fuel power plants demands pressures of up to 6 bar and a minimum temperature of 40 ^{o}C. By tuning their architecture, we show that COPs reach to 3 mmol CO_2/g sorbent at 6 bar and 45 ^{o}C. High and low pressure capacities make these porous polymer structures viable alternatives to amine scrubbers.

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발표코드: **POLY2-5**
발표분야: Synthesis and Application of Microporous Polymer Networks
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 정유성

Organic Sol-Gel Synthesis of Porous Covalent Molecular Networks

박지웅

광주과학기술원(GIST) 신소재공학부

Polymerization of rigid organic building blocks with multiple reactive functional groups yields microporous organic networks whose pore sizes approach molecular length scales. We present the first sol-gel processable, microporous organic molecular networks which are synthesized via a two-stage mechanism involving the formation of colloidal dispersions and the subsequent growth to monolithic networks by solvent evaporation, analogous to the sol-gel synthesis of inorganic oxide networks. The molecular networks synthesized via the organic sol-gel method are readily processed into coatings, free-standing films, nanoparticles with desired functionalities and sizes, and nanocomposites with other polymer matrices. Of particular interest is that the organic sol-gel method offers exceptionally simple ways to fabricate porous molecular network membranes. The potentials of the organic-sol-gel-based porous molecular networks as new ultra- or nanofiltration membranes will be discussed.

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장소: 일산KINTEX
발표코드: **POLY3-1**
발표분야: Current Trends in Polymer Sensors Research
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 곽기섭

Porphyrin-based sensors for selective ion binding

장우동

연세대학교 화학과

Porphyrins and chlorophylls are essential pigments in natural system. In biological systems, porphyrins and chlorophylls perform many essential functions, such as oxygen transport, active site in enzyme, and light harvesting. The functional porphyrin derivatives in biological systems provide various motivations for the design of biomimetic functional materials. Using the porphyrin moieties, we recently have designed several types of receptor molecules for the bindings of anionic and cationic species. The design of synthetic receptors is an important issue in supramolecular chemistry. Hydrogen bonding and electrostatic interactions allow the binding and transport of anions in biological systems, such as sulfate- and phosphate-binding proteins. Along this line, several indole-based anion receptors have been developed, in which the -NH protons in the indole moieties bind strongly to several anions via hydrogen bonds. It is well known that zinc porphyrin works as a Lewis acid by accepting axial ligands with lone pairs of electrons. By combining zinc porphyrins and biindole, we designed a new type of molecular tweezers and macrocyclic receptor for the simultaneous binding of DABCO as well as anionic guests. The molecular tweezers and macrocycle exhibited strong positive allosteric effect when the guest molecules binding into the cavities.

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장소: 일산KINTEX

발표코드: **POLY3-2**

발표분야: Current Trends in Polymer Sensors Research

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 곽기섭

Coordination Polymer Gels with Important Environmental and Biological Applications

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 on the applications of gel forming functional ligands and metal ions to sensing, drug-delivery and catalysis that have been developed over the past three to five years. Selected 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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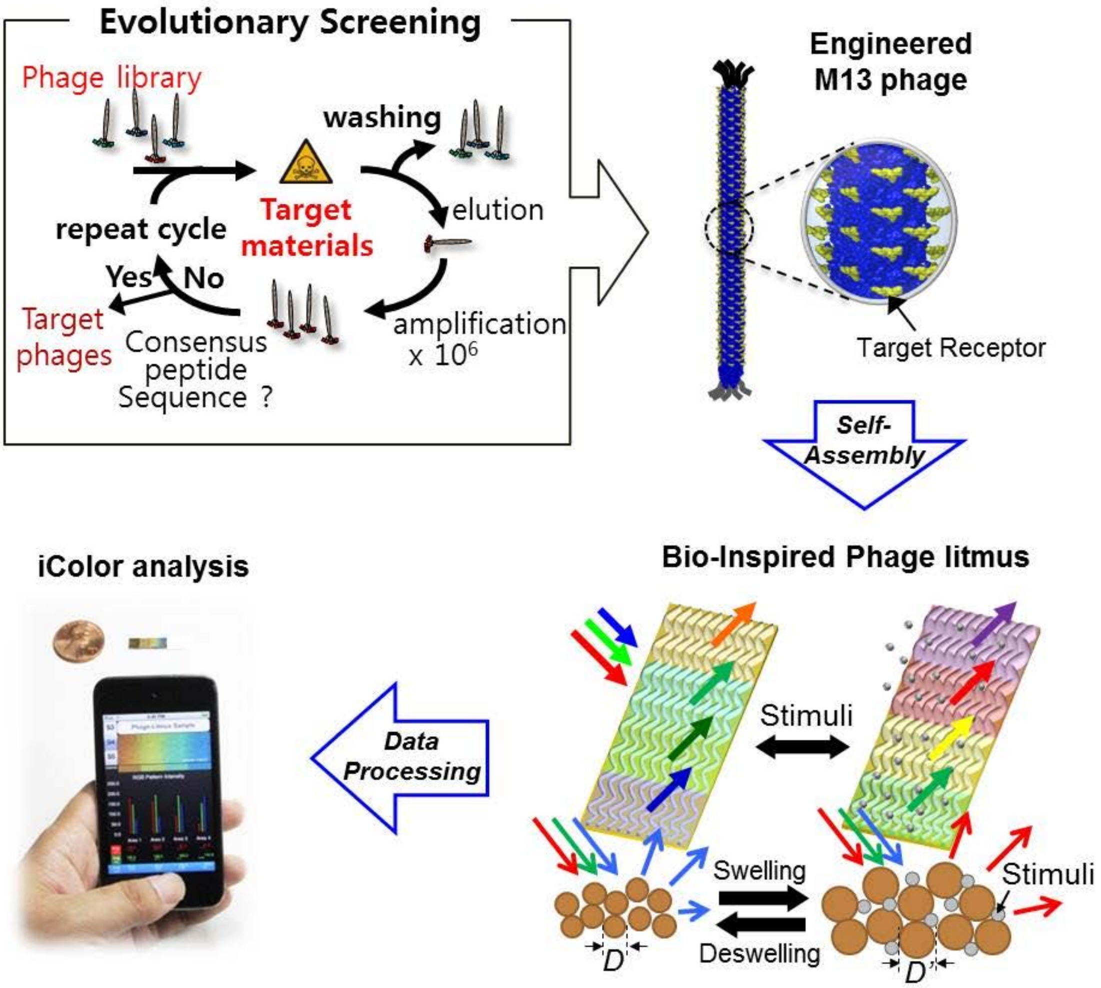
발표분야: Current Trends in Polymer Sensors Research
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 곽기섭

Phage Litmus: Biomimetic Virus-Based Colorimetric Sensors for Explosive Detection

오진우

부산대학교 나노소재공학과

Nature utilizes various of the colorization process. Some species of birds can express their mood of tempers by changing their collagen structures on skin. For example, turkey can change their skin color by expansion of the collagen structures, which are associated with the distinct color changes. Here, we developed bioinspired virus-based colorimetric sensors which can be genetically tuned for target molecule. Using M 13 bacteriophage, we fabricated responsive self-assembled color matrices composed of quasi-ordered fiber bundle structures. These virus matrices can exhibit color change by stimuli through fiber bundle structure modulation. Upon exposure of volatile organic compounds, the resulting multi-colored matrices exhibited distinct color changes with different ratios that can be recognized by the naked eyes. Using the directed evolutionary approaches, we genetically engineered the virus matrix to incorporate binding motif for explosive detection (i.e., trinitrotoluene (TNT), and polybrominated diphenyl ethers (PBDEs)). Through utilizing a common handheld device (i.e., iPhone), we could distinguish TNT molecules down to 20 ppb in a selective manner. Our novel biomimetic virus colorimetric sensor can overcome current limitation for low response selectivity.


Evolutionary Screening
Phage library
washing
Target materials
elution
repeat cycle
Yes
No
Target phages
Consensus peptide Sequence ?
amplification x 10⁶
Engineered M13 phage
Target Receptor
Self-Assembly
Bio-Inspired Phage litmus
Stimuli
Swelling
Deswelling
Stimuli
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D'
Data Processing
iColor analysis

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발표코드: **POLY3-4**
발표분야: Current Trends in Polymer Sensors Research
발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 오진우

Transformation of the Programmed 2D Structures to the 3D Objects

정광운

전북대학교 고분자.나노 공학과

Color-tunable three-dimensional (3D) actuators were successfully fabricated by the combination of the physical principle of actuators with the basic concept of photonic crystals, By controlling the d-spacings and the refractive index contrasts of the self-assembled 3D colloidal photonic crystals, colours of the photonic actuators were tuned. The reversible 3D photonic actuators transformed from the programmed 2D structures via the bending, twisting and folding mechanisms may be applied in the field of mechanical actuators, and optoelectronic and bio-mimetic devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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발표분야: Current Trends in Polymer Sensors Research
발표종류: 심포지엄, 발표일시: 금 12:10, 좌장: 오진우

Fluorescent conjugated polymers as biological and chemical stimuli-responsive platforms

이택승

충남대학교 유기소재섬유시스템공학과

Fluorescent conjugated polymers are being extensively investigated for their potential applications in the fields of optoelectronics, microelectronics, and chemical and biological sensors. Especially, water-soluble conjugated polymers have been attracted a great deal of attention because of their unique optoelectronic properties, which may serve as a basis for a new generation of optoelectronic devices and biochemical detection such as DNA, proteins, and biological agents. Their peculiar properties stem from the combination of optoelectronic properties of conventional conjugated polymers and water solubility induced by ionic nature of polyelectrolytes. Their optoelectronic properties can be easily tuned through the structural alteration of the conjugated structure of the polymer backbones, and the ionic functionality endows them with exceptional features such as electrostatic interaction with oppositely charged species, a high sensitivity toward fluorescence quenchers and fluorescence change with aggregation.The aggregation-induced blue-to-green solution fluorescence change can be subsequently used for sensing of oppositely charged species. In a dilute, well-dissolved ionic conjugated polymer solution, exciton transport can be approximated by a one-dimensional random walk within an isolated polymer chain. However, if the polymers are aggregated within close proximity to each other, interchain exciton migration becomes possible, and a three-dimensional random walk becomes available to the migrating exciton. Using this mechanism, charged conjugated polymer could detect protein through their electrostatic interaction.

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발표코드: **POLY3-6**
발표분야: Current Trends in Polymer Sensors Research
발표종류: 심포지엄, 발표일시: 금 12:40, 좌장: 오진우

Novel liquid crystal sensors for protein detections

박수영

경북대학교 고분자공학과

5CB (nematic liquid crystal, 4-cyano-4?-pentylbiphenyl) microdroplets coated with PAA-b-LCP (PAA: poly(acrylic acid), PAA: poly(4-cyanobiphenyl-4-oxyundecylacrylate)) and PNIPAM-b-LCP (PNIPAM : poly(N-isopropylacrylamide)) were successfully made via microfluidics. Their functionalized surfaces of the 5CB microcroplets were examined for detection of several proteins such as lysozyme (LSZ) and bovine serum albumin (BSA) which could be easily visualized with an optical microscope under crossed polarizers by the radial to bipolar configurational change of the 5CB. This transition was strongly dependent on the electrostatic state of the PAA chain and the hydrophilic/hydrophobic state of the PNIPAM chain, which were controlled by pH and temperature of the aqueous protein solutions, respectively. This study demonstrated a simple approach for the development of a liquid crystal-based sensor for label-free detection of proteins, which may have diverse applications in various biomedical fields.

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발표코드: **IND1-1**

발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 유복렬

저배위 실리콘 화학종의 합성과 반응성 응용

한준수

한국과학기술연구원(KIST) 물질구조제어연구단

Si-Si 간의 이중결합, 삼중결합 및 carbene 의 유사체인 silylene 과 같은 저배위 실리콘 화학종은 실리콘 화합물의 직접합성, 열분해 반응 및 기상법에 의한 박막형성 과정 등의 중간체로 제안되어 왔으나 고반응성 및 불안정성으로 인하여 그 확인이 불가능했었다. 따라서 입체장해가 큰 치환체를 도입하는 방법으로 실온에서 안정한 저배위 실리콘 화학종을 합성하여 그 반응성 및 특성을 연구하고 있다. 본 발표에서는 실온에서 안정한 Si-Si 간의 이중결합, 삼중결합의 저배위 실리콘 화학종의 합성방법과 그 특성 및 반응성에 관한 결과를 보고하고자 한다.

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발표코드: **IND1-2**
발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 유복렬

Synthesis and Applications of Silafluorene Derivatives having Catity Structure

손홍래

조선대학교 화학과

Silole and silafluorene showing the striking optical properties such as an aggregation-induced emission enhancement (AIEE) were used for chemical- and bio-sensor applications. Silole derivatives exhibit weak photoluminescence (PL) in common organic solvents, but if they become nanoaggregates (NA), their efficiency of PL is surprisingly increased by few decade times. Silole derivatives exhibited FRET between polysilane and silole derivatives to give highly photoluminescent silole-cooperated organic nanoparticles. Silole derivatives have also been shown to have potential as chemosensors for detecting explosives. For example, poly(tetraphenyl)silole has been shown to detect nitroaromatics, including TNT, with high sensitivity. However the silole derivatives were not able to detect other type of explosives such as nitroamines and nitrate esters.Silafluorene derivatives containing iptycene moiety in the benzene ring were synthesized and their electronic and photonic behaviors have been investigated. Their emission behaviors and quantum yield for these compounds were investigated to characterize optical property for possible applications such as an explosive sensor and OLED. The iptycene silafluorene derivatives were used as a chemosensor to detect nitroamines, nitroaromatics and nitrate esters. The detection efficiency of silafluorene derivatives for TNT exhibited 100 times higher than that of silole derivatives. X-ray single crystal structure of dimethyliptycenesilafluorene revealed that the packing diagram of dimethyliptycenesilafluorene possessed a cavity structure in the solid state. The size of cavity was about 1.2 nm. The formation of cavity might allow grabbing of explosive molecules to increase the detection efficiency for explosives.

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장소: 일산KINTEX
발표코드: **IND1-3**
발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 유복렬

Big Is Beautiful: Carbosilane Dendrimers Its Preparation and Usability

김정균

동아대학교 화학과

This is a report on novel carbosilane dendrimers containing branches with Si-C and Si-O-C bonds. Introduction of organic moieties into the dendrimers is performed by hydrosilation of carbon-carbon double/triple bonds. Versatile organic or organometallic moieties are introduced onto the peripheral regions of dendrimers by coupling and complexation reactions, which clearly demonstrates their potential for variation. Dendrimers of unique architecture containing a single kind of multi-functionality have been of increasing interest during the last three decades. Their shapes, sizes, and structures are defined by their preparation and characterization.

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장소: 일산KINTEX
발표코드: **IND1-4**
발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites
발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 손홍래

Siloxane Block Copolymers for the Enhancements of Nanolithography and Nonvolatile Memories

정연식

한국과학기술원(KAIST) 신소재공학과

The self-assembly of Si-containing block copolymer (BCP) thin films and simple plasma oxidation can produce tailored SiOx nanostructures with tunable geometry, size, and density. To begin with, this talk will present how the self-assembly of Si-containing BCPs can be utilized for sub-10 nm pattern formation with a high throughput. Recent results on the self-assembly of siloxane BCPs for the achievement of sub-10 nm resolution, fast pattern generation, transfer-printing capability onto nonplanar substrates, and device applications for nonvolatile memories will be introduced. This talk will also report the direct formation of ordered memristor nanostructures on metal and graphene electrodes by the self-assembly of Si-containing BCPs. This approach offers a practical pathway to fabricate high-density resistive memory devices without using high-cost lithography and pattern-transfer processes. Finally, this talk will present a novel approach that can relieve the power consumption issue of phase-change memories by incorporating a thin SiOx layer formed by BCP self-assembly, which locally blocks the contact between a heater electrode and a phase-change material and reduces the phase-change volume. The writing current decreases by 5 times (corresponding to a power reduction of 1/20) as the occupying area fraction of SiOx nanostructures varies.

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발표코드: **IND1-5**

발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites

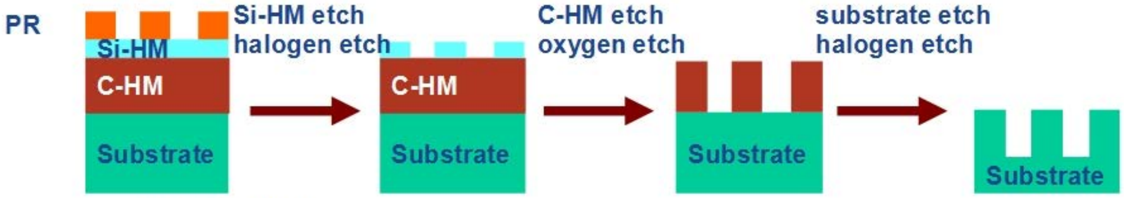
발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 손홍래

Silicon Materials for Spin-On Hardmask Process

조현모

연세대학교 실리콘 신소재 센터

In the recent semiconductor manufacturing, as linewidths decrease, thinner photoresists (PRs) are adopted to prevent collapse of patterned PR caused by high aspect ratios. But, the thin photoresists could not fully provide deeper etched patterns on substrates in ArF (193 nm) lithography process. To solve this problem trilayer schemes have been designed (Figure 1). The trilayer stack consists of a PR, an oxygen plasma-resistant hardmask (usually Si-HM) which serves as a mask when patterns of Si-HM is transfer to a C-HM, and a halogen plasma-resistant HM (usually C-HM) which serves as a mask when patterns of C-HM is transfer to substrates. The etch rate of silicon-containing material is low for oxygen plasma and is high for halogen plasma, while the etch rate of organic material is low for halogen one and is high for oxygen one. Such etch selectivities of organic and inorganic materials enable to make deep etched pattern.Since Si-HM is under-layer of PR in trilayer scheme, Si-HM should absorb 193 nm light for anti-reflecting at ArF exposure step to make well-established PR pattern. Thus, deep UV (193 nm) absorption as well as oxygen plasma-resistance is required for Si-HM materials. Even though a high silicon or a silica content in Si-HM is necessary to achieve high oxygen plasma-resistance, aryl groups (usually phenyl groups) have been incorporated into Si-HM materials to meet optical property, resulting the increase of an organic content to make oxygen plasma-resistance lower. To resolve this issue, we have investigated to get optimized Si-HM materials which increase a silicon or a silica content of Si-HM along with proper optical property at 193 nm. In this presentation, those results will be presented in detail.


PR
Si-HM
C-HM
Substrate
Si-HM etch
halogen etch
C-HM
Substrate
C-HM etch
oxygen etch
Substrate
substrate etch
halogen etch
Substrate

HM = HardMask

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장소: 일산KINTEX
발표코드: **IND1-6**
발표분야: Recent Trends in High Functional Silicon-Containing Polymers and Fine Composites
발표종류: 심포지엄, 발표일시: 목 11:45, 좌장: 손홍래

Development of the Futuristic Silicone Encapsulant for LED

김우한

제일모직 LEDSE

Optically transparent polymers have been researched in various applications such as the fabrication of microlenses, optical coatings, and the encapsulation for optoelectronic devices [1]. With the increasing demands for high performance in these applications, a high refractive index and high realiability are important for the optical efficiency and lifetime of the devices [2]. These reliabilities require stable transparency and resistance to external chemical aggression or thermal decomposition for high power devices which need high current and thus high thermal load are involved in [3]. Encapsulation materials for optoelectronic devices such as light emitting diodes (LEDs) are especially sensitive to thermal stability and moisture / gas permeability, because moisture / gas permeation through encapsulation material causes the corrosion of metal lead frame and reflector. Thermal decomposition decreases transparency and reduces the light extraction efficiency from these devices. For example, device reliability and lifetime in high-brightness LEDs can be limited by the capability of the encapsulation materials [4]. Also, a high refractive index in the encapsulation material is required for high efficiency light extraction from an LED, significantly improving its illumination performance. Thus, the key factors of LED encapsulation materials are excellent transparency, high refractive index, and high resistance to heat, moisture, gas, and chemical reactions. Thermal stability at high temperature and high resistance in moisture / gas permeation are the most desirable combination for use in high power LED encapsulation and would bring the long lifetime and high efficiency of device performance. We confirmed that Cheil’s polysiloxane has a sufficient hardness to protect the LED from thermal stress during operation and from external forces. Also, these polysiloxanes has high resistance of oxygen and moisture permeation comparing with commercial polysiloxanes. These properties are the most important advantages for use as LED encapsulation.

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발표분야: Recent Trends in Carbon-Containing Materials
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 전용석

Raman analysis of the micro-structure and oxidation behaviors of the commercial carbon fibers

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전남대학교 고분자 섬유 시스템공학과 [1]대구대학교 과학교육학부 [2]전남대학교 신화학소재공학과

The micro-structure and defect of the carbon fibers are the determining factors of their physical and mechanical properties. The R values (Intensity of D/Intensity of G band) were determined by the Raman analysis and the values were visualized with various colors. The carbon fiber is sensitively oxidized depending on the contact area of the micro-domain of the carbon fiber at above 500℃ and the property limits their application condition. This study includes the oxidation dependence on the micro structures of the carbon fibers. In general, the more crystalline fibers, the higher the oxidation resistive was. The diameter reduction ratio value at 50wt% burn-off and surface morphologies deduced to 4 classifications of the oxidation mechanism as: oxidation from the surface of the fiber due to its dense microstructure as high modulus polyacrylonitrile(PAN) based fiber; oxidation from the large crystallite surface through the diffusion of oxygen along the pores among as high modulus pitch based graphitized fiber; oxidation from the relatively small crystallite surface due to the porous structure with low crystallinity as rayon based carbon fiber; and oxidation showing the characteristics of the medium of 1st and 2nd cases as PAN based carbon fiber.

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발표코드: **IND2-2**

발표분야: Recent Trends in Carbon-Containing Materials

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 전용석

탄소계 복합소재의 제조 및 응용

양철민

한국과학기술연구원 (KIST) 복합소재기술연구소

최근 탄소계 복합소재는 우주항공/자동차, 전기/전자, 에너지/환경 등의 분야로 적용범위가 급속히 확대되고 있는 추세이다. 이러한 추세에 따라 경량이면서 고강도, 다기능성, 그리고 성형가공성이 우수한 탄소계 고분자 복합소재의 제조 및 응용 기술이 크게 주목 받고 있다. 고분자소재는 다양한 장점에도 불구하고 금속 등 기존소재와 비교해서 매우 낮은 기계적 물성을 보이기 때문에, 탄소계 보강재를 고분자와 복합화함으로써 고분자소재의 고강도화와 동시에 다양한 기능성을 부여하여 제품의 부가가치를 극대화하는 연구개발이 활발히 진행되어 오고 있다. 국내의 경우, 탄소소재 및 복합소재에 대한 핵심기술을 확보하지 못해 국내 수요의 대부분을 수입에 의존하고 있는 상황이다. 또한, 탄소계 복합소재는 다양한 활용성과 우수한 성능에도 불구하고 소재 가격이 고가이고, 대량생산의 한계, 요소기술의 미확보 등이 시장확대의 걸림돌이 되고 있다. 본 발표에서는 탄소섬유강화 고분자 복합소재와 나노분산 고분자 복합소재, 그리고 에너지 및 전자분야에 적용되고 있는 탄소계 복합소재의 제조 및 응용에 있어서의 요소기술 및 개발동향에 대해 소개하고자 한다.

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발표코드: **IND2-3**
발표분야: Recent Trends in Carbon-Containing Materials
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 전용석

Ordered mesoporous porphyrinic carbon catalysts with Pt-like electrocatalytic activity for oxygen reduction

주상훈

울산과학기술대학교(UNIST) 나노생명화학공학부

The high cost of polymer electrolyte fuel cell (PEFC) systems, predominantly dictated by the platinum-based cathode catalysts for the oxygen reduction reaction (ORR), has critically impeded the widespread application of PEFCs. Therefore, the quest for low-cost yet high-performance non-precious metal catalysts has been of prime importance in recent years. However, the ORR activity of the non-precious metal catalysts is still fairly inferior to the Pt-based catalysts. In this presentation, the preparation of a new class of self-supported, transition metal-doped ordered mesoporous porphyrinic carbon (M-OMPC; M = Fe, Co, or FeCo) catalysts with high surface areas and tunable pore structures will be presented. Of M-OMPC catalysts, FeCo-OMPC exhibited an extraordinarily high ORR activity in an acidic medium, which was the best among the non-precious metal catalysts reported in the literature, and outperformed the carbon-supported Pt (Pt/C) catalyst. Furthermore, the FeCo-OMPC showed superior long-term durability and methanol-tolerance in ORR. The weakening of the interaction between oxygen atom and the FeCo-OMPC compared to Pt/C as well as high surface area of the former could be responsible for its significantly high ORR activity.

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발표코드: **IND2-4**
발표분야: Recent Trends in Carbon-Containing Materials
발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 양철민

TiO2 nanoparticles loaded on graphene/carbon composite nanofibers by electrospinning for increased photocatalysis

김보혜[*] 김창효[1] 양갑승[2,*]

대구대학교 과학교육학부 [1]전남대학교 고분자섬유시스템공학과 [2]전남대학교 고분자 섬유 시스템공학과

Graphene/carbon composite nanofibers (CCNFs) with attached TiO2 nanoparticles (TiO2-CCNF) were prepared, and their photocatalytic degradation ability under visible light irradiation was assessed. They were characterized using scanning and transmission electron microscopy, X-ray diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy, and ultraviolet?visible diffuse spectroscopy. The results suggest that the presence of graphene embedded in the composite fibers prevents TiO2 particle agglomeration and aids the uniform dispersion of TiO2 on the fibers. In the photodegradation of methylene blue, a significant increase in the reaction rate was observed with TiO2 -CCNF materials under visible light. This increase is due to the high migration efficiency of photoinduced electrons and the inhibition of charge?carrier recombination due to the electronic interaction between TiO2 and graphene. The TiO2-CCNF materials could be used for multiple degradation cycles without a decrease in photocatalytic activity.

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발표코드: **IND2-5**
발표분야: Recent Trends in Carbon-Containing Materials
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 양철민

Carbon materials applications for dye sensitized solar cells.

전용석

울산과학기술대학교(UNIST) 친환경에너지공학부

Dye-sensitized solar cells (DSSCs) have attracted much attention because of their advantages like low cost, easy fabrication, and high solar-to-electricity conversion efficiency. Since they can be fabricated on transparent and flexible substrate, they offer very promising potential for real applications such as building integrated photovoltaic system, automobile window photovoltaic system, and portable solar cell embedded in flexible display system. The typical DSSC consists of a dye-sensitized mesoscopic TiO2 photoanode, a Pt counter electrode, electrolyte with I3-/I- redox couple. Operation of the DSSC is initiated by light-induced oxidation of dye molecules. The oxidized dye molecules accept electrons from iodide ions in electrolyte, and the resulted tri-iodide ions are reduced back to iodide ions at the counter electrode. One of most important challenges in the recent development of DSSCs is to substitute the Pt counter electrode with maintaining high conversion efficiency because it is a rare and expensive material and so a barrier for large-scale fabrication. Requirements of materials to replace Pt in the counter electrode are high charge exchange current during redox reaction (high electrocatalytic activity), resistance to corrosive electrolyte environments containing iodide, and transparency. So far, many research efforts have been made to find possible substituents which are CoS and carbonaceous materials like carbon black, carbon nanotubes, and graphene. Coating of such carbon materials should be thick for high surface area because they show low charge exchange current, providing a disadvantage of an opaque DSSC. In this talk, a few carbon materials such as hybrid films of graphene oxide (GO)/metal and medussa-like nano materials will be introduced to improve conversion efficiency of DSSC and to replace the Pt counter electrode.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR1-1**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 문회리

Pore Modification of Metal-Organic Frameworks for Hydrogen Storage and Carbon Dioxide Capture

백명현

서울대학교 화학부

We have modified the pore spaces of metal-organic frameworks (MOFs) by various strategies in order to enhance their hydrogen storage and carbon dioxide capture abilities. Inclusion of crown ethers in a MOF significantly increases the isosteric heat of the hydrogen adsorption in the MOF. Fabrication of metal (Pd, Mg) nanoparticles within the pores of the MOFs increases the hydrogen storage capacities of the MOFs. In particular, a MOF embedded with Mg nano crystals stores hydrogen by physical adsorption at low temperatures and by chemical absorption at high temperatures, exhibiting synergistic effects on both adsorptions. Impregnation of various metal ions in the pores of an anionic MOF, and the pore functionalization by attaching some pendant groups at the organic linkers of the MOFs significantly enhance the selective carbon dioxide capture abilities of the MOFs at room temperature.

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발표코드: **INOR1-2**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 문회리

Design, preparation, and modification of metal-organic frameworks for valued applications

김자헌

숭실대학교 화학과

Researches on MOFs are currently facing many challenges for their industrial applications mainly due to their high preparation cost and low chemical stabilities. In order to resolve these problems, we have focused on developing both specialty and cheap MOFs with respect to their proper applications. In an effort to introduce specific function, some highly porous MOFs have been extensively functioalized with amines for post-synthetic modification. For cheap but efficient MOF adsorbents, known MOFs have been treated with aqueous solution to enlarge their pore sizes or even generate mesopores. Furthermore, various composite materials composed MOFs and other nanomaterials have been considered and prepared for their specific or bulk applications in the field of storage and separation. Our recent and on-going research works for exploring many-valued MOFs will be presented and discussed.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR1-3**

발표분야: New Frontiers in Metal-Organic Frameworks

발표종류: 심포지엄, 발표일시: 목 09:55, 좌장: 문회리

A Kinetic Approach for Preparation of Porous Networks Based on Structure Science

Masaki Kawano

포항공과대학교 첨단재료과학부

The diversity of networking process that can be dominated by weak intermolecular interactions is not only the source of complexity but also attractive points. Indeed, weak intermolecular interactions play crucial roles in emergence of biological functions. Although a huge number of efforts have been made to obtain desired thermally stable systems, there is still no clear load map to obtain the intermediate phase which is of key importance to generate dynamic function. We propose a new approach to prepare porous materials using kinetic assembly of metal ions and multi-interactive ligands. Interactive ligands make the potential surface of networking sharper to enable trapping of metastable phases. From each metastable phase, we can prepare unique coordination networks which cannot be prepared directly under harsh conditions. In this talk, we will introduce the past three years achievements in our WCU program at POSTECH about molecular design of multi-interactive ligands, selective kinetic assembly of coordination networks, the emergence of unique functions, and the application of crystalline porous networks for direct observation of reactive species by ab initio powder structure analysis.

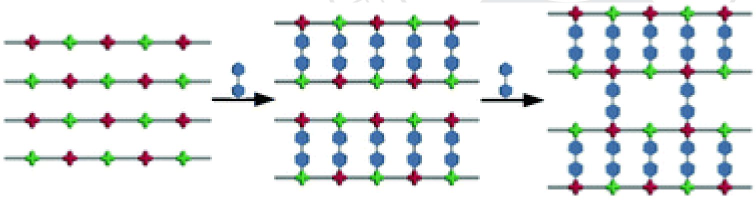
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR1-4**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 정유성

Sequential Self-Assembly in Metal-Organic Frameworks

최원영

울산과학기술대학교(UNIST) 화학과

Despite of phenomenal success in Metal-Organic Frameworks, the synthetic protocol is largely limited to traditional "one-pot" synthesis. This presentation discusses the use of sequential self-assembly in the construction of metal?organic frameworks through the systematic insertion, replacement, and removal of organic structural building units. We review previous and current works that can be classified as such sequential self-assembly in multidimensional MOFs.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR1-5**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 정유성

Nano-to-microgram scale X-ray analysis using porous complexes

Makoto Fujita

The University of Tokyo, POSTECH

X-ray single crystal diffraction (SCD) analysis has the intrinsic limitation that the target molecules must be obtained as single crystals. Here, we report a new protocol for SCD analysis that does not require the crystallization of the sample. In our method, tiny crystals of porous complexes are soaked in the solution of a target, where the complexes can absorb the target molecules. The crystallographic analysis clearly determines the absorbed guest structures along with the host frameworks. As the SCD analysis is carried out with only one tiny crystal, the required sample amount is of the nano-to-microgram order. We demonstrate that even ~50 ng of a sample is enough to be analyzed. When combined with high performance liquid chromatography (HPLC), multiple fractions were directly characterized, establishing a prototypical LC-SCD analysis. Furthermore, the structure of a scarce marine natural product was unambiguously determined using only 5 ?g of the compound.

References:

1. Y. Inokuma, T. Arai, and M. Fujita *Nature Chem.* 2010, 2, 780-783.
2. Y. Inokuma, G.-H. Ning, and M. Fujita *Angew. Chem. Int. Ed.* 2012, *51*, 2379-2381.
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일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR1-6**

발표분야: New Frontiers in Metal-Organic Frameworks

발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 정유성

Nanoporous Covalent Organic Polymers

YAVUZCAFERTAYYAR

한국과학기술원(KAIST) EEWS대학원

Carbon dioxide capture and separation is an unresolved challenge tampering the feasibility of fossil fuels for energy production. Porous materials have long been evaluated for next generation CO_2 adsorbents. Crystallinity, however, is not needed for trapping gases as periodicity or order is not required in the sorbent solids. A good analogy would be that gases are like animals and simple caves would suffice to house them; crystal palaces are not necessary. Porous polymers - robust, inexpensive and amorphous - show promise as feasible materials for the capture of CO_2 from warm exhaust fumes. We report the syntheses of porous covalent organic polymers (COPs) with CO_2 adsorption capacities of up to 5616 mg/g (a world record - measured at high pressures, i.e. 200 bar) and industrially relevant temperatures (as warm as 65 ^{o}C). COPs are stable in boiling water for at least one week, in air up to 400 ^{o}C and theoretical calculations refer to an amorphous extended framework as density is likely the main reason for exceptional CO_2 capacities. COPs also show near infinite CO_2/H_2 selectivity and the highest CO_2/N_2 selectivity (288) to date. The latter is found to be due to a new concept of N_2-phobicity. Post combustion carbon capture from fossil fuel power plants demands pressures of up to 6 bar and a minimum temperature of 40 ^{o}C. By tuning their architecture, we show that COPs reach to 3 mmol CO_2/g sorbent at 6 bar and 45 ^{o}C. High and low pressure capacities make these porous polymer structures viable alternatives to amine scrubbers.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR1-7**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 정유성

Metal-Organic Frameworks for CO2 Separation and Capture

배윤상* Christopher E. Wilmer[1] Omar K. Farha[1] Joseph T. Hupp[1] Randall Q. Snurr[1]

연세대학교 화공생명공학과 [1]Northwestern University, USA

A significant challenge in selective CO2 separation and capture by adsorption is the design of new adsorbents with improved properties. Metal-organic frameworks (MOFs) are a new class of nanoporous materials synthesized in a “building-block” approach that may open up new options for understanding and designing sorbent properties. MOFs are synthesized by the self-assembly of metal or metal-oxide vertices interconnected by rigid organic linker molecules. The rational synthesis approach opens up the possibility of incorporating a wide variety of functional groups into the materials. This presentation will provide several MOF design strategies for obtaining high CO2 selectivities from CO2/CH4 and CO2/N2 mixtures. One of the strategies is the creation of open metal sites by removing the coordinated solvents. The other strategy is the post-synthesis modification of MOFs by incorporating highly polar ligands in the pores. Another is chemical reduction through alkali metal doping. We have also created over 137,000 hypothetical MOFs on the computer and screened them for CO2/CH4 and CO2/N2 separations using GCMC simulations. From the large amount of data obtained, we found clear correlations between purely structural characteristics (e.g., pore size, surface area, and pore volume), as well as chemical characteristics (i.e., functional groups), with five adsorbent evaluation criteria taken from the engineering literature. These structure?property relationships can serve as a map for experimental synthesis going forward.

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장소: 일산KINTEX
발표코드: **INOR1-8**
발표분야: New Frontiers in Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 12:05, 좌장: 정유성

MOF-Derived Materials for Novel Applications

양승재 박종래[1,*]

서울대학교 공과대학/재료공학부 [1]서울대학교 재료공학부

Metal organic frameworks (MOFs) represent an emerging class of materials that have attracted extensive research interest due to their tunable porosity and versatile functionality. Most studies, thus, are directed toward improving pore characteristics and introducing hetero-functionality by changing ligand and metal oxide cluster and, conclusively, numerous applications have been investigated, including gas storage/separation, catalyst, sensing, and gas chromatography. MOFs are 3D crystalline porous materials comprised of metal oxide centers and organic ligands, joined periodically to form a crystalline porous array. Taken together, it is presumed that all materials, i.e. conductor (metal), semiconductor (metal oxide), and insulator (organic species), can be derived from MOFs precursor. These unique structural characteristics have motivated the development of facile preparations of novel MOF-derived materials, such as metal oxide quantum dots@porous carbon, carbon-coated MOF, and hierarchically porous carbon. The resultant MOF-derived materials exhibited promising performances in the various applications involving moisture-resistant coating, lithium ion anode, blackish water treatment, photocatalyst, and gas storage.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR2-1**
발표분야: Catalytic Reaction Using Transition-Metal Complexes
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 장혜영

Reactions of Late Transition Metal Hydrides and Alkyls with Molecular Oxygen

Karen I. Goldberg

Department of Chemistry, University of Washington, USA

From environmental and economic standpoints, molecular oxygen represents an ideal oxidant for chemical transformations. It is readily available, inexpensive (particularly if used without separation from air) and environmentally benign. However, more expensive and/or hazardous oxidants are often employed in oxidation reactions. Further understanding of how transition metal complexes react with molecular oxygen will assist in efforts to develop new selective homogeneous catalytic reactions that effectively utilize this abundant and environmentally friendly oxidant. One potential high value use of oxygen as an oxidant would be in selective alkane functionalization. A variety of late transition metal complexes have been shown to activate alkane C-H bonds to generate metal alkyl and alkyl hydride complexes. To accomplish alkane functionalization, such late metal species need to undergo further reaction. If oxygen is to be used as an oxidant, the reactivity of these species with oxygen needs to be understood. With this goal in mind, the reactions of a variety of late transition metal alkyls, hydrides and alkyl hydride complexes with molecular oxygen have been investigated. The insertion of oxygen into metal-hydride bonds to form metal-hydroperoxides, the insertion of oxygen into metal-alkyl bonds to form metal-alkylperoxides and oxygen-induced reductive elimination have all been observed. Mechanistic investigations and our nascent understanding of the scope of these oxygen reactions with late transition metal complexes will be presented.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR2-2**
발표분야: Catalytic Reaction Using Transition-Metal Complexes
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 장혜영

Metallocene-Catalyzed Synthesis and Properties of Various Functionalized Polyethylenes

박명환

충북대학교 화학교육과

Single-site group 4 metallocene catalytic systems have enabled us to produce polyolefins with the tailored polymer architecture in terms of molecular weight, functionalities, and degree of incorporation of functional groups, which in turn may lead to intriguing properties. In particular, polyethylenes with pendent groups such as triarylamine, triarylborane, and *ortho*-carborane can be considered as a novel class of functionalized polyolefins as well as implement intrinsic properties of side-groups. A proper choice of the catalytic system may provide an effective route to control the amount of various functional moieties in the polymer chain. In this regard, the details of the foregoing chemistry will be presented along with their properties.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR2-3**

발표분야: Catalytic Reaction Using Transition-Metal Complexes

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 장혜영

N-Heterocyclic Carbene Ruthenium, Palladium, and Gold Complexes: Synthesis, Structure, and Catalysis

홍순혁

서울대학교 화학과

The use of N-heterocyclic carbene (NHC) ligands in homogeneous catalysis has now become one of the most extensively studied fields in organometallic chemistry. A breakthrough came when Arduengo isolated stable free carbenes derived from imidazolium salts. It is considered that NHCs behave like tertiary phosphines in many aspects with stronger sigma-donor properties. The strong sigma-donating ability of NHCs confers several advantages such as stronger binding, greater thermal stability and increased basicity. Although many examples show that NHC binds to the metal through C2, it has been shown that C4 and C5 of carbene can also be used for the binding, since the first discovery by Crabtree and co-workers. Carbenes of the latter type, so-called "abnormal" NHCs or mesoionic NHCs, are considered as even stronger sigma-donors than traditional imidazolin-2-ylidenes, which may offer new opportunities in catalysis. Our group has been involved in the development of normal or abnormal (mesoionic) NHC-based transition metal complexes for better catalysis in C-C and C-X bond formation reactions. Syntheses, structural characterization, weak interactions, and catalysis of recently developed NHC-based Ru, Pd, and Au complexes will be presented.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR2-4**

발표분야: Catalytic Reaction Using Transition-Metal Complexes

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 장혜영

Transition-Metal Catalyzed Synthesis of Functionalized Polyolefins and their Application to OLEDs, OPVs, and Chemosensors

이민형

울산대학교 화학과

Organometallic chemistry is one of the key areas associated with modern chemical industry. From the traditional petro- and fine chemistry, in recent years, it provides core aspects in the optoelectronic applications such as OLEDs, OPVs, and chemosensors. For example, transition metal catalysis allows for the synthesis of a variety of new functionalized polymers which can be used as efficient layer materials in OLEDs or electron-accepting material in OPVs. When phosphorescent heavy metal complexes are combined with organoboron moiety, it can provide novel photophysical properties which are useful in designing turn-on anion sensors. In this contribution, recent examples of OLEDs, OPVs, and anion sensor applications of organometallic chemistry will be presented.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR2-5**

발표분야: Catalytic Reaction Using Transition-Metal Complexes

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 박명환

Transition-metal Catalyzed Asymmetric Reactions under Photo-oxidation and Air oxidation Conditions

장혜영

아주대학교 화학과

Asymmetric amino catalysis have been provided a wide range of enantiomerically enriched organic compounds which are the key structure for pharmaceuticals and natural product synthesis. In the context of expanding the scope of aminocatalysis, various transition metal complexes have been introduced to asymmetric organocatalytic reactions, rendering unexpected bond formations with high levels of stereoselectivity. In this presentation, our recent accomplishments regarding asymmetric photo-oxidation and copper-catalyzed oxidation for organocatalytic reactions for multi-substitution of aldehydes will be presented.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR2-6**

발표분야: Catalytic Reaction Using Transition-Metal Complexes

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 박명환

Metal Complexes having N-rich Ligands: Synthesis and Catalytic Studies in the Ring Opening Polymerization of Lactide

이준승

전남대학교 화학과

A large variety of new group 4 catalytic systems have been reported as effective catalysts for polyolefin and copolymers of ethylene with higher α-olefins.1 Their use for the ring opening polymerization (ROP) of cyclic esters, especially lactide (LA), is a relatively unexplored area, though some group 4 catalysts have applied to ROP of LA since 2001.3 Titanium alkoxides are typical catalytic systems; however, the chlorotitanium system without alkoxide or amides, in which chloride can play the role of an initiating group, are very rare. Until now, only two examples of chlorotitanium complexes for ROP of LA have been reported in the literature. Moreover, researches of group 4 metallocene complexes containing the cyclopentadienyl (Cp) ligand for the ROP of LA is another unexplored area. Herein we , we report the synthesis and characterization of novel half and non-organometallic complexes containing triazole or tetrazole ligands, along with their catalytic behavior in the ring-opening polymerization of lactides.

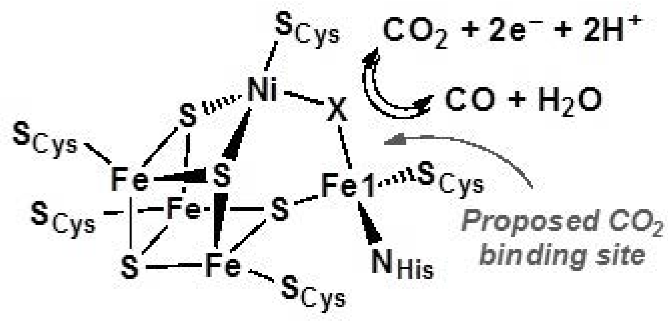
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR2-7**
발표분야: Catalytic Reaction Using Transition-Metal Complexes
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 박명환

Activation of Carbon Dioxide at the Single Nickel Center; Inspired by CODH Chemistry

이윤호

한국과학기술원 화학과

Transformation of carbon dioxide to useful chemicals is an eminent topic in recent chemical research due to its relevance to the global energy and environmental issues. In particular, its adduct formation with transition metals has been interested in not only producing a crucial intermediate to absorb the atmospheric CO2 but utilizing CO2 as a C1 source in chemical syntheses. Many examples in the organometallic field were reported where metal-CO2 species can be isolated and converted mostly to metal-CO, oxalate or formic acid. Unfortunately, their catalytic conversion is still limited. In nature, an efficient catalytic interconversion between CO2 and CO occurs at the Ni,Fe-bimetallic active site of carbon monoxide dehydrogenase (CODH) revealing the prominent methodology to utilize carbon dioxide as an energy carrier. A series of structural data of CODH were recently reported including substrate bound species where the binding mode of CO2 was structurally exhibited. A key interaction with CO2 occurs at a nickel center, where a Lewis acid, a Fe ion is closely located to stabilize the anionic form of the substrate. A zero valent nickel is hypothesized for binding of CO2 through the oxidative addition with the concomitant formation of Ni-carbon bond to produce Ni(II)-COO? species. We believe that understanding the fundamental interaction of a Ni ion with CO2 in the CODH active site environment would be crucial for accomplishing the excellent efficiency of the CO2 activation in developing the catalyst. In our laboratory the activation of carbon dioxide is currently explored in particular, with [PNP]Ni scaffold utilizing a tridentate amidodiphosphino pincer ligand and [NP3]Ni species with a tetradentate ligand. A mononuclear Ni(II) carboxylic acid (-COOH) and its analogous Ni(II) formate (-OCOH) species will be introduced as well-defined nickel complexes to investigate the interaction between a nickel ion and a CO2 molecule. This square planar nickel model system is structurally reminiscent to the active site geometry of CODH where a carbon atom of -COOH moiety is coordinated to revealing a Ni(II)-1η-COO? binding mode. Details of the stoichiometric interconversion of CO2 and CO at the single nickel center will be discussed.



일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR2-8**

발표분야: Catalytic Reaction Using Transition-Metal Complexes

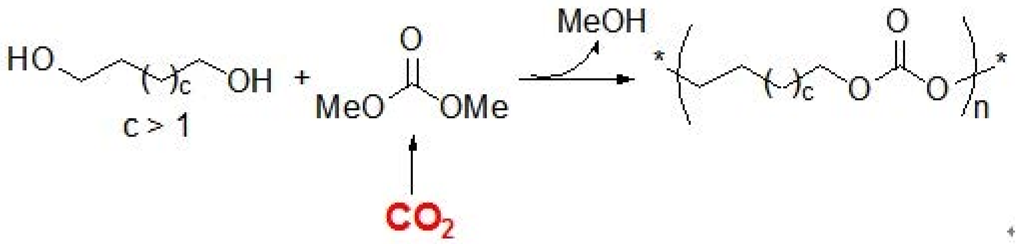
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 박명환

Preparation of Bio-Degradable High-Molecular-Weight Aliphatic Polycarbonates Using CO2 as a Feedstock

이분열

아주대학교 분자과학기술학과

Aliphatic polycarbonates are an attractive material. They are biodegradable and basically the carbonate fractions can be derived from carbon dioxide. The aliphatic polycarbonates in which the carbonate linkage is connected by a space of two carbons can be prepared through copolymerization of CO2 and epoxide. The aliphatic polycarbonates in which the carbonate linkage is connected by a space of more than three carbons such as poly(1,4-butylene carbonate) (PBC) and poly(hexamethylene carbonate) (PHC) can be prepared by condensation polymerization of dimethyl carbonate and aliphatic diols. Dimethyl carbonate was prepared in industry using hazardous phosgene but currently it is benignly produced in a large scale using carbon dioxide. An aliphatic diol, 1,4-butanediol is an inexpensive chemical produced in a large scale in industry. PBC is attractively semi-crystalline polymer (Tm, 60oC) and also bio-degradable. However, there have been few reports that describe successful preparation of high-molecular-weight aliphatic polycarbonate through the condensation polymerization of dimethyl carbonate and aliphatic diols. Here, we disclose a preparation strategy for high-molecular-weight aliphatic polycarbonates of which Mw values are in the range of 100000-300000.



일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS1-1**

발표분야: Environmental Science Based on Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김영독

Oxidation and Reduction on metal oxides: the role of defects in photo- and thermal-chemistry

Cynthia Friend

Department of Chemistry & Chemical Biology, Harvard University, USA

TBA

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS1-2**
발표분야: Environmental Science Based on Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김영독

The development of Ambient Pressure XPS and its applications to surface chemistry

문봉진

광주과학기술원(GIST) 물리광과학부

X-ray photoelectron spectroscopy (XPS) is one of the major tools in the fields of surface chemistry due to its excellent capabilities in studying surface chemical and electronic properties. However, due to the short inelastic attenuation lengths of photoelectrons, as well as the requirement of high vacuum in the electron spectrometer, only the model studies or ex-situ systems have been carried out, and thus creating so-called “pressure-gap”. In an effort to bridge this pressure-gap, the ambient pressure x-ray photoelectron spectroscopy (AP-XPS) has been continuously developed and now puts a new road map in the world of surface science with use of synchrotron radiation source. In this presentation, the basic principles and the latest instrumental development of AP-XPS will be presented. Also, the application of AP-XPS to various fields of surface chemistry will be introduced, e.g. surface catalysis, oxidation dynamics, and environmental science.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS1-3**
발표분야: Environmental Science Based on Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 김영독

Hierarchically driven 1-dimensional nanostructures as highly efficient electrochemical sensing elements

김명화

이화여자대학교 화학 나노과학과

Quasi one-dimensional (1-D) nanostructure materials have been of great interest as the most promising architectures to enhance the electrocatalytic activity due to their much higher surface area, higher mass transport rate, and amendable control of more complex hybrid nanostructures. Particularly, electrochemical nanosensors based on 1-D nanostructures demonstrate immense surface area-to-volume ratios that allow improved sensitivity, portability, small size for reduced power consumption and heat generation and a reduced cost of materials. Thus, rational design and facile synthesis of hierarchical architectures based on 1-D nanostructures are currently of a great interest as unique building blocks with novel functions toward the development of advanced nanoscale electrochemical devices. It means that secondary 1-D nanostructures directly grow in a radial direction on a primary 1-D backbone, resulting in higher dimensionality structures and capability of achieving parallel connectivity and interconnection. In this study, thus, we introduce a facile synthetic strategy to grow hierarchically driven metal oxide 1-dimensional structures via a simple vapor phase transport process as well as their electrochemical performances as efficient electrocatalysts for a variety of applications. This rational engineering of a nanoscale architecture based on the direct formation of the hierarchical 1-dimensional (1-D) nanostructures on an electrode can offer a useful platform for high performance electrochemical biosensors, enabling the efficient, ultrasensitive detection of biologically important molecules.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS1-4**
발표분야: Environmental Science Based on Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 김명화

Catalytic decomposition of NO over TiO_2(110)

김유권

아주대학교 자연과학부

We performed a systematic investigation into the interactions of NO with a TiO_2(110) substrate using temperature-programmed desorption (TPD) and x-ray photoemission spectroscopy (XPS) techniques to understand catalytic processes associated with catalytic NO decomposition over TiO2-based catalysts. We find that NO readily decomposes on a well-prepared TiO_2(110) surface to induce a spontaneous desorption of N_2O leaving oxygen atoms behind at the substrate temperatures as low as 50 K. Our experimental data suggest that the low-temperature N_2O desorption channel is closely related to surface charges located on Ti atoms. NO reactivity is also found to vary significantly depending on the surface structure of the TiO_2 surfaces. For example, surface hydroxyls are found to react with NO to induce a formation of NH_3 which desorbs at around 400 K. We show how the reactivity of NO can be controlled by the coadsorption of other simple molecules.

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Understanding underlying processes in solid electrolyte membrane reactors

엄성현

고등기술연구원 신소재공정센터

A membrane reactor is a chemical reactor in which at least one of the reactants or products is supplied or removed partly or wholly through a membrane. The use of a membrane rather than a conventional reactor offers several advantages, the main one being that it combines reaction and separation in a single unit. Solid electrolyte (SE) membrane reactors are equipped with ion conducting membranes, which ideally are impermeable for non-charged reaction species. These reactors work as electrochemical cells where the oxidation and reduction reactions are coupled and are carried out separately on catalyst/electrodes layers located on different sides of the electrolyte.Of late, extensive research on electrochemical membrane reactor applications is strongly concentrated in the high temperature range using either oxygen ion conducting or proton conducting inorganic ceramic membranes, because the majority of industrially important catalytic processes occur in a temperature range between 300°C and 800°C.The objective of this presentation is to give a brief overview on the current status and the future trends in the development and application of electrochemical reactors equipped with proton conducting solid electrolyte materials used as membranes in these reactors.Interesting applications combining steam electrolysis with NO reduction, dehydrogenative methane coupling for co-production of ethylene and hydrogen, carbon dioxide conversion toward carbon monoxide, and hydrogen pump will be presented in a way that can help chemists understand underlying processes in solid electrolyte membrane reactors.

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Challenges and Opportunities in Ultra-Deep Desulfurization

이용걸

단국대학교 화학공학과

Environmental regulations for reducing motor vehicle emissions has put considerable pressure on the refining industry worldwide to produce cleaner fuels, and has motivated much research for the development of new hydrotreating catalysts. Among alternatives to the widely used sulfides are transition-metal carbides, nitrides, and phosphides. Metal phosphides are a novel catalyst group for deep hydrotreating and have received much attention due to their high activity for hydrodesulfurization (HDS) and hydrodenitrogenation (HDN) of petroleum feedstocks. Previous studies of silica-supported Ni2P employed a low surface area (90 m2 g-1) support. It is the objective of this work to investigate a mesoporous siliceous material (790 m2 g-1) as support. Particular attention is placed on understanding the effect of nitrogen, sulfur and aromatic compounds on the catalytic behavior, as these compounds are reported to inhibit HDS. The present study also includes the use of X-ray absorption fine structure (XAFS) spectroscopy to study the structure of the finely dispersed phosphide phases before and after reaction. As will be shown the samples after use show evidence for the formation of a surface phospho-sulfide phase of very high activity.

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Infrared spectroscopic studies of hydrated aniline ions: time-resolved dissociation dynamics

박승민

경희대학교 화학과

Van der Waals clusters containing an aromatic compound and solvent molecules permit us to investigate “weak” intermolecular interactions which play a significant role in a great variety of physical, chemical, and biological processes. Most of all, hydrated clusters have attracted extensive research interest as hydrogen bonding is certainly the most fundamental interaction of solvation processes. Recently, infrared spectroscopic studies of such clusters in gas phase combined with ab initio calculations proved to be highly powerful to provide important information for a clear understanding of geometric structures, intermolecular interactions, conformational dynamics, and proton transfer processes in solvated molecular systems. Besides, the branching ratio and mode selectivity in IR predissociation of hydrogen-bonded ternary clusters were examined with an aid of tandem mass spectroscopy. Here, we present experimental results on time-resolved IR predissociation dynamics of hydrated aniline cluster ions by excitation of different vibrational modes such as free NH of aniline+, symmetric and anti-symmetric bonded NH of aniline+, free OH of water, symmetric and anti-symmetric bonded OH of water.

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Controlled Assembly and Plasmonic Properties of Core-Satellite Nanostructures

윤상운

단국대학교 화학과

The assembly of noble metal nanoparticles offers an appealing means to control and enhance the plasmonic properties of nanostructures. However, making nanoassemblies with easily modifiable gap distances with high efficiency has been challenging. In this talk, I will present a novel strategy to assemble metal nanoparticles into Janus-type asymmetric core-satellite nanostructures. I will discuss the plasmonic properties of the resulting core-satellite nanoassemblies with a focus on the plasmon coupling in the range of less than 3 nm interparticle gap distances and SERS activity of the assemblies.

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Gas-phase spectroscopy of jet-cooled acetaminophens by REMPI, UV-UV, and IR-UV hole-burning techniques

최명룡

경상대학교 화학과

The conformational structures of jet-cooled acetaminophen (hereafter referred to as AAP, also known as N-acetyl-para-aminophenol or paracetamol) were investigated in the gas phase by resonant 2-photon ionization and UV-UV hole-burning spectroscopy [PCCP, 13, 16537 (2011)]. In contrast to the results from a previous study [PCCP, 12, 4147 (2010)], two nearly isoenergetic conformers were distinctly found in a supersonic molecular beam expansion and positively identified as the cis and trans isomers of acetaminophen by UV-UV hole-burning spectroscopy. Recently, UV-UV hole-burning spectra of 4-AAP exhibited 4 different species, which were attributed to the two independent transitions of the ground $0a_1$ and hot 1e internal rotational level with an aid of IR dip spectroscopy [PCCP, 15, 957 (2013)]. Further spectroscopic investigation of 2- and 3-AAP and AAP-derivatives (phenacetine and metacetine) with an aid of IR dip spectroscopy will also be presented and discussed.

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Theranostic application of upconversion nanoparticle

김형민

국민대학교 생명나노화학과

Recently, upconversion fluorophores, which emit shorter wavelength light than excitation energy, have been proposed as in vivo optical imaging probe. Different from conventional multiphoton imaging scheme, the upconversion process relies on multiple metastable energy levels. Because a near-infrared (NIR) continuous-wave (CW) diode laser can be used as an excitation source, it can increase the penetration depth and suppress autofluorescence in biological samples. Moreover, UCNPs have high photostability and exhibit neither photoblinking nor photobleaching. In this study, we used the energy conversion process of UCNPs not only to optically image the tumor site of mouse but also to apply photodynamic therapy (PDT). Administered PDT drugs (photosensitizers) are activated by upconverted light; they generate cytotoxic reactive oxygen species (ROS) from surrounding water molecules and induce cell death.

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Molecule-Silicon Nanostructure Hybrid Materials for the Control of Charge Storage and Transport

정현담

전남대학교 화학과

This lab has initiated compelling research into silicon quantum dots (Si QD) solids and nanocomposites in order to utilize their synergetic benefits with quantum dot solids through fabrication of Si QD thin films. The issues of oxidation concerning the Si QD thin films were confirmed using Fourier transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS). We compared optical gaps of four Si QDs of the same size but different capping molecules: Otc-, TMS-, and Phe-Si QDs by means of UV-vis and PL. Optical gap was gradually decreased from Otc-Si QD to TMS-Si QD and then to Phe-Si QD. The decrease in optical gap of Si QD was attributed to the delocalization of confined carriers from Si QD core to the conjugated capping layer perceived from the Si-C=C- termination. Silicon quantum dots-polystyrene nanocomposite (SiQD-PS NC) was synthesized by post-functionalization of hydrogen-terminated SiQDs with a styrene monomer using the thermally induced surface-initiated polymerization approach. The resultant nanocomposite contains SiQDs capped with polystyrene chains of different lengths, which form the quantum well structure that gives the nanocomposite its positive charge trapping property, which was deduced from the C-V characteristics of its thin films. In the OTFT device using the nanocomposite, the transfer curve of the transistor was controllably shifted to the negative direction by varying applied gate voltage, indicating the memory function due to charge trapping. The electron transport properties of conjugated molecules with silicon electrodes were studied using non-equilibriums Green’s function/density functional theory (NEGF-DEF) formalism in ATK package.

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Vertical Nanostructure Arrays for Cellular Interface Application

윤명한

광주과학기술원(GIST) 신소재공학부

Recently, vertical nanostructure arrays have been drawing much attention due to their unexpected applications in biological science such as intracellular delivery of biomolecules, electrophysiological stimulation, guiding axons in neuronal culture, and etc. To further investigate the potential for the sophisticated neuronal interfaces, it is indispensible to secure a reliable method for fabricating vertical nanostructure arrays and ensure the long-term viability of neuronal culture on these substrates. In this presentation, we report a newly-developed fabrication method for well-dispersed vertical silicon nanowire arrays (vSNAs) with fine control over their geometric parameters (e.g., length, diameter, density). The specific position of vSNA was determined using general photolithography. Unlike typical vSNA fabrication methods such as chemical vapor deposition and reactive ion etching, our method relies on a combination of wet chemical etching and nanosphere lithography, which enables relatively low-cost and wafer-scale preparation of vSNAs. We also report the viability test of human fibroblast and rat embryonic (E18) hippocampal neurons cultured on the vSNA substrates with a variety of geometric factors tested. From our preliminary results, we anticipate that our vSNAs substrates can be employed as a useful platform for cellular interfaces in the research fields of biotechnology, biophysics, and bioelectronics.

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Solution processed organic electronic devices based on highly ordered organic semiconducting crystals and dielectrics

표승문* 박승언

건국대학교 화학과

Many types of organic based electronic and optoelectronic devices such as light-emitting diodes, thin-film transistor, complementary inverter and non-volatile memory device have been demonstrated, and some of them have been commercialized. In this presentation, we propose a simple solution process for the formation of highly ordered organic semiconducting crystals for high performance opto-electronic devices. In addition, we have fabricated organic electronic devices based on highly ordered organic semiconducting crystals and polymeric gate dielectrics and their performance has been evaluated in diverse measurement conditions. The devices discussed here include organic field-effect transistor and phototransistor and organic complementary inverters.

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Quantitative characterization of inorganic materials using high resolution Rutherford backscattering spectroscopy

이형익

삼성전자 종합기술원 분석그룹

Rutherford backscattering spectroscopy (RBS) 혹은 MEIS (medium energy ion scattering spectroscopy)는 샘플을 파괴시키지 않고 깊이에 따른 조성변화 및 정량분석을 상당한 신뢰성을 가지고 측정할 수 있어 반도체 산업의 연구개발에 필수적인 장비로 사용되고 있다. 이에 삼성 종합기술원에서는 통상적인 MEIS 장비보다 최대 500 keV 까지 에너지를 높이고, 분해능은 MEIS 수준을 가져, 얇은 막도 무리 없이 측정할 수 있는 high resolution RBS 장비를 도입하여 사용하고 있다. 반도체 물질의 공정조건 확보를 위한 정량분석, 두께 및 밀도분석, ion implantation 에 의한 defect 분석, 박막 속에 들어 있는 수소의 정량평가, XPS/SIMS 등과 연계한 기초적 연구에 주로 활용되고 있다. 본 발표에서는 high resolution RBS 를 이용하여 SiN:H, quantum dot 등의 정량분석 및 최근 SIMS, XPS 등에서 활발히 이용되고 있는 Gas Cluster Ion Bean (GCIB)의 유무기 물질의 surface damage 평가에 대한 기초적 연구 결과를 중심으로 발표할 예정이다.

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Analysis of Inorganic Components within Patterned Thin Films using SIMS

어재호 조성찬[1]

삼성모바일디스플레이(주) 분석기술그룹 [1]삼성디스플레이(주) OLED사업부 생산기술팀

Liquid Crystal Displays (LCDs) have now become a part of the major components in the field of larger graphics interface thanks to the splendid picture quality along with the thin form-factor that realizes various application areas imaginable. Though it is one of the electronic devices, the very heart of it is composed of a diversity of organic and inorganic compounds that are mixed into a wide range of compositions for necessary properties. In addition, they are built into multi-layer structures forming interfaces with each other. Because of this structural complexity, the materials have to be prepared following strict guidelines not to interfere the functionalities of the adjacent layers. To make matters worse, both the interfacial and surface properties are not easily defined from the bulk structures due to the lack of the three dimensional interactions. Secondary ion mass spectrometry (SIMS) plays an important role in this type of characterizations: interfacial layer compositions, diffusiveness of certain matters, and so forth, to determine whether or not the device is to perform as designed. However, care should be taken during such analytical approach because the primary ions at high kinetic energy can lead to a variety of artifacts with the momentum transfer to the sample. In the mean time, inter-layer structures interpreted from such affected data prevent engineers from correctly correlating the transfer curves of thin film transistors (TFTs) with the process parameters. Aforementioned vagueness results in a display product of poor image quality as the TFTs control the brightness of each pixel to assemble a picture to display. That is not the only experimental parameter that may push the analytical chemists into confusion and such factors include the incidence angle, sample roughness, conductance of the sample, to name a few. The current presentation covers recent achievement that allows better understanding of the characteristics of TFTs in the pixel layouts and tidbits about how such data should be obtained overcoming practical limitations.

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발표분야: Recent Advances in Inorganic Material Analysis

발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 조성찬

Direct visualization of self-assembled nanostructures by TEM

이은지

충남대학교 분석과학기술학과

Research in bio- and electrical material science and engineering has advanced to where it is possible to make complex nanostructures by the rational design of self-assembling natural and synthetic molecules. The comprehensive characterization of the designed nanostructure in terms of function and structure represents a central step in nanotechnology research. In this repect, Transmission Electron Microscopy (TEM) have led to the direct visualization analysis of soft matter and self-assembled organic-inorganic hybrid nanostructures which contribute to a better understanding of their formation and functional capabilities. In this talk, I will review the different TEM techniques used to characterize nanostructure and future challenges.

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Kinetics of semiconductor nanowire nucleation In situ transmission electron microscopy study

김봉중* J. Tersoff[1] E. A. Stach[2] F. M. Ross[1]

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The effect of size on phase stability and phase transformations is of both fundamental and appliedinterest. For example, during the nucleation and growth of self-assembled nanowires from nanoscalemetal catalysts, the phase of the catalyst determines properties such as the growth rate and the structure ofthe nanowire. Based on our interest in Si and Ge nanowires catalyzed using Au, we have examined phasestability in the Si-Au and Ge-Au systems. Observations were made *in situ* in an ultra high vacuumtransmission electron microscope that has gas delivery capabilities. We start with either size-selectedaerosol particles or with evaporated and agglomerated Au films on electron transparent SiN membranes.The samples are heated by direct current, and Si or Ge is supplied by flowing the chemical vapordeposition precursor gases, disilane or digermane through a capillary into the polepiece region.For Si-Au, the transformation takes place as Si is added to the particle, and it can be seen that thereaction proceeds from the surface inwards, so that at intermediate times the system consists of a solid Auparticle surrounded by liquid AuSi. [1] Modeling the kinetics of this transformation demonstrates that theAu-AuSi interface energy becomes important in modifying phase stability when the Au size becomessmall. Analysis shows a substantial shift in the liquidus line, and a discontinuous change in the liquidcomposition at the transition. On further addition of Si, the AuSi eutectic liquid droplet becomessupersaturated with Si and eventually Si is precipitated. This nucleation event shows complex kinetics [2],as the nucleus rapidly jumps to a large volume and then grows more slowly at a rate dependent on thesupply of Si. The jump size can be used to determine the supersaturation of Si in AuSi at the moment ofnucleation. A comparison of kinetics at a range of temperatures, pressures and droplet sizes showsconsistent behavior: supersaturation is not dependent on droplet volume, leading to predictable

nucleationkinetics, which may be important in forming Si nanowires controllably. In the Ge-Au system, we findmore complex kinetics. [3] Above the eutectic temperature, the behavior of the system is similar to that ofthe Au-Si system, with formation of a liquid AuGe phase followed by precipitation of Ge. However,below the eutectic temperature, a liquid phase also forms, and solid Ge precipitates from this liquid. Weobserved liquid AuGe below the eutectic temperature. The liquid phase persists due to a robustsupercooling that is stabilized by the supersaturation of Ge arising from the growth process.

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발표분야: Recent Advances in Inorganic Material Analysis

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Thermodynamics of covalent and noncovalent chemistry on carbon nanotubes using photoluminescence: Importance of Self Assembly of Surfactants

주상용

연세대학교 화학과

In spite of the broad scientific attention that single walled carbon nanotubes (SWNTs) have charmed thus far, their lack of chirally-pure nanotubes confines the effective utilization in in both academic research and high-end applications. At the heart of such nanotube purification, the binding affinities between SWNTs and self-assembled surfactants play a key role and current state of the art in nanotube separation exploits cosurfactants for enhancing sorting efficiency. However, the deterministic design rule of utilization of cosurfactant in the sorting scheme is still unknown. In this contribution, we provide flavin mononucleotide (FMN)-wrapped SWNTs as a platform for exchanging with other cosurfactants and reaction with diazonium salt. The determined equilibrium constants from various surfactants originate from the native stability between nanotube and the initial surfactant and provide quantitative information of relative binding affinity and binding mode of various cosurfactants towards each (n,m) nanotubes. Temperature-programmed photoluminescence experiments provide the effects of the combination of two surfactants on the resulting PL, absorption, and thermodynamic parameters. This highlights the importance of surfactant arrangement of surfactant on carbon nanotubes.ACKNOWLEDGMENTS This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2011-0015154).

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Rapid monitoring of CFP-10 during culture of Mycobacterium tuberculosis by using a magnetophoretic immunoassay

이재범

부산대학교 나노메디컬공학과

We introduce a rapid and robust sensing kit using sandwich-type magnetophoretic immunoassay (MPI) for the colorimetric detection of a secreted tuberculosis (TB)-associated antigen, CFP-10, in cultures of Mycobacterium tuberculosis (Mtb). Detection using this assay relies on the antigen-specific formation of complexes between Au nanoparticles (NPs) and magnetic microparticles (MMPs), such that magnetophoresis in the presence of CFP-10 decreases the plasmon absorbance of the assay solution due to the removal of Au NPs. The MPI offers rapid (results are obtained in 10 min), quantitative, and qualitative monitoring of CFP-10 expression in a detection range from 10 to 10,000 pg/mL with a detection limit of 10 pg/mL. Assay validation was performed by monitoring CFP-10 secreted during the Mtb culture. The data revealed a linear relationship between the concentration of CFP-10 in culture supernatants and the duration of Mtb culture. Thus, it shows high potential that the rapid and robust MPI sensing kit can be used for early TB diagnosis through immunoassay detection of TB-specific antigens in Mtb culture with further clinical investigation.

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Homogeneous electrochemical monitoring of enzyme activity towards cost-effective, portable biosensor

신익수

숭실대학교 화학과

The development of portable, easy-to-use, fast, inexpensive, and sensitive enzyme assay for point-of-care analysis of diseases is of an importance forward in public health, forensic analysis, food industry, and environmental monitoring. Most of the strategies proposed today are based on fluorescent-based optical detection methods that are not so easily amenable to the development of cost-effective and low-power handheld analysis. Electrochemical detection methods can offer an answer for these limitations since they are inherently robust, simple, inexpensive and easy to miniaturize. Until now few efforts have been made to employ electrochemical method in enzyme assay. In the talk, homogeneous label-free electrochemical detection strategy which relies on an enzymatic reaction will be discussed. Our approach offers simple, sensitive monitoring for enzyme activity, and some of the results are promising and comparable with the typical fluorescence assays.

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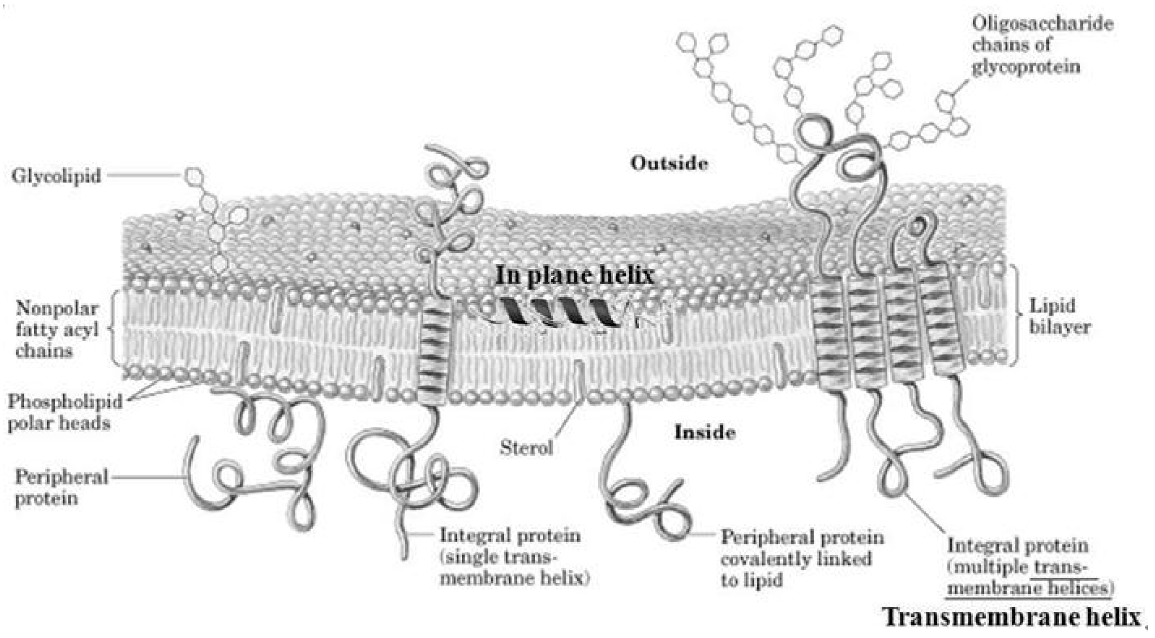
발표코드: **ANAL2-1**
발표분야: Recent Advances in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 황금숙

Structural analysis of disease-related membrane proteins using NMR

김용애

한국외국어대학교 화학과

Cell membranes contain numerous proteins and it is estimated that about 30% of the approximately 25,000 human genes code for membrane proteins. Transmembrane proteins (TMPs) are embedded in the cell membranes and act as a gatekeeper to regulate the movement of materials such as ions, hormones, nutrients, and signaling molecules into and out of cells. The majority of them are involved in major disease processes in the body and more than 50% of all TMPs have been deemed possible pharmaceutical targets. In spite of the biological and medical importance of TMPs, their structure and molecular mechanisms are poorly understood compared to the extensive structural and functional data available for soluble proteins. This inequality is due to the abundance of hydrophobic sequences, which can make it difficult to express and purify large amounts of TMPs and make them refractory to many biophysical/biochemical and structural analyses. Solid-state NMR experiments on lipid bilayer samples are especially valuable for the studies of membrane proteins. Here we will present the optimized results of large scale growth and purification to get disease related membrane proteins like developmental processes related Syndecan-4 receptor, dementia related Amyloid, and antimicrobacterial peptide of bovine milk, Lactophoricin. And we will also present the solid-state NMR spectra of mechanically aligned planar lipid bilayer samples and magnetically oriented bicelle samples of disease related membrane proteins.


Oligosaccharide chains of glycoprotein
Glycolipid
Outside
In plane helix
Nonpolar fatty acyl chains
Lipid bilayer
Phospholipid polar heads
Inside
Sterol
Peripheral protein
Integral protein (single transmembrane helix)
Peripheral protein covalently linked to lipid
Integral protein (multiple transmembrane helices)
Transmembrane helix

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발표코드: **ANAL2-2**
발표분야: Recent Advances in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 황금숙

SERS-based quantitative evaluation of proteins

정영미[*] Lei Chen[1] Bing Zhao[1]

강원대학교 화학과 [1]State Key Laboratory of Supramolecular Structure and Materials, Jilin University

Surface-enhanced Raman scattering (SERS) has recently received much attention due to its considerable potential for high selectivity and sensitivity. The recent advances in SERS-based biomolecular detection (e.g., protein, DNA and cells) have benefited from the nondestructive nature of the SERS technique. A rapid and highly sensitive bicinchoninic acid (BCA) reagent-based protein quantitative evaluation method by using competitive resonance Raman (RR) and surface-enhanced resonance Raman scattering (SERRS) methods will be introduced.

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발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 황금숙

Analysis of metabolite by mass spectrometry: Application to DMPK and metabolomics

정병화

한국과학기술연구원(KIST) 분자인식연구센터

Observations of positive and negative impacts of xenobiotic and endogenous metabolism have led to the numerous discoveries in contemporary biomedical sciences. In fact, identification of xenobiotic metabolites and metabolic pathways has become an indispensable part of drug metabolism and chemical toxicology research since the results from these studies establish the scientific basis for understanding molecular mechanisms of chemical-induced beneficial or toxicological effects, and discovery of endogenous metabolite and related metabolic pathway is also very important to find out biomarker and mechanisms for disease, drug action, toxicity. In particular, endogenous metabolite is the phenotype of many actions in the body, so it is a very convenient and important tool to predict many actions in the body produced by drug or disease.For the purpose of investigating the discovery of metabolite for drug and the change of endogenous metabolism by any kind of stimulus, the reliable and sensitive analytical tool is essential.Nowadays many challenges and development has been continuously made in the area of analytical instrument and mass spectrometry becomes one of the most potential tools for this type of investigation with great sensitivity and selectivity to analyze metabolite both of quantitatively and qualitatively.In this presentation, several examples of analysis of xenobiotic and endogenous metabolites will be investigated. Metabolomic approach which was made for the metabolite profiling and discovery of the biomarkers will be also described.

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‘q titration’ and Membrane Mimetic Systems for Protein NMR Study

손우성

차의과학대학교 약학대학 약학과

Membrane proteins are prevalent in nature where one-third of the genes in organisms ranging in complexity from bacteria to humans are translated into helical membrane proteins. They have many unique biological functions as receptors and enzymes, transporters of ions and organic molecules and human diseases result from mutations in membrane proteins and most drugs act by binding to membrane protein receptors. NMR (Nuclear Magnetic Resonance) spectroscopy can provide plenty of information about the structure and dynamics of membrane proteins in membrane mimetics including detergent micelles or lipid bilayers. The recent development of sophisticated NMR techniques, protein expression systems and isotope labeling methods significantly extended the applicability of NMR spectroscopy for membrane proteins. And optimization of membrane mimetic environment is essential to get NMR spectrum of good resolution in combination with uniformly and partially labeled membrane proteins. ‘q-Titration’ refers to the systematic comparison of signal intensities in solution NMR spectra of uniformly ^{15}N labeled membrane proteins solubilized in micelles and isotropic bicelles as a function of the molar ratios (q) of the long-chain lipids (typically DMPC) to short-chain lipids (typically DHPC). In general, as q increases, the protein resonances broaden and correspondingly have reduced intensities due to the overall slowing of protein reorientation. Since the protein backbone signals do not broaden uniformly, the differences in line widths (and intensities) enable the narrower (more intense) signals associated with mobile residues to be differentiated from the broader (less intense) signals associated with structured residues. In this talk, recent progresses on membrane mimetic systems will be presented together with ‘q titration’ method. It will include state-of-the-art methods for NMR study such as thiol reactive tagging, nanodisc, and alignment in the magnetic field.

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발표분야: Recent Advances in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 정병화

Muti-platform metabolomics approach for discovering biomarkers and understanding metabolic pathway

황금숙

한국기초과학지원연구원 통합대사체연구그룹

Metabolites are small molecules that are chemically transformed during metabolism, and serve as direct signatures of biochemical activity and are therefore easier to correlate with phenotype. Therefore, metabolite profiling, or metabolomics, has become a powerful approach that has been widely applied in different fields such as disease diagnosis, toxicology, plant science and pharmaceutical and environmental research. Since the metabolites have very diverse property in complex mixtures, no single analytical platform can be applied to detect all metabolites in biological samples. The integrated analytical approaches are beneficial to increase the coverage of detected metabolites that is not able to be achieved by single analytical technique. Metabolite profiles have been used for discovering biomarkers and identifying molecular signatures and pathways. In this study, the metabolic change and signatures were investigated by integrating NMR based global (untargeted) profiling data and different type of analytical data, demonstrating that integrated metabolite profiling conducted through a joint analysis of the data gives specific advantages in terms of sensitivity and confidence of pathway associations. This study suggests that integrative analysis provide sensitive and reproducible detection of various metabolites in a biological sample, and therefore, integrated metabolite profiling is a powerful approach for promoting the discovery of novel biomarkers and understanding metabolic pathway.

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발표분야: Recent Advances in Analytical Chemistry
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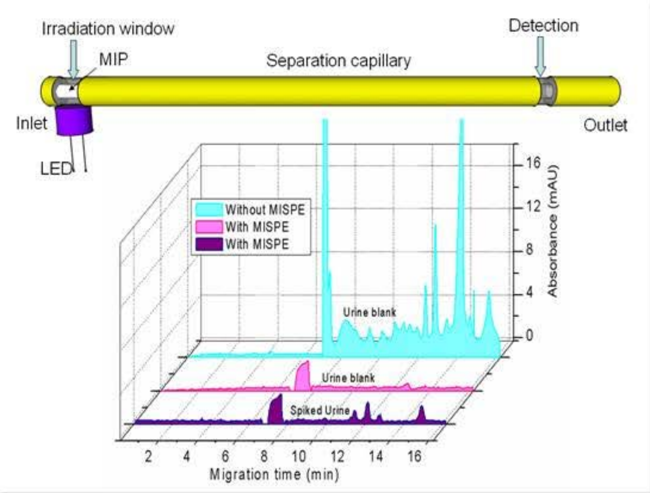
LED-induced In-column Molecularly Imprinting for Solid Phase Extraction/Capillary Electropohresis

이용일

창원대학교 화학과

A novel in-column and open-tubular molecularly-imprinted solid phase extraction (MISPE) concentrator was constructed for capillary electrophoresis (CE) that consisted of a miniaturized light emitting diode for inducing polymerization (LEDIP). The strategy was based on directly coating a short layer of MIP material (about 3 mm long) at the inlet end of the inner wall of the separation capillary using LED irradiation, thus accompanying the advantages of simplicity, zero dead volume, and ease of automation. A methyltestosterone imprinted in-column SPE concentrator was used as a model system for evaluating its operational performance. Based on a 15.3 μL sample injection (15 min at flow rate of 1.02 μL min-1), the MISPE concentrator provided an about 200-fold increase in sensitivity with a low loss of separation efficiency over conventional hydrodynamic injection. This in-column MISPE was used for the extraction of methyltestosterone and its analogues from a urine sample, showing the high affinity and selectivity, with recoveries for MISPE-CE analysis of the spiked sample ranging from 90% to 107%. The miniaturized LEDIP system is also suitable for the on-line renewing the MISPE concentrator conveniently.


Irradiation window
MIP
Separation capillary
Detection
Inlet
Outlet
LED
Without MISPE
With MISPE
With MISPE
Urine blank
Urine blank
Spiked Urine
Absorbance (mAU)
0
4
8
12
16
2
4
6
8
10
12
14
16
Migration time (min)

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발표코드: **ANAL2-7**
발표분야: Recent Advances in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 정병화

Chip-Based Analytical Platforms for Chemo/Bioanalysis

김주훈

경희대학교 화학과

There are two main topics presented here. One is functionalization of chip surfaces with nanomaterials for fabrication of novel chip-based analytical platforms. Two types of surface decoration methods will be mainly discussed: electrochemical decoration of glassy carbon surfaces and covalent decoration of chemically converted graphene (CCG) surfaces. First, amine-terminated polyamidoamine (PAMAM) dendrimers were immobilized on glassy carbon electrodes (GCEs) via electrooxidative coupling of the terminal amine groups of dendrimers. The immobilization approach was applied to build bifunctional nanostructures acting as catalytic layers for chemical and biological reactions. Second, a universal method was reported for preparation of nanoparticle-decorated CCG composites, on which size-monodisperse nanoparticles were uniformly distributed with preservation of their original size, via covalent immobilization of DENs. The method allowed universal attachment of multiple nanoparticles with distinctively different sizes and compositions on the same CCG sheet with good control over particle sizes in the range of 1 to 2 nm. The other topic is application of the fabricated chip-based analytical platforms for chemo/bioanalysis. A brief description will be presented how the chip-based analytical platforms can be applied as electrochemical, optical, and electrochemiluminescence (ECL) sensor chips based on various transduction techniques.

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장소: 일산KINTEX

발표코드: **BIO1-1**

발표분야: Cell Penetrating Peptide, CPP

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이연

Argninine-rich Cell-penetrating Peptides and their Application to Intracellular Delivery

Shiroh Futaki

Kyoto University

Arginine-rich cell-penetrating peptides (CPPs) have been gathering considerable research interests due to their ability to bring exogenous molecules into cells [1,2]. In this presentation, factors that contribute to efficient cellular uptake of arginine-rich CPPs, including membrane-associate proteoglycans and macropinocyotosis, are summarized, together with examples for the application to of CPPs to intracellular delivery of bioactive molecules. Also introduced is our study on the biodistribution of arginine-rich CPPs in tumor-xenografted nude mice after intravenous injection of fluorescently labeled CPPs, using in vivo imaging [3]. The CPPs used included HIV-1 Tat (48-60), penetratin, and the L- and D-enantiomers of oligoarginines (8, 12, and 16 residues), all of which are reported to have high cell penetration. Among the tested peptides, high accumulation in tumors was observed for the D-form of octaarginine (r8), and glycosaminoglycans played a key role. Injection of an r8-doxorubicin conjugate (4mg doxorubicin/kg) effectively suppressed tumor proliferation, with no significant decrease in mouse weight, whereas administration of doxorubicin itself (6mg/kg), yielding a similar degree of tumor-growth suppression, resulted in significant weight loss. These results suggest the potential of r8 as a prototypic tumor-targeting vector.[1] Nakase et al., Acc. Chem. Res. 45, 1132 (2012);[2] Futaki et al., Curr. Pharm. Des. in press.[3] Nakase et al., J. Control. Release 159, 181 (2012)

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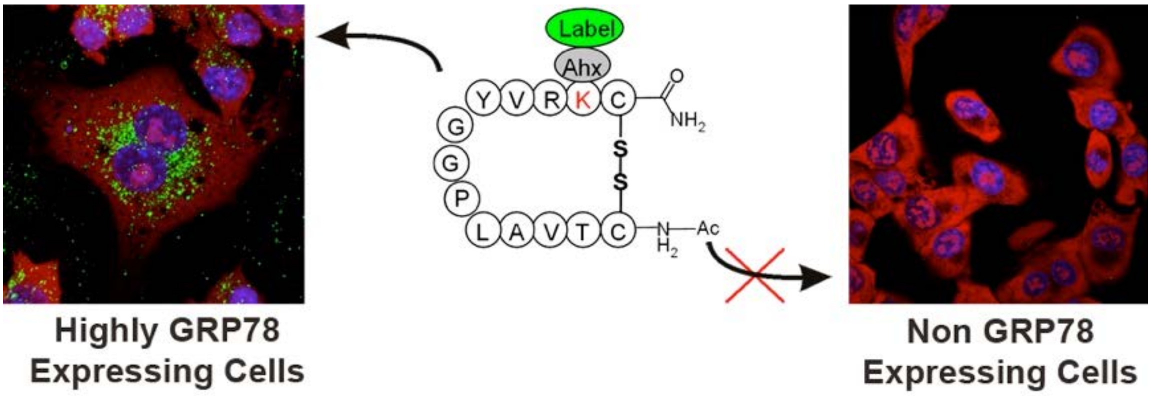
발표분야: Cell Penetrating Peptide, CPP
발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 이연

Targeting heat shock protiens on cancer cells: Selection, characterization, and cell-penetrating properties of a peptidic GRP78 ligand

김영수

한국과학기술연구원(KIST) 뇌의약연구단

Peptidic ligands can be used for specific cell targeting and the delivery of payloads into the target cell. Here we describe the screening of a pool of cyclic peptide phage display libraries using whole-cell panning against human melanoma cell line Me6652/4. This strategy resulted in the selection of the cyclic 13-mer Pep42, CTVALPGGYVRVC, which showed preferential internalization into melanoma cell line Me6652/4 versus the reference cell line Me6652/56. This translocation is a receptor- mediated process that does not require electrostatic interactions nor does it involve transfer to the lysosomal compartment. The cellular receptor for Pep42 was identified as the surface membrane form of glucose-regulated protein 78 (GRP78), a member of the heat shock protein family and a marker on malignant cancer cells. The cellular uptake and intracellular trafficking of Pep42-quantum dot conjugates was monitored by confocal laser microscopy and co-localization within the endoplasmic reticulum was observed. The uptake of Pep42 could be blocked by a monoclonal antibody against the identified receptor. Furthermore, Pep42 was shown to target specifically GRP78 expressing cancer cells. The in vitro cytotoxicity of a Pep42-taxol conjugate was evaluated by flow cytometry wherein the conjugate was shown to induce apoptosis and was more effective in promoting programmed cell death in Me6652/4 cells. In summary, the data presented suggest that cyclic peptide Pep42 might be a powerful tool in the construction of drug conjugates designed to selectively kill malignant cancer cells.


Label
Ahx
Y V R K C
G
G
P
L A V T C
NH2
S
S
N H2 Ac
Highly GRP78 Expressing Cells
Non GRP78 Expressing Cells

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **BIO1-3**

발표분야: Cell Penetrating Peptide, CPP

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 이연

Designed Peptide Libraries for Cell Analyses

Hisakazu Mihara

Tokyo Institute of technology

As advances in genome-wide sciences, the protein-detection microarrays have been promising technologies providing high-throughput detection for proteins of interest. To realize such a practical protein-detection system, development of capturing agents is one of the important steps. Peptides are the promising candidates for capturing agents of protein-detection chips. Peptide de novo designing strategy for alpha-helix, beta-sheet and beta-loop enables peptide microarrays to mimic protein-protein interactions and discriminate protein structures. Thus, we have attempted to develop designed peptide microarrays for protein detection and cell characterization. Fluorescent peptide libraries with designed sequences for alpha-helix, beta-sheet and beta-loop were constructed, and each compound was immobilized or deposited on a spot to afford designed peptide microarrays. Fluorescence data of protein binding were demonstrated to show color-coded patterns regarded as protein fingerprints (PFP).Furthermore, these peptide library and microarray are also applied for cell assay systems. A peptide library designed for alpha-helix was constructed by chemical synthesis. Peptides expressing a high cell-penetrating (CPP) activity were screened, and then cell types were discriminated and profiled using the cell fingerprint (CFP) with the CPP activity of the library. Throughout these studies, it has been demonstrated that the designed peptide microarray is one of useful tools for protein and cell chip technologies.

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발표분야: Cell Penetrating Peptide, CPP
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Efficient intracellular delivery based on pH-sensitive amide derivatives

이연

서울대학교 화학부

Efficient and safe intracellular delivery of biomolecules is essential for gene- and protein-based pharmaceutics. Various methods have been developed for overcoming the barriers of cell membrane and endosomal membrane during the intracellular delivery. In this presentation, the technology based on the pH-sensitive amide derivatives, which can be degraded rapidly at early endosomal pH value of 5.5, will be discussed. Most of amide bonds can be degraded only at very acidic pHs below 2, but malec acid amide can be degraded at pH 3. Also, its derivatives, citraconic acid amide or cis-aconitic acid amide can be degraded at milder pH values, around 5-6. Moreover, its charges are converted from negative to positive during the degradation process. Inspired from the interesting characteristics, we applied the maleic acid amide derivatives to the delivery of large biomolecules, such as DNA, siRNA, protein, or antibodies. The delivery efficiency and cytotoxicity will be carefully considered for the development of more efficient, specific and safe delivery carriers.

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장소: 일산KINTEX

발표코드: **BIO1-5**

발표분야: Cell Penetrating Peptide, CPP

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 최수혁

Post-antibody Medicines “MicroAntibodies”: Generation of Molecular-targeting Peptides by Directed Evolution in Phage-displayed Libraries

Ikuo Fujii

Osaka Prefecture University

At present, antibodies are indisputably the most successful reagents in molecular targeting therapy. However, use of antibodies has been limited due to the biophysical properties, immunogenicity, non-cell permeability, high cost to manufacture, and so on. To enable new applications where antibodies show some limitations, we have developed an alternative-binding molecule with non-immunoglobulin domain. The molecule is a helix-loop-helix peptide, which is stable against natural enzymes in vivo and is too small to be non-immunogenic. We constructed a phage-displayed library of the helix-loop-helix peptides and then screened the library for G-CSF receptor. Finally, the screened binding peptides were cyclized by introduction of a disulfide-bond linkage into the N- and C-termini. The cyclic peptide showed strong binding affinity (Kd of 4 nM) to the receptor. This semi-rational strategy, which combines directed evolution with de novo designed peptides, provides a new way to generate structured functional peptides for useful tools in the field of chemical biology as well as alternatives to antibody medicines. Here, feasibility for the medical application, biological activity, cell permeability, immunogenicity, and in vivo stability, will be discussed in detail.

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발표코드: **BIO1-6**
발표분야: Cell Penetrating Peptide, CPP
발표종류: 심포지엄, 발표일시: 목 11:25, 좌장: 최수혁

Conformational flexibility and the positive charges are the key factors in bacterial cell selectivity and membrane penetration of peptoid substituted analog of Piscidin

김양미

건국대학교 생명공학과

Piscidin 1 (Pis-1) is a novel cytotoxic peptide with a cationic alpha helical structure isolated from the mast cells of hybrid striped bass. In this study, we designed Pis-1 analogs which have bent structures and investigated their motional properties using NMR spectroscopy. Pis-1[PG] with a substitution of Pro8 for Gly8 in Pis-1 had higher bacterial cell selectivity than Pis-1. We designed peptoid residue-substituted peptide, Pis-1[NkG], in which Gly8 of Pis-1 was replaced with Nlys (Lys peptoid residue). Pis 1[NkG] had higher antibacterial activity and anti-inflammatory activity with lower cytotoxicity against mammalian cells than Pis-1 and Pis-1[PG]. Both peptides had a three-turn helix in the C-terminal region and a bent structure in the center. Pis-1[PG] has a rigid bent structure at Pro8 whereas Pis-1[NkG] existed as a dynamic equilibrium of two conformers with a flexible hinge structure at Nlys8. Depolarization of the membrane potential of Staphylococcus aureus and confocal laser-scanning microscopy study revealed that Pis-1[NkG] effectively penetrated the bacterial cell membrane and accumulated in the cytoplasm, whereas Pis 1[PG] did not penetrate the membrane but remained outside or on the cell surface. Introduction of a lysine peptoid provided conformational flexibility and increased the positive charge at the hinge region; both factors facilitated penetration of the bacterial cell membrane and conferred bacterial cell selectivity on Pis-1[NkG].

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장소: 일산KINTEX

발표코드: **BIO2-1**

발표분야: Protein Chemistry

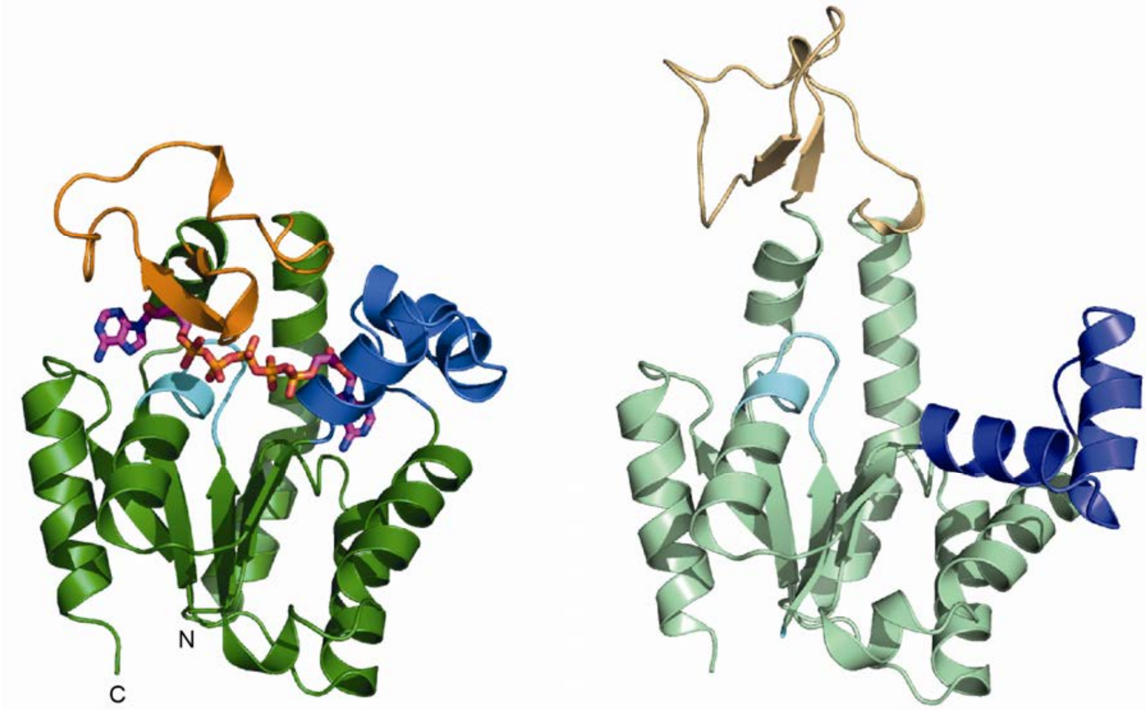
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이상호

Structural basis for pneumococcal growth by adenylate kinase

이상호

성균관대학교 생명과학과

Pneumococcal infection claims more than 1.6 million deaths worldwide. Capsular polysaccharides (CPS) act as major virulence factors by protecting pneumococci from host. Synthesis of CPS requires energy supply by ATP hydrolysis and adenylate kinases (AdKs) constitute a major family of enzymes to regulate cellular ATP level. However, it remains poorly understood whether AdKs act as a virulence factor in pneumococcal diseases. Here we show that AdK from *Streptococcus pneumoniae* (SpAdK) is essential in pneumococcal growth by crystallographic and functional studies. We determined the crystal structure of SpAdK in two conformations: ligand-free open form and closed in complex with a two-substrate mimic inhibitor adenosine pentaphosphate (Ap5A). Arg-89 was identified as the key active site residue, suppressing pneumococcal growth both in non-capsular and capsular strains when mutated. Expression of wild-type *adk* gene in fucose-inducible strains rescued growth defect, but not Arg-89 mutant gene. Cellular ATP level increased in proportion to the expression level of wild-type *adk* gene. Taken together, our results support that SpAdK regulates pneumococcal growth via its enzymatic activity.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일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **BIO2-2**
발표분야: Protein Chemistry
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이상호

Regulating Activities of the Ubiquitin-Proteasome System through Small-Molecule Inhibitors and Activators

<u>이민재</u>

경희대학교 응용화학과

Rates of proteolysis are a function of cell’s physiological state and are controlled differentially for individual proteins, affecting a variety of regulatory pathways both in normal and pathological conditions. The ubiquitin-proteasome system is responsible for the degradation of most intracellular proteins in eukaryotes, where substrates were marked for degradation by the attachment of polyubiquitin chains that is required for subsequent recognition and breakdown by the proteasome. As our knowledge of biological processes in the system has grown for the last 30 years, so have the ties between the system and various human diseases including cancers, metabolic diseases, and neurodegenerative diseases. In this presentation, I intend to provide an example of studies which were involved in small-molecule inhibitor/activator development in the ubiquitin-proteasome system through rational design and high-throughput screening, and its application to modulate its biochemical and functional outputs. The focus is on the proteasome and the N-end rule pathway. The small-molecule activator of the proteasome accelerated the degradation of various proteotoxic proteins including tau. Heterobivalent inhibitors of the N-end rule pathway were also successfully applied to mammalian cells and delayed the degradation of target substrates. These small molecules potentially provides a novel, mechanism-modifying method for the treatment and prevention of human diseases.

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장소: 일산KINTEX

발표코드: **BIO2-3**

발표분야: Protein Chemistry

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 이상호

Structural basis of apoptosis inhibition by apoptosis inhibitor 5

이병일

국립암센터 연구소 바이오분자기능연구과

Apoptosis inhibitor 5 (API5) is an anti-apoptotic protein that is upregulated in various cancer cells. Here, we present the crystal structure of human API5. API5 exhibits an elongated all alpha-helical structure. The N-terminal half of API5 is similar to the HEAT repeat and the C-terminal half is similar to the Armadillo-like (ARM) repeat. HEAT and ARM repeats have been implicated in protein-protein interactions, suggesting that the cellular roles of API5 may be to mediate protein-protein interactions. Various components of multiprotein complexes have been identified as API5-interacting protein partners, suggesting that API5 may act as a scaffold for multiprotein complexes. API5 exists as a monomer, and the functionally important heptad leucine repeat does not contain the predicted leucine zipper structure. Additionally, Lys251, which can be acetylated in cells, plays important roles in transactivation mediated by API5 and the inhibition of apoptosis under serum deprivation conditions. The acetylation of this lysine also affects the stability of API5 in cells.

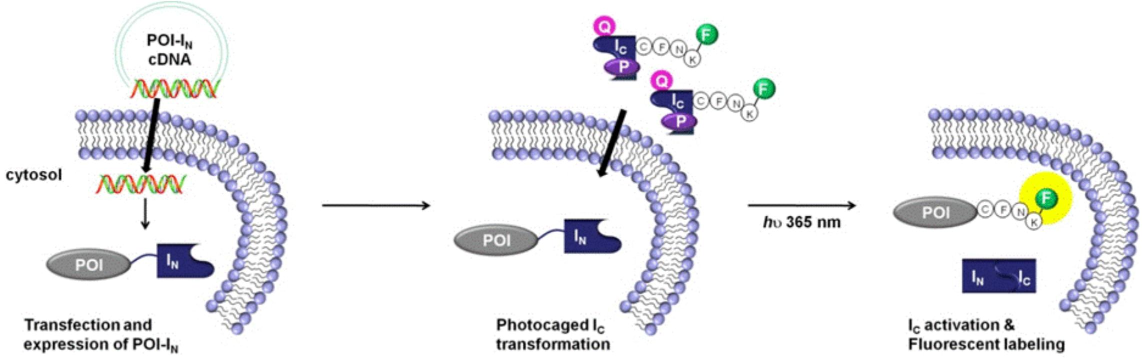
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **BIO2-4**
발표분야: Protein Chemistry
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 이상호

Photo-activatable fluorescent labeling of recombinant proteins in live cells

권영은

동국대학교 의생명공학과

Recombinant proteins containing an N-terminal fragment of split-inteins were selectively labeled with a fluorescent dye in live cells through an amide bond. This approach allows introduction of various ligands with diverse physical properties to a target protein. Such in situ addition of small probes perturbs the properties of target proteins much less than does green fluorescent proteins and enables monitoring the functions and locations of target proteins in live cells. Additionally, the use of photo-chemical switch allows the necessary temporal control for studying the function of proteins with increased sensitivity. This system provides a novel and effective approach to control the fluorescent tagging of proteins in live cells using light as an external stimulus.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **BIO2-5**
발표분야: Protein Chemistry
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 이상호

Development of platform technology for next generation antibody therapeutics

김용성

아주대학교 응용화학생명공학과

The use of monoclonal antibodies (mAbs), which specifically bind to target molecules with high affinity, is of interest for many pharmaceutical and industrial applications. As of January 2013 there are 33 mAb therapeutics approved in either the US or EU in various indications, mainly cancers and autoimmune/inflammatory diseases. However, the clinical efficacy of mAbs approved for solid-tumor cancer therapy is relatively low as a single agent showing response rates of 8% - 18% even for the qualified patients for particular mAb. Also, market competition becomes very high due to coming-soon biosimilar mAbs. Therefore there are great needs for the development of innovative mAbs against new targets and next-generation mAbs with superior profiles to current mAbs. Next-generation antibody will show greater clinical efficacy, reduced side-effects, and more convenient administrations.In this talk, I will discuss our effort to develop proprietary platform technology for next generation antibody therapeutics, including bispecific antibody, tumor tissue penetrating antibody, and cell-penetrating antibody for targeting of intracellular molecules.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN1-1**
발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이상기

Metal Catalyzed Carbonylation and Cyclization Reactions

Howard Alper

University of Ottawa, Ottawa, Canada

Transition metal catalyzed reactions are of genuine value for organic synthesis. Results will be presented for the hydroformylation, and direct reductive hydroformylation, of olefins to alcohols, the cyclization of heterocycles and acyclic compounds with heterocumulenes, and intramolecular cyclocarbonylation affording medium and large ring macrocycles. Very recent results on the oxidative carbonylation of o-hydroxystyrenes to coumarins, and the direct carbonylation of indoles by C-H bond activation will be described.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-2**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 이상기

Highly Selective Catalytic Reactions of Enoldiazoacetates

Michael P. Doyle

University of Maryland, College Park, MD 20742 USA

A new class of stable diazo compounds provides access to chemical transformations that have not been possible previously. This presentation will focus on catalytic processes with easily prepared enoldiazoacetates that include cycloaddition reactions that operate by vinylogous processes through metal carbene intermediates. Metal vinylcarbenes are susceptible to both [3 + 3]- and [2 + 3]-cycloaddition reactions[1,2] with nitrones, azomethine ylides, and hydrazones, and stereocontrol that generally exceeds 90% ee and 95% de is achieved when these reactions are performed with Hashimoto's chiral phthalimide-amino acid ligated dirhodium catalysts. The divergent activities of copper and dirhodium catalysts is evident in these reactions, with copper directing reactant enoldiazoacetates along an acid-catalyzed pathway, and dirhodium taking the reactants through a metal carbene pathway. A more precise understanding of catalysis in these reactions allows predictability in their applications for synthesis.

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2. Xu,X.; Qian, Y.; Zavalij, P. Y.; Doyle, M. P. *J. Am. Chem. Soc.* 2013, *135*, 1244-1247.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-3**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 이상기

Synergy between Complex Total Synthesis and New Recation Development:Synthesis of Haouamine A and Transition Metal Catalyzed Free Radical Reactions

이철범

서울대학교 화학부

Discussed in this talk will be recent studies in our laboratories that have been focused on the chemical synthesis of complex natural products. The marine natural product *haouamine A* is an alkaloid that possesses a unique 11-membered azacyclophane moiety within a complex fused-bridged polycyclic molecular architecture and selective antitumor activities. In order to address challenges associated with the synthesis of this novel target, our approach has been based on new methods and strategies emanating from the unprecedented catalytic reactivity of transition metal complexes. Examples will be given on how the transition metal catalysis is applied to resolve difficult issues encountered during the total synthesis campaign. Also described will be how the discoveries from a target-oriented synthesis have led to the development of new catalytic methods of potentially broad utility. In particular, two new transition-metal-catalyzed radical reactions will be described, which mediate reductive transformations of organohalides by making use of SET mechanisms effected by nickel and iridium catalyses, respectively.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-4**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

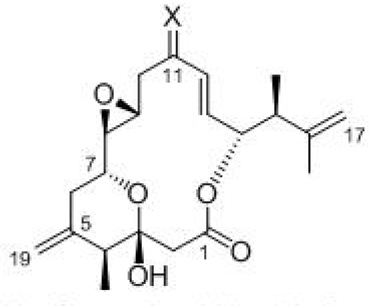
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 이희윤

First Convergent and Enantioselective Total Synthesis of (-)-Amphidinolide O and (-)-Amphidinolide P

이덕형

서강대학교 화학과

Amphidinolide family compounds (A-H and J-Y) were isolated by Kabayashi group and have attracted much attention of the synthetic community because of their unusual structural features and cytotoxic activities. (+)-Amphidinolide O and (+)-amphidinolide P are related closely in structure to each other and have shown *in vitro* cytotoxicity against murine lymphoma L1210 (IC_{50} = 1.7 and 3.6 μg/mL) and human epidermoid carcinoma KB cells (IC_{50} = 1.6 and 5.8 μg/mL). Two natural products possess a novel fifteen-membered macrolide structure with an epoxide at C_8-C_9, one double bond at C_{12}-C_{13}, two exo-methylene groups at C_5 and C_{16}, and one 6-membered ring bridged hemiacetal moiety. They have different functional groups only at C_{11} position (amphidinolide O has a C_{11} carbonyl group, but amphidinolide P possess an C_{11} exo-methylene group). From these structural similarities, we report first total synthesis of (-)-amphidinolide O and (-)-amphidinolide P through the convergent synthetic strategy. We were also able to determine the absolute stereochemistry of them ambiguously.



X = O : *ent*-Amphidinolide O
X = CH_2 : *ent*-Amphidinolide P

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-5**

발표분야: Current Trends in Organic Chemistry: Catalysis and Synthesis

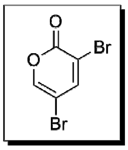
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 이희윤

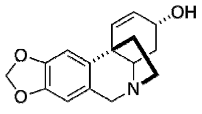
Strategic application of regioselective coupling/Diels-Alder reactions of 3,5-dibromo-2-pyrone towards the total synthesis of alkaloid natural products

조천규

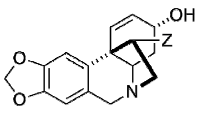
한양대학교 화학과

During the past few years, we have explored the Diels-Alder chemistry of 3,5-dibromo-2-pyrone as a new enophile synthon. Its synthetic versatility has been further exuberated by the discovery that either of the two C-Br groups can be selectively functionalized through transition metal catalyzed coupling reactions. The resultant 3- or 5-substituted 2-pyrones are potent neutral dienes, and can undergo cycloaddition reaction to afford an array of densely functionalized cyclohexenes. Ever since then, we have explored the potential applicability of the rich chemistry embedded in the 2-pyrone cycloadducts toward target oriented synthesis. Our earlier efforts in this context were not so fruitful, resulting in either complete failure (on pondaplin) or only limited success (on phomactin A and rapiculin). A few examples later, we began to prove the effectiveness of our concept which resulted in the successful total syntheses of (±)-trans-dihydronarciclasine, (±)-joubertinamine, (±)-mesembrine, (±)-crinine, (±)-crinamine, (±)-galanthamine, (±)-aspidospermidine, (±)-pancratistatin and (±)-lycorine. Presented herein are the synopses of our past results and recent progress on the total synthesis of Amaryllidaceae and Sceletium family alkaloids.

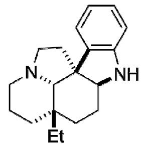




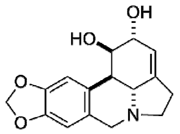
Crinine



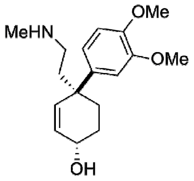
Crinamine



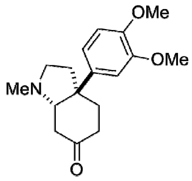
Aspidospermidine



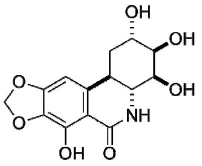
Lycorine



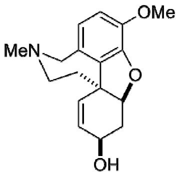
Joubertinamine



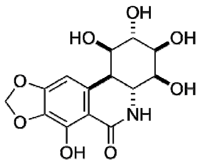
Mesembrine



trans-Dihydronarciclasine



Galanthamine



Pancratistatin

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN2-1**
발표분야: Current Trends in Organic Chemistry: Functional Organic Materials
발표종류: 분과기념강연, 발표일시: 목 14:30, 좌장: 이필호

Catalytic Access to Gold Carbenoids and Their Applications in Organic Synthesis

신승훈

한양대학교 화학과

Recent focus in our laboratory deals with development of N-O bond redox chemistry catalyzed by gold complexes.[1-3] Of particular interest in this area is the equivalence of alkynes to alpha-oxo carbenoids. Catalytically generated Au-carbenoids enables a number of interesting tandem reactions, such as [3+2]-dipolar cycloadditions of azomethine ylides,[1] tandem Mannich reaction,[2] and N-H insertion/annulation.[3] These examples show that the N-O bond substrates derived from cheap hydroxylamines are appealing oxidants for generation and utilization of carbene intermediates.Second aspect in this presentation deals with new reactivity of acceptor-substituted alkynes.[4-6] Despite long-standing interests in the reactions of 1,n-enynes particularly in the area of gold catalysis, there are few intermolecular processes. To enhance and exploit the intermolecular reactivity of alkynes, we adopted to use acceptor-polarized alkynes and successfully developed a variety of inter-molecular reactivity. Alkenes function as nucleophilic components in such reactions, most likely involving cyclopropyl gold carbenoids as intermediates. This led to [4+2] annulations of delta-lactones, and unprecedented enyne cross metathesis product. Diversification of alkyne component reveals new reactions, such as kinetic resolution of E/Z olefin mixtures with a high selectivity. Change of olefinic component into allylic ether led to a new intermolecular [3,3]-sigmatropic rearrangement, an equivalent of classical Claisen rearrangement

References

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6.(a) Koo, J.; Park, H. ?S.; Shin, S. Tetrahedron Lett. 2013, 54, 834. (b) Yeom, H. -S.; Shin, S. Org. Biomol. Chem. 2013, 11, 1089.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN2-2**
발표분야: Current Trends in Organic Chemistry: Functional Organic Materials
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 윤주영

Transition Metal Complexes and C_{60}-Organic Chromophore Dyads as Triplet Photosensitizers: Molecular Design and Applications in Upconversion and Photocatalysis

Jianzhang Zhao

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dailian, P. R. China

Triplet photosensitizers are versatile organic materials, which are very useful for applications in the areas of photodynamic therapy (PDT),[1] photocatalysis,[2] and triplet-triplet annihilation (TTA) based upconversion.[3] Traditional triplet photosensitizers are limited to porphyrin compounds and transition metal complexes. However, traditional transition metal complexes show weak absorption in visible spectral region and the lifetime of the triplet excited states is short, both feature are detrimental to the application of triplet photosensitizers. Heavy atom-free triplet photosensitizers are rarely reported. Recently we prepared a series of Ru(II), Ir(III), Pt(II) and Re(I) complexes that show strong absorption of visible light and long-lived triplet excited states.[4] We also propose to use C_{60}-organic chromophore dyads as heavy atom-free triplet photosensitizers, which show strong absorption of visible light and long-lived triplet excited states. These new triplet photosensitizers were successfully used in photocatalysis and TTA upconversion.

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일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN2-3**

발표분야: Current Trends in Organic Chemistry: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 윤주영

Functional Organic Adhesives Inspired by Marine Mussels

이해신

한국과학기술원(KAIST) 화학과

This presentation will cover recent development of adhesive organic chemistry inspired by marine mussels. Recently, it was reported that catecholamines are rich in the mussel adhesive proteins. There are two different types of catecholamines. One is a class of small molecules, which include dopamine, norepinephrine, epinephrine, and many others. The other is polymers, and the representative example is biopigment melanin. Melanin forms by oxidative polymerization of small molecule catecholamines, and its chemical structures are not precisely known due to complexity at a molecular level. Catecholamine has a long history of study focusing on biology and biochemistry in human body. Recently, however, it was found that catecholamine has an excellent property in surface adhesion. In particular, catecholamine chemistry exhibits functionalizing surfaces of virtually any materials, which is different from existing surface chemistry such as self-assembled monolayer (SAM) deposition, layer-by-layer (LbL) assembly, and others. This presentation will cover some utilities of the unique properties of catecholamine focusing on functional organic molecules.

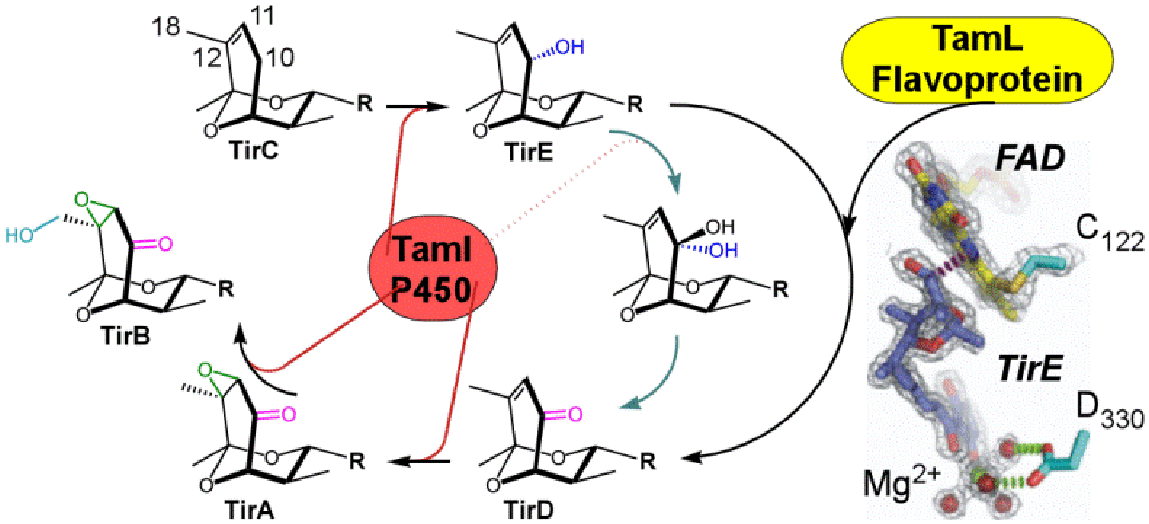
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN2-4**
발표분야: Current Trends in Organic Chemistry: Functional Organic Materials
발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 장우동

Characterizing and engineering diverse C-H bond activation catalysts from microbial natural product systems

David H. Sherman

Life Science Institute, Department of Medicinal Chemistry, Chemistry, and Microbiology & Immunology, University of Michigan, Ann Arbor, MI USA

Over the past decade, we have expanded our analysis and engineering of a broad class of monooxygenases from diverse natural product pathways. Cytochrome P450s and flavin oxidases are among the most widely distributed groups of enzymes in nature, catalyzing the oxidation of natural product and xenobiotic small molecules. Although hundreds of monooxygenases have been examined in the oxidative metabolism of drugs, only a small number have been studied in bacterial and fungal secondary metabolism, especially in macrolide antibiotic biosynthetic pathways. In most of these systems, hydroxylation and/or epoxidation reactions occur in the late stages of biosynthesis after macrolide formation by the polyketide synthase (PKS). In addition to significant increases in biological potency, hydroxylation provides potential sites for chemical modification and further enhancement of bioactivities. Thus, the creation of novel macrolide analogs through in vivo metabolic engineering and in vitro chemoenzymatic synthesis warrants a concomitant effort towards the development of monooxygenases with defined substrate specificities. Over the past several years, our work has focused on expanding knowledge of substrate flexibility and functionality of a range of P450 monooxygenases from macrolide and selects other natural product systems, including fungal alkaloids. Our progress has provided fascinating new insights into the molecular mechanisms of these biocatalysts, and their ability to generate novel products by hydroxylation, epoxidation, pinacol rearrangements, pyran ring formation and other transformations operating on both natural and unnatural substrates. This information is directing protein engineering/substrate engineering efforts to better understand the function and positional specificity of individual enzymes, as well as their ability to catalyze a range of oxidative reactions. Our program brings complementary approaches of synthetic chemistry to create diverse substrates, biochemistry to investigate and develop engineered monoxygenases with versatile substrate selectivity, and X-ray and NMR-based methods to obtain high resolution structural information for mechanistic understanding of these remarkable proteins.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN2-5**
발표분야: Current Trends in Organic Chemistry: Functional Organic Materials
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 장우동

Bioconjugate Chemistry Is Essential for Nano-biomedicine Applications

전상용

한국과학기술원(KAIST) 생명과학과

Bioconjugation involves the linking of two or more molecules to form a novel complex having the combined properties of its individual components. Natural or synthetic compounds with their individual activities can be chemically combined to create unique substances possessing carefully engineered characteristics. The technology of bioconjugation has affected nearly every discipline, including life sciences and pharmaceutical and medical fields. In this lecture I will share with you some of my own experience on how bioconjugation has been utilized for nano-biomedical applications by having a couple of actual bioconjugation examples used in the field.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MEDI-1**
발표분야: Molecular Targeted Therapeutics with Kinase Inhibitors
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 남기엽

Therapeutic Implications of Novel Small-Molecule Inhibitor to MET & RON as Receptor Tyrosine Kinase in Human Cancer

진동훈

서울아산병원 아산생명과학연구원 암연구단

The met proto-oncogene product MET, the receptor for hepatocyte growth factor (HGF), has been implicated in tumorigenesis and metastatic progression. Point mutations of MET are also aberrantly activated in many types of human malignancies and their deregulated activity is correlated with tumor growth, invasion, and metastasis. MET has therefore attracted considerable attention as a potential target in anticancer therapy. Here, we report that the novel MET kinase inhibitor, AC1, inhibits various constitutively active mutant forms of MET as well as HGF-activated wild-type MET. AC1 inhibited the proliferation of cells expressing activated MET, and promoted the regression of tumors formed from such cells in a mouse xenograft model through anti-angiogenic and pro-apoptotic actions. AC1 also inhibited HGF-stimulated activation of MET signaling in the presence or absence of serum. Furthermore, in tests of 27 different MET variants, AC1 inhibited 15 of the 17 MET variants that exhibited autophosphorylation with nanomolar potency; only F1218I and M1149T variants were not inhibited by AC1. Notably, AC1 inhibited three MET variants that are resistant to the MET inhibitors SU11274, NVP-BVU972, and PHA665752. Together, these results suggest that AC1 can be used as a potent agent for the therapy of human malignancies bearing MET point mutations or expressing activated MET. The macrophage-stimulating protein receptor tyrosine kinase (RON) is a member of the c-MET receptor tyrosine kinase family. RON, like c-MET, is also expressed and deregulated in a variety of human cancers including breast, gastric, gallbladder, lung and colon. Its biological functions are involved cell proliferation, migration, and invasion. For this reason, it has been suggested RON as a potent target for cancer therapy. However, small-molecule kinase inhibitors of RON activity that have been tested in vitro and in vivo to validate RON as a potential target in solid tumors were not developed, to data. Here, we demonstrated that AC2, identified as a novel inhibitor of RON, strongly induces tumor regression, especially in colon

and gastric cancer. AC2 potently inhibited the kinase activity of RON with IC50 of 9 nmole/L. AC2 also inhibited macrophage-stimulating protein (MSP)-dependent cellular signaling, cell proliferation, invasion, and migration. Importantly, AC2 significantly inhibited activities of various RON mutants including constitutively activeforms. Consistently, this compound inhibited RON mutants-mediated tumor formation, cellular events, colony formation, migration, and invasion, and promoted the regression of tumors formed from such cells in a mouse xenograft model. In addition, AC2 also inhibited the activity of c-MET, VEGFR2, and Lck, and these molecules-mediated signaling and cellular events. Together, these results suggest that AC2 can be used as a potent agent for the therapy of human malignancies bearing RON and its mutations or expressing activated RON, especially colon and gastric cancer.

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장소: 일산KINTEX
발표코드: **MEDI-2**
발표분야: Molecular Targeted Therapeutics with Kinase Inhibitors
발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 남기엽

Discovery of selective small molecules targeting EGFR addicted cancers.

민경훈

중앙대학교 약학대학

Inhibition of aberrantly activated kinases has been demonstrated to be one of the many cancer specific targeting strategies. Epidermal growth factor receptor (EGFR) is an attractive therapeutic target for human cancers including colon cancer and non-small cell lung cancer (NSCLC). Unfortunately, targeting wtEGFR is not enough to regulate uncontrolled tumor growth mediated by abnormal EGFR expression. Some NSCLC respond to EGFR tyrosine kinase inhibitors (TKIs), gefitinib and erlotinib. However, in most cases, acquired resistance to EGFR TKIs was developed within a year after initiation of therapy. A secondary mutation of EGFR (T790M) is responsible for half of patients with the acquired resistance to gefitinib or erlotinib. Therefore, development of TKIs targeting EGFR-T790M for resistant NSCLC or targeting other additional oncogenic kinases for other cancers with aberrant EGFR expression has been a key subject for overcoming the resistance in EGFR addicted cancers. Herein, a series of MK compounds exhibited over 1000-fold difference in potency against EGFR T790M compared to EGFR wild type. In addition, part of them inhibited selectively wtEGFR and VEGFR, which may be able to be applied to other cancers.

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장소: 일산KINTEX

발표코드: **MEDI-3**

발표분야: Molecular Targeted Therapeutics with Kinase Inhibitors

발표종류: 심포지엄, 발표일시: 목 15:35, 좌장: 남기엽

synthesis and global kinase profiling for 14-membered resorcylic acid lactones

심태보

한국과학기술연구원(KIST) 화학키노믹스연구센터

Naturally occurring 14-membered resorcylic acid lactones (RALs) such as hypothemycin turned out to be covalent kinase inhibitors. In an endeavor of enriching our small molecule kinase inhibitors discovery programs we have explored 14-membered resorcylic acid lactones as covalent kinase inhibitors. This presentation includes synthesis and global kinase profiling data for these 14-membered resorcylic acid lactones.

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장소: 일산KINTEX
발표코드: **MEDI-4**
발표분야: Molecular Targeted Therapeutics with Kinase Inhibitors
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 함정엽

Discovery of a Novel Class of Highly Potent, Selective, ATP-Competitive, and Orally Bioavailable mTOR inhibitor (XL388).

백태곤

CJ제일제당 제약연구소 신약연구센터

A series of novel, highly, selective and ATP-competitive mTOR inhibitors have been identified based on a benzoxazepine scaffold. Lead optimization resulted in the discovery of inhibitors with low nanomolar activity and greater than 1000-fold selectivity over the closely related PI3K kinases. Oral administration of mTOR inhibitor (XL388) to athymic nude mice implanted with human tumor xenografts afforded significant and dose-dependent antitumor activity.

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장소: 일산KINTEX

발표코드: **MEDI-5**

발표분야: Molecular Targeted Therapeutics with Kinase Inhibitors

발표종류: 심포지엄, 발표일시: 목 16:55, 좌장: 함정엽

Kinase drug discovery for non-oncology indications

YOONTAEYOUNG

동아제약 혁신신약 연구소

While kinases play critical roles in virtually all intracellular signaling processes, efforts to harness kinase inhibition for a therapeutic application have largely been confined to the oncology area. One of the major difficulties of non-oncology application of kinase inhibitors is the fear of unexpected toxicity primarily due to the 'off-target' kinase activity. However, as the recent FDA approval of tofacitinib for rheumatoid arthritis exemplifies, the kinase field has matured enough that development of highly selective inhibitors is becoming increasingly possible and non-oncology applications are within practical reach. In this talk, three cases of early discovery kinase programs aimed at cardiovascular and infectious disease applications will be briefly discussed (PKD for heart failure, WNK kinase for hypertension, and PI4K for hepatitis C virus infection). Emphasis will be placed on the development and use of tool compounds in (in)validation of the target kinases.

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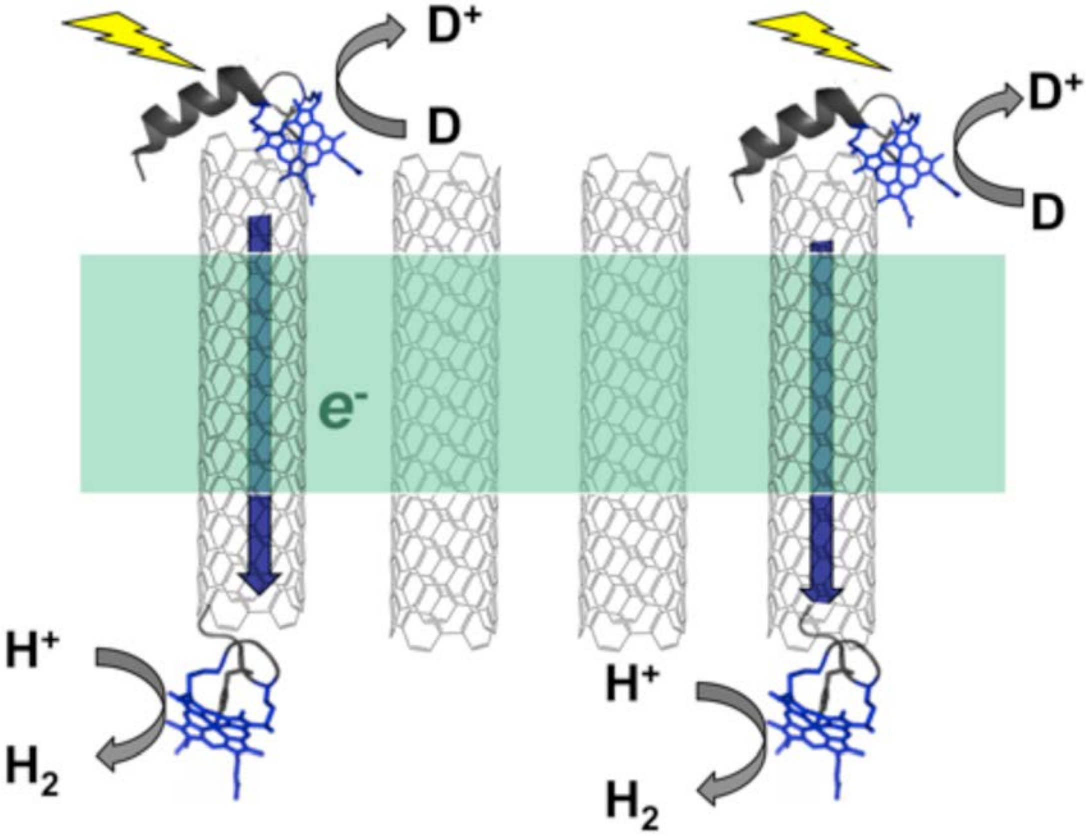
발표코드: **MAT1-1**
발표분야: Advances in Photovoltaics and Photocatalysis
발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 김승주

Bio-nano Constructs for Solar Fuels

Lenore Kubie Erin C. Kleingardner Jesse G. Kleingardner Richard S. Eisenberg[*] Todd D. Krauss[*] Kara L. Bren[*]

Department of Chemistry, University of Rochester, Rochester, NY 14627, USA

The successful utilization of the clean energy carrier hydrogen (H_2) as a fuel requires methods for H_2 production using primary energy sources not based on fossil fuels. Of possible primary energy sources, solar offers the greatest long-term impact because of its abundance and availability. Our team is engineering bio-inspired nanoscale assemblies to capture visible light and transfer photogenerated electrons to a catalyst at which proton reduction occurs to yield H_2 (Fig. 1). The assemblies make use of a membrane support for orientation and compartmentalization of the components. The target assembly possesses a modular design with three components: (1) zinc-substituted heme proteins (cytochromes) and porphyrin-peptide conjugates that yield reducing electrons upon illumination, (2) a carbon nanotube membrane for rapid charge separation, and (3) bioinspired proton-reducing catalysts based on earth-abundant metals. The presentation will focus on the development of novel biosynthetic methods for the preparation of porphyrin-peptide conjugates and the use of these biomolecules for photoinduced electron transfer to nanotubes and for catalytic hydrogen generation.



D+
D
D+
D
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H2
H+
H2

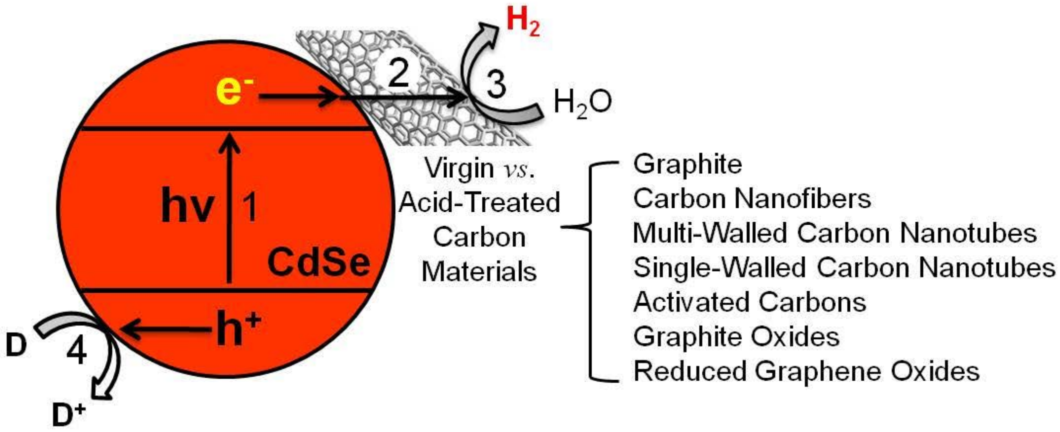
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT1-2**
발표분야: Advances in Photovoltaics and Photocatalysis
발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 김승주

Carbon-Catalyzed Solar Hydrogen Production

박현웅

경북대학교 에너지공학부

Recently, carbon materials of relatively low cost have been reported as an alternative to platinum group metals in semiconductor based-photoconversion systems. The primary reason for the coupling of semiconductors with carbon materials appears to be the unique physicochemical properties of carbon materials. We note that even though a number of papers have appeared regarding the application of diverse carbon materials in the photoconversion systems, no systematic comparison of carbon materials for their effects have been reported yet. The aim of this study is to address (1) which physicochemical property of carbon materials is the primary factor catalyzing solar hydrogen in water? (2) why do carbon materials have different catalytic effects? (3) to what extent can the carbon materials enhance solar hydrogen production? For this aim, we have employed five different commercially available carbon materials (activated carbons, carbon fibers, multi-walled nanotubes, single-walled nanotubes, and graphites) and two carbon materials converted from the commercial graphite (graphite oxides and reduced graphene oxides). For solar hydrogen, CdSe and CdS as model semiconductors were synthesized on these carbon materials. The carbon materials were tested without and with acid treatment because the surface treatment was expected to change the physiochemical properties of the carbon materials, which in turn may affect the solar hydrogen efficiency as well.


H$_2$
2
3
e$^-$
H$_2$O
hv
1
CdSe
h$^+$
D
4
D$^+$
Virgin *vs.* Acid-Treated Carbon Materials
Graphite
Carbon Nanofibers
Multi-Walled Carbon Nanotubes
Single-Walled Carbon Nanotubes
Activated Carbons
Graphite Oxides
Reduced Graphene Oxides

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장소: 일산KINTEX
발표코드: **MAT1-3**
발표분야: Advances in Photovoltaics and Photocatalysis
발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 인수일

IDEAL DYE-SENSITIZED SOLAR CELLS WITH HIGH EFFICEINCY AND LONG-TERM STABILITY

박태호

포항공과대학교 화학공학과

In both academia and industry, tremendous effort has been devoted to improving the power conversion efficiency of dye-sensitized solar cells (DSCs) to exploit their high efficiency and low production costs. The efficiency of a DSC is determined by the short circuit current density (Jsc), the open circuit voltage (Voc), and the fill factor (FF). These key parameters are strongly governed by the characteristics of the TiO2/dye/electrolyte interface, at which many electrochemical reactions occur. Modifications of the interfacial properties can alter the conduction band edge and shield the trap states of TiO2, thereby influencing Voc, Jsc, and the recombination reaction of the photoinduced electrons with any oxidized species. In addition, interfacial recombination pathways act as a loss mechanism in competition with the transport processes. In this talk, we present nanoporous network polymer nanocomposites with tunable pore size for size-dependent selective ion transport via the surface-induced cross-linking polymerization of methyl methacrylate (MMA) and 1,6-hexanediol diacrylate (HDDA) on the surfaces of nanocrystalline TiO2 particles. The morphologies of the porous network polymer layer and nanopores were investigated by transmission electron microscopy (TEM), field emission scanning electron microscopy (FE-SEM), and Brunauer-Emmett-Teller (BET) experiments. The porous layer size-selectively screened the ions that contacted the nanocrystalline TiO2 particles, as demonstrated by ion conductivity measurements, electrochemical impedance spectroscopy (EIS), and transient absorption spectroscopy (TAS).

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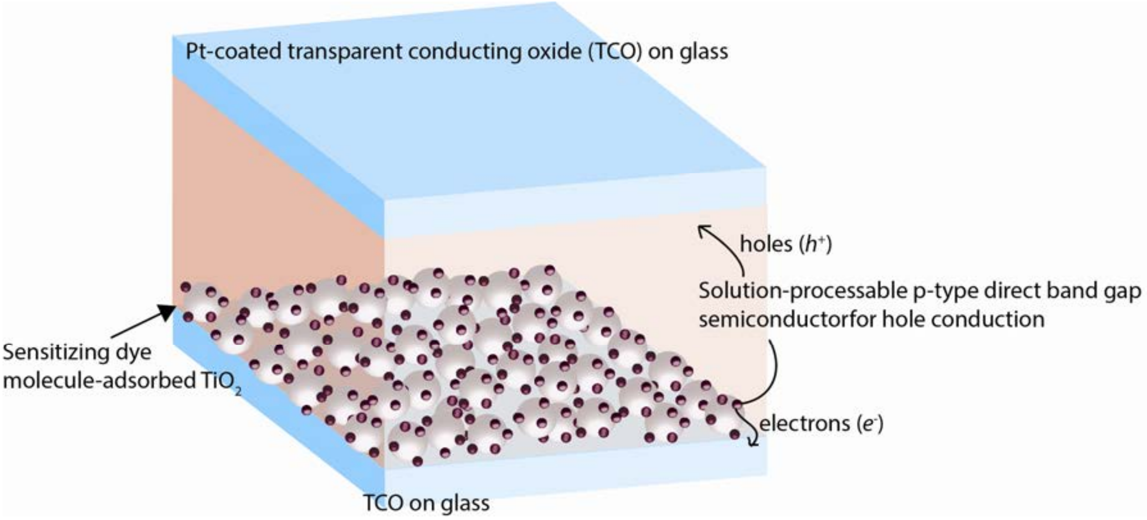
발표코드: **MAT1-4**
발표분야: Advances in Photovoltaics and Photocatalysis
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 인수일

Soluble p-type inorganic semiconductors for high efficiency all-solid-state dye-sensitized solar cells

정인

한국과학기술원(KAIST) 나노과학기술대학원

Dye-sensitized solar cells (DSCs) are low-cost photovoltaic devices that enable to convert sunlight to electricity with relatively high power conversion efficiency. They are promising alternatives to highly expensive, conventional solid-state solar cell technology based on materials such as Si, CdTe and $CuIn_{1-x}Ga_xSe_2$. Despite many advantages, the presence of organic liquid electrolytes that results in their inevitable problems of leakage, high volatility and complex chemistry, significantly limit long-term stability and performance significantly and ultimately prohibit commercialization of this technology. In spite of significant efforts to replace liquid electrolytes, the efficiencies of the resulting DSCs remain modest. Here I demonstrate that the p-type inorganic semiconductors $CsSnI_{3-x}F_x$ can replace the problematic organic liquid electrolytes in DSCs. $CsSnI_3$ consists of inexpensive and earth-abundant elements and exhibits remarkably high hole mobility and direct band gap at 1.3 eV. It is solution-processable at room temperature resulting in all-solid-state DSCs (ssDSCs. The resulting ssDSCs are made of $CsSnI_{3-x}F_x$, nanoporous TiO_2 and the N719 Ru dye, and show power conversion efficiencies up to 10%.


Pt-coated transparent conducting oxide (TCO) on glass
holes (h^+)
Solution-processable p-type direct band gap semiconductorfor hole conduction
Sensitizing dye molecule-adsorbed TiO_2
electrons (e^-)
TCO on glass

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장소: 일산KINTEX
발표코드: **MAT1-5**
발표분야: Advances in Photovoltaics and Photocatalysis
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 인수일

비진공 습식 공정에 의한 CIGS 및 CZTS 박막 태양전지 개발 동향

안세진

한국에너지기술연구원 태양에너지연구단

칼코파라이트 구조의 $CuInSe_2$(CIS) 계 화합물은 직접천이형 반도체로서 높은 광흡수 계수 ($1x10^5 cm^{-1}$)와 밴드갭 조절의 용이성 및 열적 안정성 등으로 인해 고효율 박막 태양전지용 광흡수층 재료로 많은 관심을 끌고 있다. CIS 계 물질에 속하는 Cu(InGa)Se2 (CIGS) 태양전지의 경우 박막 태양전지 중 세계 최고 효율인 20.3 %를 달성한 바 있다. 그러나 이러한 우수한 성능에도 불구하고 CIS 계 박막 증착 시 동시증발장치나 스퍼터링 장치와 같은 고가 진공장비를 사용해야 한다는 점이 CIS 박막 태양전지 상용화의 걸림돌이 되고 있는데, 이는 장비 특성상 공정단가가 높고 대면적화가 어렵기 때문이다. 따라서 기술개발 이후의 상용화 단계를 고려할 때 CIS 박막 모듈 단가를 획기적으로 낮출 수 있는 새로운 기술이 필수적이다. 이러한 관점에서 용액 및 나노 입자 전구체를 비진공 습식 방식으로 코팅하여 CIS 광흡수층을 제조하는 기술이 CIS 태양전지의 저가화 및 대면적화를 가능케 하는 차세대 기술로 인식되고 있다. 본 세미나에서는 다양한 형태의 용액 또는 입자 전구체를 이용한 CIS 광흡수층 제조 기술 개발 현황 및 각 기술별 특징을 소개하고자 한다. 이와 더불어, 최근 CIGS 의 저가형 대체 물질로 각광받고 있는 CZTS ($Cu_2ZnSn(S,Se)_4$)계 박막 형성을 위한 비진공 습식 공정 개발 동향도 함께 소개하고자 한다.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-1**

발표분야: Nanomaterials for Bio-Medical Applications

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김태일

Antigen Presenting Imageable Gold Nanoparticle Vaccines for Effective Cancer Immunotherapy

전상용

한국과학기술원(KAIST) 생명과학과

Vaccines against cancers and chronic viral diseases should induce potent humoral immune responses as well as cytotoxic T cell responses. Nanoparticulate carriers that mimic viral properties in terms of size, geometry and antigen display may be appropriate candidates for induction of such responses. Their size enables them to reach local LNs directly and interact with APCs to trigger antigen-specific immune responses. Furthermore, linkage of TLR ligands to antigen-displaying nanoparticles can effectively lead to activation of DCs engulfing nanoparticulate vaccines and facilitate induction of T cell responses. In this regard, we showed that a GNP-based antigen carrier system could potentially serve as a vaccine for cancer prevention and treatment. GNPs displaying RFP as a model antigen and CpG ODN as a TLR9 ligand reached target LNs, where they interacted with DCs, potently inducing antibody production through a Th1-driven pathway and priming CTL responses in an antigen-specific manner. As a result, GNP-based vaccines exhibited significant antitumor efficacy in RFP expressing melanoma tumor models. Taken together, these findings suggest GNP-based antigen delivery systems may be a useful vaccine technology able to prevent and/or treat a variety of ailments.

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장소: 일산KINTEX
발표코드: **MAT2-2**
발표분야: Nanomaterials for Bio-Medical Applications
발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 김태일

Synthesis and Application of Theranostic Nanocontainer with a Shape- and Size-predetermined Cavity

이광렬

고려대학교 화학과

Theranosis has been introduced for monitoring therapeutic response of a tumor toward antiproliferative chemotherapeutic agents, and nanoparticle-based theranostic systems have been widely developed. However, for successful clinical translation of nanoparticle-based theranostic systems with therapeutic efficacy enhancements, theranostic nanoparticles need to be designed to efficiently deliver therapeutic cargo to a tumor in a target-specific fashion, which would greatly enhance the safety and efficacy of cancer treatment due to mitigated nanomaterial-originated toxicity from minimal usage of diagnostic nanocontainers. The theranostic nanocontainers, hitherto developed, however do not satisfy the very first requirement, namely, high drug loading efficiency. We hypothesized that hollow inorganic nanocontainers with a hydrophobic cavity can enhance the loading efficiency of hydrophobic chemotherapeutic drugs. Herein, as a proof of concept, we report a novel one-pot synthetic process, which utilizes shape- and size- controlled nanoparticles as removable template cores, to form hollow nanocontainers with a shape- and size-predetermined hydrophobic cavity. The resulting nanocontainers fulfilled the dual requirements of delivering an effective dose of an anticancer drug to tumour tissue and enabling image-contrast monitoring of nanocontainer fate through T2-weighted magnetic resonance imaging, thereby helping achieve the optimal balance between diagnostic and therapeutic moieties in an all-in-one theranostic nanoplatform. The nanoparticle-templating strategy could be further exploited for preparation of various hollow nanostructures with predesigned cavity size and shape that should lead to great advances in nanoparticle-based theranostic systems.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-3**

발표분야: Nanomaterials for Bio-Medical Applications

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김태일

Nanotechnology Meet Immunology: Nanomaterials for Enhanced Immunity

임용택

충남대학교 분석과학기술대학원 분석과학기술학과

The design and chemical synthesis of multifunctional nanomaterials have been providing potential applications in biomedical fields such as molecular imaging and drug delivery. Recently, bio-derived and/or synthetic nanostructured materials capable of modulating the immune system have been also issues of interest in immunology-related nanomedicine fields. In this talk, the recent research results on the development of nanostructured materials for enhanced immunity would be presented. I will introduce the chemical strategy for the combination of nanostructured materials and bioactive compounds to improve both anti-cancer immunity and vaccine delivery efficiency.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT2-4**
발표분야: Nanomaterials for Bio-Medical Applications
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 오제민

Toxicity and Toxkcokinetics of Inorganic Nanoparticles in vitro and in vivo

최수진

서울여자대학교 식품공학

Along with the extensive development of nanomaterials for biological and medical applications, a growing concern about their potential toxicological effects on humans has been raised in recent years. Human body may be intentionally or unconsciously exposed to diverse types of nanoparticles by several routes due to the expanded production and use of artificial nanomaterials in a variety of fields. And it is certain that the toxicity of nanomaterials with large surface area and high reactivity may not be predictable from the known properties of bulk-sized materials. It is, therefore, highly required to understand the biological response of nanoparticles and toxicity mechanism as well. We evaluated the cellular uptake behaviors of inorganic nanoparticles such as anionic nanoclays and zinc oxide nanoparticles in cell lines and their toxicity mechanism was also investigated. Moreover, their intracellular trafficking pathway and toxicokinetics were determined in human cell as well as in animals, focusing on endo-exocytic pathway, pharmacokinetics, tissue distribution, and excretion profiles. These results will be useful for practical biological and medical applications of inorganic nanoparticles with safe and biocompatible level.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT2-5**
발표분야: Nanomaterials for Bio-Medical Applications
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 오제민

Using Gold Nanorods for Thyroid Cell Targeting

장원희

동국대학교 생명과학과

Nanoparticles (NPs), particles with a length scale below the order of 100 nm, exhibit very different properties compared with their bulk materials, largely due to quantum confinement effect. Due to their promising future in applications, many NPs are now being used or under extensive studies to be used in many different fields including biomedical, electronic, and semiconductor industries. Among them, biomedical applications of NPs are of particular interest with many useful application potentials such as bioimaging, biosensing, and cancer therapies. Recently, applications of NPs for gene delivery into cells were reported. In addition, NPs have attracted much attention as photothermal therapeutic agents in hyperthermia therapies. In order to utilize NPs for various biomedical applications, especially for in vivo applications, the toxicities of NPs have to be correctly assessed. Here we show that the surface gold nanorods had very little toxicity and that antibody-conjugated gold nanorods can specifically bind to ethanol-fixed or live thyroid cells. Together, the data suggest that the gold nanorods can be used for various theragnostic applications that require thyroid cancer cell targeting.

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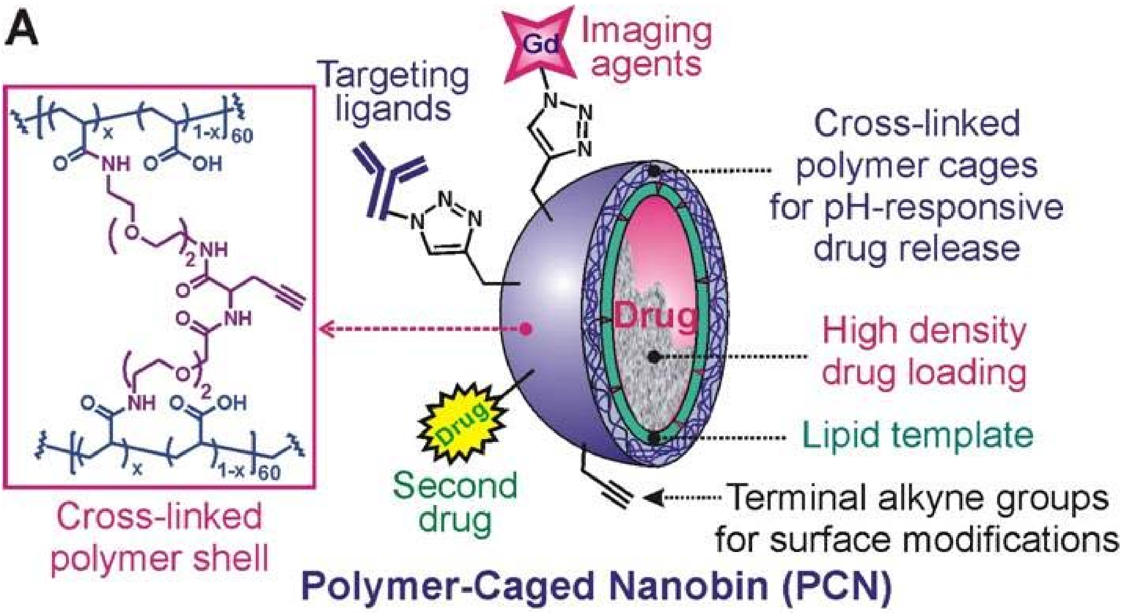
장소: 일산KINTEX
발표코드: **MAT2-6**
발표분야: Nanomaterials for Bio-Medical Applications
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 오제민

Lipid-Based Polymer-Caged Nanobins as a Modular pH-Responsive Delivery Platform for Cancer Chemotherapy

이상민

가톨릭대학교 화학과

Although liposomes have the potential to decrease the toxic side effects often associated with conventional small-molecule chemotherapy, bare liposomes are often unstable in biological environments, leading to low shelf-life and short circulation time. Additionally, they lack the specific triggers that can release the encapsulated drug under predefined condition. To overcome these limitations, clickable polymer-caged nanobins (PCNs) were prepared from liposome templates using a cholesterol-terminated poly(acrylic acid) that can be cross-linked with alkyne-functionalized diamine linker to create a protective shell around the liposome core and make it more stable. These PCNs possess pH-responsive characteristics that can be used to trigger the release of encapsulated anticancer drugs inside the liposomal core under mild acidic conditions. Given these design advantages, PCN can effectively inhibit in vivo tumor growth in a murine model of breast cancer. Importantly, PCN was well-tolerated by mice and drug-encapsulation attenuated the adverse toxicity of drugs. Furthermore, the PCN strategy allows for the additional incorporation of targeting groups and other drugs into the protective shell. With an alkyne-functionalized diamine cross-linker, azide-modified targeting ligands can be orthogonally linked to the shell via click ligation. Additionally, cisplatin-prodrug can be conjugated to the unmodified acrylate groups on the protective shells of the PCNs to provide a new strategy for combination chemotherapy regimens, enhancing the synergy in the combination of two agents. With readily modifiable surface chemistry and pH-sensitive drug-releasing triggers, PCNs constitutes a highly versatile delivery platform that can be used with conventional liposomal technology.


A
Targeting ligands
Gd
Imaging agents
Cross-linked polymer cages for pH-responsive drug release
Drug
High density drug loading
Lipid template
Drug
Second drug
Terminal alkyne groups for surface modifications
Cross-linked polymer shell
Polymer-Caged Nanobin (PCN)
x
1-x
60
NH
OH
O
2
N
N
N

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT2-7**
발표분야: Nanomaterials for Bio-Medical Applications
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 오제민

Multidentate Oligomeric Ligands for Quantum Dots, Iron Oxide and Gold Nanoparticles with Enhanced Biocompatibility

나현빈

명지대학교 화학공학과

Inorganic nanocrystals, such as quantum dots (QDs), metal and metal oxide nanoparticles (NPs) exhibit unique size- and composition-dependent properties, and they offer great promises for use in biomedical applications, including magnetic resonance imaging (MRI) and optical imaging/sensing. High quality NPs which are prepared using high temperature reaction of organometallic precursors, and they are mainly hydrophobic and not compatible to biological system. Surface processing is essential to render these NPs biocompatible and further endow them with functionalities.

Versatile surface-functionalization strategy based on ligand exchange can be applied to an array of inorganic nanocrystals, including QDs, gold and iron oxide nanoparticles (NPs). The strategy is based on designing a set of multifunctional oligomers, consisting of a short backbone, on which were laterally grafted several poly(ethylene glycol) (PEG), or other hydrophilic moieties, and either thioctic acid (TA), dihydrolipoic acid (DHLA) or dopamine as anchors on NPs. Here the TA and DLHA groups allow strong anchoring onto Au NPs and QDs, while catechols exhibit a specific affinity to iron oxide NPs. Rapid ligand exchange of the hydrophobic ligand takes place, resulting in aqueous dispersions of nanoparticles that exhibit remarkable colloidal stability over a broad range of conditions. Furthermore, by inserting controllable fractions of end-functionalized PEGs (such as PEG-COOH, PEG-N_3 and PEG-NH_2) the NPs become reactive and easy to couple to a variety of target biomolecules.

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발표코드: **ELEC1-1**
발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 박성호

Size-dependent shape transition in lead sulfide quantum dots

최혜경 김용현[1,*] 정소희[2,*]

과학기술연합대학원대학교(UST) 나노메카트로닉스학과 [1]한국과학기술원(KAIST) 나노과학기술대학원 [2]한국기계연구원 나노기계연구본부

PbS nanocrystal quantum dots (NQDs) are very promising for applications in solution- processed photovoltaic device because of their large bulk exciton Bohr radius (20 nm) and size-tunability over the entire near-infrared wavelength region. PbS NQDs, however, have poor air stability for large size PbS NQDs. In this research, we firstly synthesized highly air stable, ultra-small PbS NQDs with diameters as small as 1.5 nm, absorbed at 480 nm using low growth temperature after fast quenching. The PbS NQDs size is controlled from 1.5 to 7.5 nm in diameter. We found a transition at 4 nm in diameter in the air-stability for varying PbS NQDs size. We show this transition is driven by shape transition from octahedron to cuboctahedron due to increasing steric hindrance as large PbS NQDs size using X-ray photoemission spectroscopy (XPS) measurements and density functional theory (DFT) calculations. These studies provide important clues on surface chemistry about air-stability and also can be very useful in the process of designing better stable PbS NQDs under ambient conditions in the future.

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발표코드: **ELEC1-2**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)

발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 박성호

Al_2O_3-passivated Silicon Nanohole Photocathode for Solar Hydrogen Evolution

최미진 방진호[1,*]

한양대학교 나노공학과 [1]한양대학교 응용화학과

Silicon nanohole (SiNH) array fabricated by metal-catalyzed electroless etching method enhanced photocurrent compared to planar Si photoelectrode due to a lower kinetic overpotential induced by a larger surface area and light-trapping effects of the SiNH surface. To further reduce the kinetic overpotential, a 1-nm-thick Al_2O_3 passivation layer was deposited onto the SiNH by atomic layer deposition (ALD). On account of its passivation effect, proton reduction kinetics became much more improved. Also, when Pt was deposited over the Al_2O_3 layer, the photocathode showed further reduced kinetic overpotential by 200 mV than the Al_2O_3-passivated SiNH array.

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발표코드: **ELEC1-3**
발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박성호

Porphyrin-based Field Effect Transistors

이석중

고려대학교 화학과

Recently, the charge-transport phenomena of organic conjugated materials have been intensively investigated because of the potential applications in electronics and optoelectronics. Among them, organic field-effect transistors (OFETs) fabricated from either thin films or well-defined single crystals (SCs) as charge-transporting layers are one of the most promising electronic devices. In particular, the unique anisotropic arrangement of organic semiconducting molecules owing to their strong intermolecular interactions is expected to have a significant influence on the OFET performance, because the larger overlap of π-orbitals between neighboring molecules may increase the bandwidth and facilitate charge-transport. In this regards, porphyrin is one of the most important π-conjugated planar molecules and they have often been employed in OFETs, organic phototransistors (OPTs), dye sensitized solar-cells (DSSC) and organic photovoltaics (OPVs). Because of their unique structure, porphyrins may provide multiple interactions such as hydrogen bonding, π?π stacking, electrostatic interactions, and metal?ligand coordination. However, the performances of recently developed porphyrin-based OFET devices show relatively low carrier mobilities in the range of 10-6 to 10-1 cm2V-1s-1. A deeper understanding of such systems has hardly been achieved because of the lack of information on the molecular packing and intermolecular arrangement (which are closely related to the OFET performance), since most porphyrin-based OFET devices are based on thin films or polycrystalline objects prepared by spin-coating or vacuum-deposition processes and showing relatively poor device performances because of the limitation in use of π-conjugation. For a high degree of crystallinity with an excellent determinacy as well as a high corresponding device performance, the extension of π-orbitals and the location of conjugative substituents on the porphyrin core may play major roles. Therefore, I like to present a series of new π-extended porphyrin derivatives and their OFET devices performances along with films and single-crystals.

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장소: 일산KINTEX

발표코드: **ELEC1-4**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)

발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 신재호

Bimetallic nanocrystals with tailored morphologies for electrocatalytic applications

한상우

한국과학기술원(KAIST) 화학과

The catalytic activity and selectivity of nanocrystals (NCs) can be tuned by controlling their morphology, because the exposed surfaces of the NCs have distinct crystallographic planes that can determine their overall catalytic properties. However, the control of the size, shape, and composition of NCs has been limited due to the complex kinetics in the reduction of cationic metal precursors and to the difficulty in finding suitable stabilizing agents. Therefore, development of an efficient synthesis route for the preparation of monodisperse bimetallic NCs is still a radical issue to study their properties and applications such as polymer electrolyte and proton exchange membrane fuel cells (PEMFCs). Herein we report facile wet-chemical synthesis routes to prepare bimetallic NCs with well-defined morphologies including Au@Pd octahedra, Au-Pd alloy octahedra, Au-Pd rhombic dodecahedra, Au-Pd nanodendrites, Pd-Cu alloy NCs, and Au@Pt heteronanostructures, and their electrocatalytic performances toward ethanol oxidation, formic acid oxidation, and oxygen reduction.

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장소: 일산KINTEX

발표코드: **ELEC1-5**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 신재호

Electrochemistry through thin and dense silica film

정택동

서울대학교 화학부

Silica has been known as a good proton-selective membrane that is robust and cost-effective. Several tens of micrometer thick glass is widely used as pH sensitive probes for commercialized pH meters. Semiconductor industry brought about the technology of silicon machining that currently makes it possible to etch and deposit nanometer scale of morphology and thickness of silicon oxide. Not only size but also density or crystallinity of silicon dioxide are now possibly under nano-control, offering unprecedented opportunities to electrochemistry. Although such well defined silica layers are electrical insulators, the protons permeating through them can serve as electron carriers that enable new electrochemistry under tight control of direct tunneling current. In this talk, we will discuss the electron transfer through a thin insulating layer of the dense SiO2 and its capability of leading to novel electrochemistry on the dielectric surface.

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발표코드: **ELEC1-6**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (I)

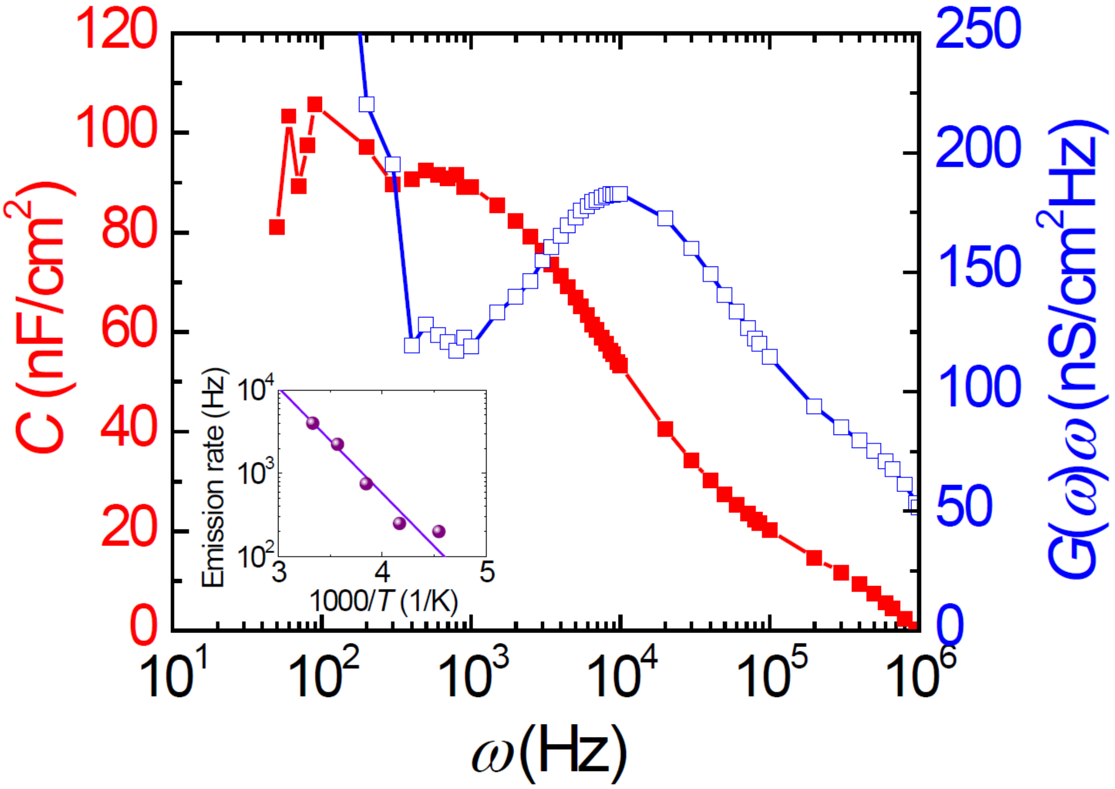
발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 신재호

Electrical characterization of solution processed chalcopyrite thin film solar cells

김동욱

이화여자대학교 물리학과

Chalcopyrite thin film solar cells have gained growing research interest due to their high energy conversion efficiency and competitive fabrication cost. We have investigated electrical properties and photovoltaic performance of CuInxGa1-xS2 (CIGS) and CuInxGa1-xS2-ySey (CIGSSe) thin film solar cells, which are fabricated by a precursor solution coating method and a subsequent multi-step heat treatment process. Both of the samples have energy conversion efficiencies of ~8%: low-band-gap CIGSSe (high-band-gap CIGS) showed higher photocurrent (higher open-circuit voltage). Such heterojunction solar cells consist of several polycrystalline thin films, whose microstructures should affect the performance of the devices. The two samples have distinct microstructures (grain size and surface topography), caused by the different preparation conditions. Thus, careful characterizations and analyses would give us important clues to improve the energy conversion efficiency. In this presentation, we will discuss the influences of the microstructures on the temperature-dependent DC and AC characteristics of the CIGS and CIGSSe thin film solar cells.


C (nF/cm^2)
120
100
80
60
40
20
0
G(ω)ω (nS/cm^{2}Hz)
250
200
150
100
50
0
10^1
10^2
10^3
10^4
10^5
10^6
ω(Hz)
Emission rate (Hz)
10^4
10^3
10^2
3
4
5
1000/T (1/K)

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ELEC2-1**
발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 박성호

Assembled quantum dot solids for energy applications

정소희

한국기계연구원 나노기계연구본부

A noticeable photoconversion efficiency of nanocrystal quantum dot solar cells has been achieved very recently, more than 7% (Ip et al., Nature Nanotechnology 2012). Understanding and controlling the carrier transport in quantum dot solids (QDS) is crucial for further improvement in efficiency. Based on the microscopic understanding of the surface properties of nanocrystal quantum dots, we created an assembled quantum dot structures for enhanced conductivity. Further, a few fundamental aspects of efficient nanocrystal quantum dots-based photovoltaics will be discussed.

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장소: 일산KINTEX

발표코드: **ELEC2-2**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 박성호

Synthesis and biomedical application of dextran coated hollow Au-Ag bimetallic nanoparticles

민달희

서울대학교 화학과

Hollow metallic nanoparticles have been implicated in many researches including the development of biosensors, thermo-sensitive therapies and diagnostic tools. Hollow nanostructures possess unique characteristics such as reduced particle density, hollow interior for high payload and tunable surface plasmon resonance. In addition, hyperthermia effect could be induced using near infrared (NIR) light, which is favorable in therapeutic applications. In this talk, we report facile synthetic strategy to prepare hollow Au-Ag bimetallic nanoparticles by using biocompatible polymer dextran as reducing agent of precursor and surface coating to enhance the structural durability against galvanic replacement reaction. In addition, surface chemistry and biomedical application of the prepared hollow Au-Ag nanoparticles will be discussed.

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발표코드: **ELEC2-3**
발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 박성호

Utilization of Semiconductor Nanoparticles for Boosting Solar Cell Efficiency

방진호

한양대학교 응용화학과

Semiconductor nanoparticles have long been utilized in solar cell applications. In this talk, a recent effort to enhance solar cell efficiency using semiconductor nanoparticles will be presented: the utilization of ZnSe nanoparticles in silicon solar cell and of Cu2ZnSn(S1?xSex)4 nanoparticles in quantum dot sensitized solar cell.Introducing a ZnSe quantum dot (QD) layer over silicon nanowire (Si NW) solar cells considerably enhanced external quantum efficiency (EQE) over broadband wavelengths. This was attributed to the combination of two major benefits of ZnSe QDs: superior light trapping and photon down-conversion.Cu2ZnSn(S1?xSex)4 nanocrystals were utilized as an alternative to Pt, which suffers from a low electrocatalytic activity and instability due to irreversible surface adsorption of sulfur species. A quantum dot sensitized solar cell constructed with Cu2ZnSn(S0.5Se0.5)4 as a counter electrode showed the highest energy conversion efficiency of 3.01%, which was even higher than that using Pt (1.24%). The compositional variations in between Cu2ZnSnS4 (x = 0) and Cu2ZnSnSe4 (x = 1) revealed that the solar cell performances were closely related to a difference in electrocatalytic activities for polysulfide reduction governed by the S/Se ratios.

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발표코드: **ELEC2-4**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)

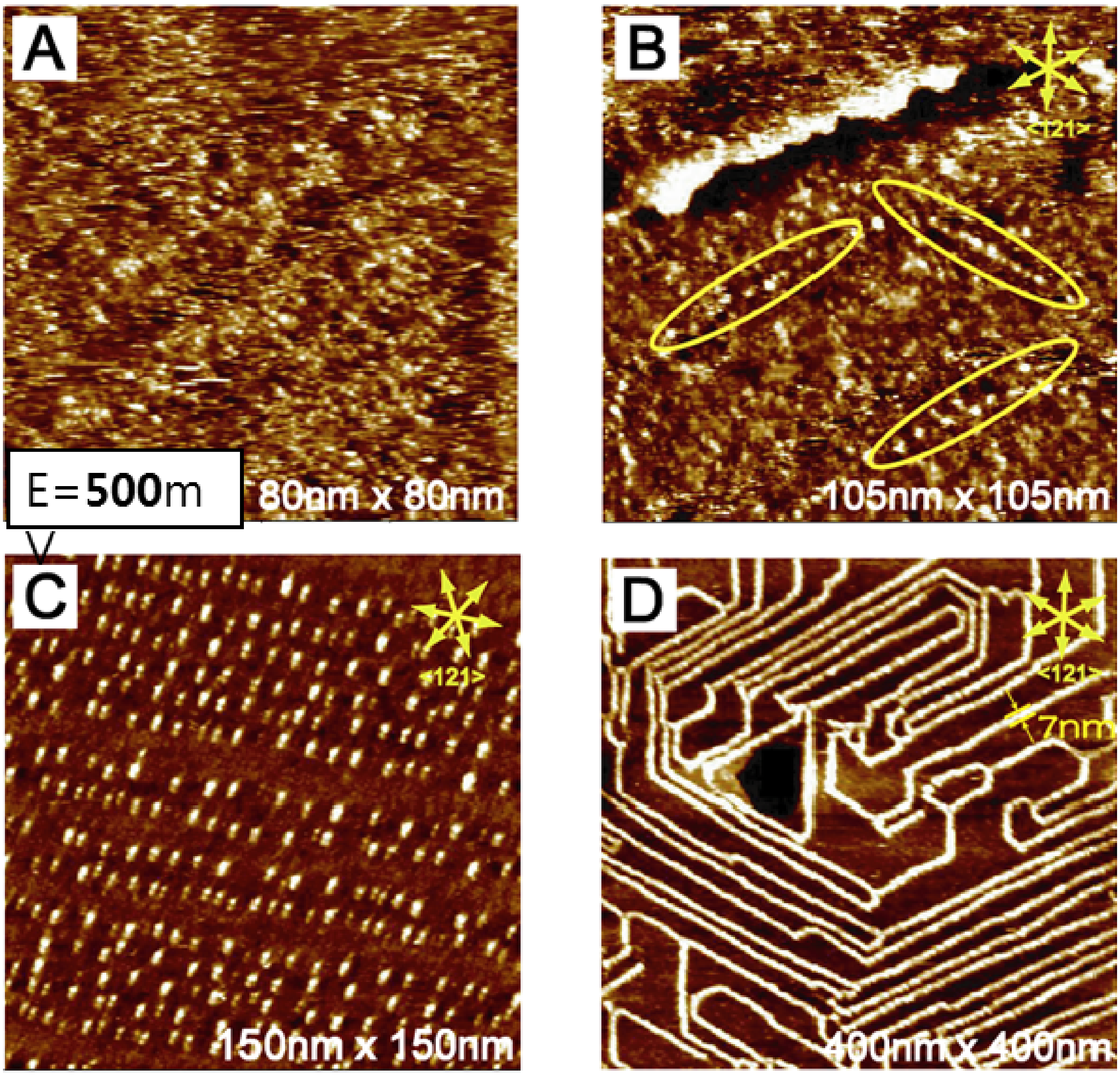
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 양해식

Electrochemical Process in Energy Conversion and Storage by in-situ STM: Strategy and Examples

Li-Jun Wan

Institute of Chemistry, Chinese Academy of Sciences

Energy conversion and storage is becoming a challenging field in electrochemistry. Effective electrode material as electrocatalyst is playing a key role in an energy conversion or storage device. On the other hand, understanding the electrochemical process taking place at the electrolyte/electrode interface is also an important issue to modify and create new electrocatalysts. In this talk, I report the preparation of various electrode materials for direct methanol fuel cell and lithium-ion battery. As a strategy, nanostructured materials were designed and prepared. For instance, the experimental results demonstrate that Pt and Pt-based nanostructured materials such as Pt naospheres, well-dispersed Pt nanoparticles on CNTs (Pt/CNT), Sn/Pt nanotube array and Pt-Fe films have better electrocatalytic property than the bulk Pt catalyst. In-situ electrochemical scanning tunneling microscopy (STM) was used to probe the interfacial process of the nanostructured materials. In situ STM results revealed the structural change of an electrode surface and adsorbants on an electrode surface. A series of STM images of picric acid on Au (111) at different potentials is shown in Fig. 1.References:1.Liang, H. P., Wan, L. J. et al., Angew. Chem. Int. Ed., 2004, 43,1540.2.Wan, L. J., Acc. Chem. Res., 2006, 39, 334.3.Guo Y.G., Hu J.S., Wan L.J., Adv. Mater., 2008, 20, 2878.4.Wen R., Wan, L.J. et al., J. Am. Chem. Soc. 2008, 130, 12123.5.Wang, J.J, Wan, L.J. et al., J. Am. Chem. Soc. 2010, 132, 12218.Fig. 1 A series of STM images of picric acid on Au (111) at different potentials


A
E=500mV
80nm x 80nm
B
<121>
105nm x 105nm
C
<121>
150nm x 150nm
D
<121>
7nm
400nm x 400nm

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발표코드: **ELEC2-5**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)

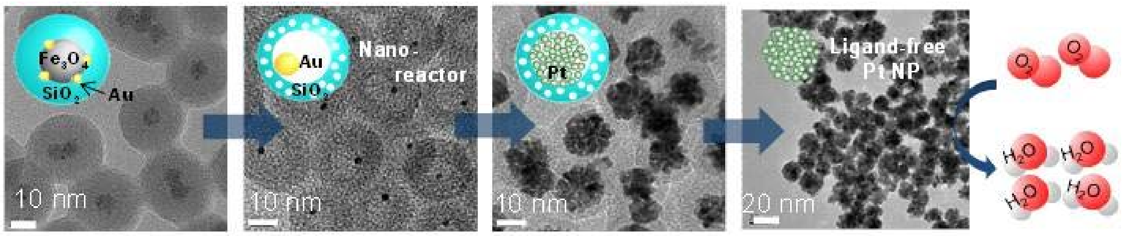
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 양해식

Nanoreactor Approach for the High Concentration Synthesis of Pt-based Nanocrystals with Enhanced Electrocatalytic Activities

이인수

포항공과대학교 화학과

Pt-based nanocrystals have been the most effective catalysts in proton-exchange membrane fuel cells. Although there has been considerable progress in the morphology controlled syntheses of metal nanocrystals through a metal-seed or block copolymer mediated process, the lack of a facile synthetic route has limited their practical applications. In particular, there is strong demand for a new synthetic method for the mass production of Pt-based nanocrystals. In this context, our research has been focused on developing a novel method which is suitable for the large-scale synthesis of the electrocatalytic metal nanocrystals. In this presentation, I will discuss the study to examine the possibility of high-concentration synthesis of Pt nanodendrites in a controllable manner through the recently developed nanoreactor approach which employs the Au@h-SiO2 nanoparticles consisting of a porous silica nanoshell and an entrapped Au nanocrystal. The hollow silica nanoreactors confine the growth of metal species inside the silica cavity and, thus, provide a consistent and well-isolated environment for the growth of nanocrystals, which enables the morphology-controlled synthesis of Pt nanodendrites even from a highly concentrated reaction suspension. Moreover, the porous silica shell could be removed readily under basic conditions, and the resulting surfactant-free Pt nanodentrites were ready for catalytic applications without additional processing to remove the surfactant molecules covering the catalytic surface. I will also present the higher effectiveness of the prepared Pt nanodendrites as an electrocatalytic material for facilitating the oxygen reduction reaction, compared to that of commercial Pt black catalysts.


Fe3O4
SiO2
Au
10 nm
Au
SiO2
Nano-reactor
10 nm
Pt
10 nm
Ligand-free Pt NP
20 nm
O2
O2
H2O
H2O
H2O
H2O

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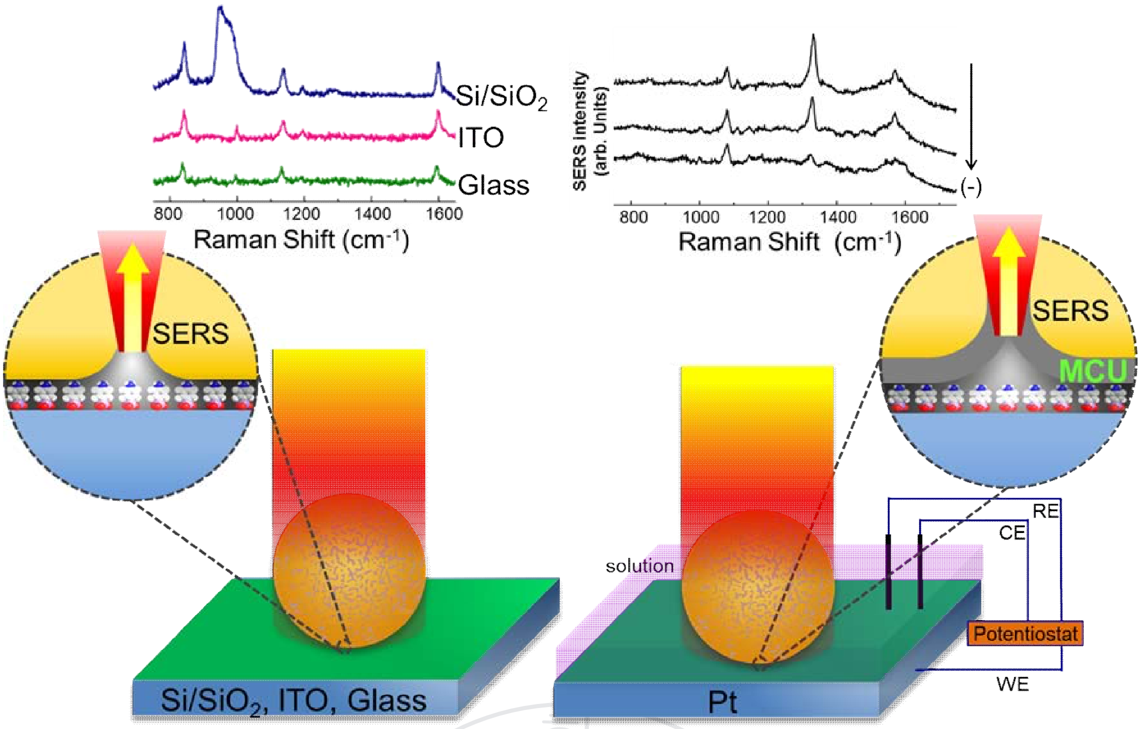
장소: 일산KINTEX
발표코드: **ELEC2-6**
발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)
발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 양해식

In-situ electrochemical Raman spectroscopy using a single gold microshell to understanding interfacial reaction

박려림 정택동*

서울대학교 화학부

Direct probing of the structure and dynamics at electrode-solution interface can provide crucial insight into heterogeneous catalysis involved in biological systems, fuel cells, solar cells, and batteries. To investigate such interfacial reactions, vibrational spectroscopy such as surface-enhanced infrared absorption spectroscopy (SEIRAS), attenuated total reflection-infrared (ATR-IR) spectroscopy, and surface-enhanced Raman scattering (SERS) spectroscopy have been proposed and utilized. Among these methods, SERS is receiving particular attention as one of the most promising techniques to monitoring the surface reaction or intermediates at electrode-solution interfaces. This is because SERS can offer molecular information with reportedly ultrahigh sensitivity down to single molecular level and most solvents including water rarely interfere with the characteristic spectra of the target molecules. We previously demonstrated that the gold microshell on a polystyrene microsphere of 1.8 ?m in diameter can serve as a strong SERS-active platform. Here a single gold microshell, which was elaborately fabricated to carry numerous hot spots on its own surface, enabled the acquisition of the SERS spectra from the molecules on non-SERS active substrates such as Si/SiO2, ITO, and glass. Self-assembled monolayer of 11-mercaptoundecanols on the gold microshell offered an easy and reliable way to electrically insulate from the underlying flat Pt electrode and accomplish in situ monitoring the electrochemical reaction with minimal interference.


Si/SiO2
ITO
Glass
800
1000
1200
1400
1600
Raman Shift (cm-1)
SERS Intensity (arb. Units)
800
1000
1200
1400
1600
Raman Shift (cm-1)
(-)
SERS
SERS
MCU
solution
RE
CE
Potentiostat
WE
Si/SiO2, ITO, Glass
Pt

일시: 2013년 4월 17~19일(수~금) 3일간

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발표코드: **ELEC2-7**

발표분야: Recent Electrochemistry in Nanoscience Breakthrough (II)

발표종류: 심포지엄, 발표일시: 목 17:25, 좌장: 양해식

Growth of Pt Shell onto Au Nanoplates : Preparation of Pt Nanoframes and Their Surface Plasmonic Behavior as Near-Infrared Sensors

장희정 박성호*

성균관대학교 화학과

In this talk, we will demonstrate how to synthesize Au@Pt core-shell nanoplates and how to apply the resulting nanostructure as a chemical sensor. Plate-like nanostructures recently gained attention in the aspect of surface plasmon resonance phenomena due to their large ratio of surface area to volume. Au nanoplates served as a seed in order to construct unprecedented Au@Pt core-shell nanoplates. Platinum provides structural stability to the nanostructure and allowed us to easily tune the peak position of surface plasmon bands. The presence or absence of Ag thin layer on Au nanoplates determines the morphology of Pt shell grown onto Au nanoplates, such as rim-preferential and uniform growth. The electron flow from the thin layer of Ag to Pt ions in the solution played a critical role in terms of controlling the deposition site of Pt atoms on the surface of Au seeds. After selectively dissolving Au core in Au@Pt nanoplates, we could successfully obtain Pt nanoframes with high homogeneity, controllable shape and thickness. As an application, we will compare their magnitude of surface plasmonic shifts by changing the dielectric medium, which is related to chemical sensor design.

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발표코드: **EVNR1-1**
발표분야: Nanoscale Insights in Environmental Chemical Reactions
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 권기덕

Application of Electrochemical Impedance Spectroscopy to Defined- and Mixed-Culture Bioanodes in Microbial Fuel Cells

정석희

연세대학교 사회환경시스템공학부

Microbial fuel cells (MFCs) employ electrochemically-active bacteria, so called exoelectrogens, on the anode and oxidize reduced material such as organic matter. Since MFCs can extract energy from organic wastewaters by using anodic bio-electrochemical oxidation coupled with cathodic reduction, they are actively investigated for achieving potential environmental applications such as wastewater treatment processes. The bioanode is composed of an anode biofilm and a conductive electrode. The main catalytic components of the bioanode are exoelectrogens. These microorganisms perform exocellular electron transfer reaction, which is the main electron transfer process in the bioanode. However, electron transfer mechanism in the bioanode is poorly understood due to its complexity and the absence of analytics. In this study, electrochemical impedance spectroscopy (EIS) was applied to mixed- and pure-culture bioanodes to understand bioanode process better. Impedance parameters of various bioanodes were successfully characterized. Methodological aspects and significant experimental results will be presented.

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Microbiological reduction of hydrogen uranyl phosphate by dissimilatory metal reducing bacteria

권만재

한국과학기술연구원(KIST) 환경연구그룹

The solubility of uranium in subsurface environments is controlled by interrelated adsorption, redox, and precipitation reactions. The current study examined the reduction of this biogenic, cell-associated hydrogen uranyl phosphate (HUP) mineral by three dissimilatory metal-reducing bacteria: Anaeromyxobacter dehalogenans strain K, Geobacter sulfurreducens strain PCA, and Shewanella putrefaciens strain CN-32, and compared it to the bioreduction of abiotically-formed and freely suspended HUP of larger particle size. Uranium speciation was determined by x-ray absorption fine structure spectroscopy (XANES and EXAFS), which showed varying extents of U(VI) reduction to U(IV). The extent of transformation to U(IV) was consistently greater with biogenic HUP than with abiotic HUP under the same experimental conditions. A greater extent of HUP reduction was observed in the presence of bicarbonate in solution, whereas a decreased extent of HUP reduction was observed with the addition of dissolved phosphate. These results indicate that the extent of U(VI) reduction is controlled by the dissolution of the HUP phase, suggesting that the metal-reducing bacteria transfer electrons to the dissolved U(VI) species, rather than to solid-phase U(VI) in the HUP mineral. Interestingly, the bioreduced U(IV) atoms were not immediately coordinated to other U(IV) atoms as found in uraninite (UO2), but were similar in structure to the phosphate-complexed U(IV) species found in ningyoite (CaU(PO4)2?H2O) even at P:U ratios as low as 1:1. The latter indicates a strong control of phosphate on the speciation of bioreduced U(IV), expressed by inhibiting the typical formation of uraninite under phosphate-free conditions.

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Greener Pathways to Organics and Nanomaterials: Sustainable Applications of Nano-Catalysts

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Sustainable Technology Division, National Risk Management Research Lab, US Environmental Protection Agency

Sustainable chemical synthetic activity involving alternate energy input, and greener reaction medium in aqueous or solvent-free conditions will be summarized for heterocyclic compounds, coupling reactions, and a variety of name reactions; these reactions are catalyzed by basic water or recyclable and reusable magnetic nano-catalysts in aqueous media using microwave (MW) irradiation.Vitamins B1, B2, C, and tea and wine polyphenols which function both as reducing and capping agents, provide extremely simple, one-pot, green synthetic methods to bulk quantities of nanomaterials in water. Shape-controlled synthesis of noble nanostructures via MW-assisted spontaneous reduction of noble metal salts using sugars will be presented. A general method has been developed for the cross-linking reaction of poly (vinyl alcohol) (PVA) with metallic systems; bimetallic systems, and SWNT, MWNT, and C-60. The strategy is extended to the formation of biodegradable carboxymethylcellulose (CMC) composite films with noble nanometals; such metal decoration and alignment of carbon nanotubes in CMC is possible using MW approach which also enables the shape-controlled bulk synthesis of Ag and Fe nanorods in poly (ethylene glycol). MW hydrothermal process delivers magnetic nanoferrites4 and micro-pine structured catalysts are obtainable in water from readily available metal salts. Sustainable route to nanoparticles using polyphenols from winery waste, or biodiesel byproduct, glycerol and their applications in catalysis, toxicity and environmental remediation will be highlighted. The comprehensive approach fulfills Green Chemistry Principles adequately and aims to generate and utilize sustainable functional nano-catalysts that will find large scale use with extreme level of waste minimization.

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발표코드: **EVNR1-4**

발표분야: Nanoscale Insights in Environmental Chemical Reactions

발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 권기덕

나노물질 기반 무기산화제의 (광)화학적 활성화 연구

이재상* 이창하[1]

한국과학기술연구원(KIST) 물자원순환연구단 [1]울산과학기술대학교(UNIST) 도시환경공학부

전통적으로 음이온성 무기산화제는 그 자체 산화력에 근거하여 제한적인 유기물질 오염 환경매질의 정화에 활용되어 왔다. 반면, 전이금속, 전자빔, 열분해, 혹은 직접 자외선 조사 등을 활용하여 이러한 무기산화제의 (광)화학적 환원반응을 촉발시킴으로써 높은 활성의 라디칼 화학종을 생성시킬 수 있으며, 이는 보다 효율적인 난분해성 유기오염물질의 산화분해를 가능케 한다. 본 연구에서는 상기한 무기산화제의 (광)화학적 활성화를 상온, 상압 조건의 나노물질 표면에서 일으킴으로써 빠른 기작의 유기오염물질 산화분해가 달성될 수 있음을 제시하였다. 나노물질 기반 무기산화제의 활성화를 통한 오염물질 산화반응의 특성화를 위해 1) 시스템 최적화, 2) 다수 오염물질종 대상 적용성 평가, 3) 관련 라디칼 산화종 규명을 통한 메커니즘 고찰, 그리고 4) 시스템의 촉매적 활용성 분석 등의 연구를 수행하였다.

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Application of computational chemistry to nano-scale environmental problem

이우진 경대승

한국과학기술원(KAIST) 건설 및 환경공학과

Physico-chemical reactions in environmental and engineered systems such as adsorption, dissolution-precipitation, complexation, and redox reaction continuously occur at complex multi-phases and their interfaces. Understanding of the reactions is crucial and essential for providing novel basic knowledge and developing environmental technologies to solve environmental problems. However, some of the reactions usually occur in a very short time and molecular level so that such limitations always have made identification of the reactions difficult and impossible. Computational chemistry methods including molecular dynamics, quantum calculation, and statistical mechanics have already made significant contributions to the understanding of molecular-level reaction mechanisms and can be applied to verify nano-scale physico-chemical reactions in the systems. We demonstrated the use of computational chemistry for advances in our understanding of complex environmental reactions by giving some examples such as molecular dynamics simulations and quantum calculations for CO_2 hydrate formation and CH_4-CO_2 hydrate replacement for solving the nano-scale environmental problems.

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발표코드: **EVNR1-6**

발표분야: Nanoscale Insights in Environmental Chemical Reactions

발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 권기덕

Metal immobilization and soil quality improvement at a military shooting range soil using soybean stover- and pine needle-derived biochars

옥용식[*] AhmadMahtab

강원대학교 바이오자원환경학과

The recent research interest in biochar has opened up its multi-disciplinary functions in science and engineering. The remediation of metal contaminated soil could be a promising exploitation of biochar. Mechanistic understandings are needed for the appropriate selection of biochar to immobilize metals in soil. In this study, biochars produced from soybean stover and pine needles pyrolyzed at 300 and 700 °C were applied as amendments to highly metal contaminated shooting range soil in laboratory incubation experiments. The characteristics of biochar were greatly influenced by the pyrolysis temperature followed by the feedstock type. Biochar significantly decreased the bioavailability and leachability of Pb (up to 88 and 65%, respectively) and Cu (up to 89 and 83%, respectively) compared to control. Contrarily, Sb was leached out to a maximum of 89% compared to control after application of biochar. Precipitation, sorption and ion-exchange were the possible mechanisms controlling metal (im)mobilization by biochar. Soybean stover-derived biochar was more effective in immobilizing Pb and Cu than pine needle-derived biochar due to relatively high O-containing functional groups. Sequential chemical extractions and thermodynamic modeling indicated that biochars resulted in geochemical transformation of metal species. Extensive spectroscopic investigations using scanning electron microscopic elemental dot mapping, and extended X-ray absorption fine structure spectroscopic (EXAFS) measurements indicated that Pb was immobilized in biochar amended soil by the formation of stable chloropyromorphite. Biochar was also effective in improving soil quality by increasing soil organic C and microbial activity. Additionally, the non-labile fraction of C in soil amended with biochars produced at 700 °C was increased, signifying the potential of these biochars towards C sequestration in soil. The results suggested that feedstock type may affect the efficacy of derived biochar in (im)mobilizing metals in soil. Special care should be taken when

applying biochar as amendment for the anionic metal/metalloid contaminated soils. Impregnation of biochar with other soil amendments could help to overcome such limitations.

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발표코드: **EVNR2-1**

발표분야: Recent Trends in Renewable Energy

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 인수일

Exceeding the Limit in Organic Solar Cells

Xiaoyang Zhu

Columbia University

This lecture aims to explore key mechanistic issues in an emerging photovoltaic technology based on organic and polymeric molecules, i.e., plastic solar cells. While there have been various predictions on whether or when photovoltaic technologies, including plastic solar cells, can be cost-competitive with electric power generation based on fossil fuels, on sometimes neglects the most important outcomes of fundamental research: the serendipity, the unpredictable, and the ground breaking discoveries that can throw the foundation of old predictions out of the window. I will present two examples from recent research in my laboratory on organic photovoltaics. The first example is within the realm of conventional theories and we aim to understand a critical step in charge separation at donor/acceptor interfaces in organic photovoltaics, namely the formation and dissociation of interfacial charge transfer excitons [1]. In particular, we show the critical role of hot charge transfer excitons in setting the fundamental time limit for charge separation in organic photovoltaics [2]. The second example illustrates the serendipity and potentially groundbreaking nature of research. We show how an intriguing physical phenomenon, exciton fission in which a singlet exciton breaks up into two triplet excitons in organic semiconductor materials, may be used to build solar cells with power conversion efficiency exceeding the fundamental limit (the so-called Shockley-Queisser limit) of conventional solar cells. We show how singlet exciton fission can occur in organic semiconductors due to a many electron quantum coherent process [3-4], and how we can efficiently extract two electrons from the quantum superposition [5].[1]M. Muntwiler, Q. Yang, W. A. Tisdale, X.-Y. Zhu, Phys. Rev. Lett. 101 (2008) 196403.[2]A. Jailaubekov, A. P. Willard, J. Tritsch, W. L. Chan, N. Sai, L. Kaake, R. I. Gearba, K. Leung, P. J. Rossky, X.-Y. Zhu, Nature Mater. 12 (2013) 66-73.[3]W.-L. Chan, M. Ligges, A. Jailaubekov, L. Kaake, L. Miaja-Avila, X.-Y. Zhu, Science 334 (2011) 1541-1545.[4]W. L. Chan, M. Ligges, X.Y. Zhu, “The energy barrier in singlet fission can be overcome

through coherent coupling and entropic gain," Nature Chem. 4 (2012) 840-845.[5] W.-L. Chan, J. R. Tritsch, X.-Y. Zhu, J. Am. Chem. Soc. 134 (2012) 18295?18302.

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발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 인수일

Multiscale Simulations On the Mechanism of Dye-Sensitized Solar Cell Systems

김형준

한국과학기술원(KAIST) EEWS대학원

To achieve the improved sustainability though the develoment of renewable energy source, it is required to understand the operational mechanism of the complex materials and systems of renewable energy systems for the development and modifications of their own properties. However, such materials or systems often consist complicated multiscale natures characterized by a sequential electron transportation, subtle balance of thermodynamic driving forces, ill-defined structural characteristics, etc; thus, it is often difficult to unveil the underlying mechanism. Thus, we use first-principles based multi-scale computational methods to understand, predict, and design the material structures for the renewable energy systems. In this talk, we discuss our recent studies on the dynamics and charge transfer mechanism of dye sensitized solar cells (DSSCs) that have been considered as promising alternatives to photovoltaic devices. From the combination of quantum mechanical simulations and molecular dynamics simulations, we discuss the complicated role of confined water molecules in DSSC electrolytes, and further suggest the new dye-regeneration pathway based on the fast inner-sphere electron transfer.

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발표코드: **EVNR2-3**

발표분야: Recent Trends in Renewable Energy

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 인수일

Preparation of Two-Dimensional Materials and Their Applications for Energy

신현석

울산과학기술대학교(UNIST) 에너지공학부

The rapid progress in graphene research has led to intensive exploration of novel 2D materials. In particular, transition metal chalcogenides, with their 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 composites of reduced graphene oxide (rGO) and metal chalcogenides, for instance, rGO/WS_2 and rGO/VS_4, and their applications for energy storage devices and hydrogen evolution.

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발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 신현석

바이오-고형연료 전소발전에 따른 폐기물 바이오매스 재생에너지 관리방안 연구

박재성

환경부 국립환경과학원 폐자원에너지연구과

신재생에너지 정책은 유럽, 미국, 일본 등 개발 국가들의 주도로 추진되어 새로운 무역장벽을 만들고 국제 질서를 개편하는데 커다란 축이 되고 있다. 한국 정부에서는 온실가스 감축, 탄소배출권 확보, 친환경 에너지 개발이라는 다각적인 차원에서 신재생에너지 정책을 추진하고 있다. 특히 신재생에너지 의무발전(RPS) 제도의 도입으로 국내 발전사들은 태양광, 풍력, 조력, 파력 등 여러 분야의 신에너지에 투자하고 있으나 가시적인 성과가 미미한 실정이다. 반면 재생에너지인 폐기물 에너지 분야는 상대적으로 접근이 용이하여 발전사들의 RPS 의무 비율을 달성하는데 큰 부분을 차지하고 있다. 그러나 폐기물 특성상 다량의 바이오매스를 함유하고 있음에도 바이오매스 에너지자원에 준하는 제도적 지원을 못 받고 있다. 본 연구에서는 최근 개정된 법에 따라 재편된 폐기물 고형연료 및 바이오-고형연료의 전소발전에 대비하고자 국내 유통 중인 고형연료의 바이오매스 함량현황을 제시하고, 고형연료의 바이오매스 함량기준을 설정을 검토하여 전소발전의 적정성 관리를 위한 바이오매스 함량관리 방안을 제시하였다. 본 연구결과는 바이오-고형연료의 품질기준 개정에 반영되어 향후 바이오-고형연료 전소 발전시 신재생에너지 공인인증서(REC) 가중치 재설정 등 제도적 지원 검토를 위한 기초자료로 활용될 예정이다.

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Bioelectrochemical system integrating reverse-electrodialysis for renewable energy production from wastewater

남주연

한국에너지기술연구원 제주글로벌연구센터

Microbial electrolysis cells (MECs) have shown advantages of efficient biomass conversion to biohydrogen gas. However, an external power source (~0.11 V in theory) is required in order to lower cathode potential to produce hydrogen (-0.41 V vs. Standard Hydrogen Electrode at pH 7). Recently, it was reported that hydrogen can be produced in MECs by using salinity difference between high and low concentration salt solutions along with organic matter degradation using electrochemically active bacteria without an external voltage supply. Reverse electrodialysis (RED) is a method for converting salinity differences between high and low concentration solutions into electrical power, and a RED stack can be integrated into a microbial electrolysis cell (MEC) between the electrodes, making a Microbial reverse-electrodialysis electrolysis cell (MREC). In this study, the MREC with a RED stack containing five cell pairs of high and low concentration salt solutions successfully produced hydrogen from wastewater without external power sources and the maximum hydrogen yield was 3.4 mol H2/mol acetate, with a hydrogen production rate of 1.6 m3 H2/m3?d at a salinity ratio of in?nite.

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Photocatalytic CO2 conversion and water splitting

인수일

대구경북과학기술원(DGIST) 에너지 시스템 공학과

The development of solar powered photo-activated materials promises to have a major impact in a variety of future applications in environmentally friendly science, such as solar energy conversion (solar fuel and photoelectrocatalysis), self-cleaning, air/water purification and artificial photosyntheiss. For this research various photocatalytic experimental systems have been designed and constructed to conduct gas/solid heterogeneous photocatalytic reactions in the UV-Vis region. Simultaneously visible light activated materials such as anion-doped TiO_2 have been successfully prepared by chemical and/or physical synthetic techniques [1]. Currently a multi-template strategy for synthesizing hollow nanocubes of CuO-$TiO_{2-x}N_x$, a new hybrid material that photocatalytically converts CO_2 into methane under solar irradiation, has been developed [2]. In addition this talk will review researches related to the direct conversion of solar energy to chemical fuels (i.e.,hydrogen) utilizing a combination of a visible or infrared light absorber such as Si with non-Pt hydrogen evolution reaction (HER) catalysts such as cubanes made of Mo_xS_y. Prof. Chorkendorff and et al. showed that the bioinspired molecular co-catalysts such as incomplete cubane-like clusters (Mo_3S_4) efficiently catalyze the evolution of hydrogen when coupled to a p-type Si semiconductor that harvests red photons in the solar spectrum. The current densities at the reversible potential match the requirement of a photoelectrochemical hydrogen production system with a solar-to-hydrogen efficiency in excess of 10% [3].[1] S. ?I. In et al., Journal of the American Chemical Society, 2007, 129 (45), 13790-13791.[2] S. ?I. In et al., Angewandte Chemie International Edition, 2012, 51, 3915-3918[3] Ib Chorkendorff et al., Nature Materials, 2011, 10, 434-438

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장소: 일산KINTEX

발표코드: **KCS-1**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 박승범

Self-Assembled Synthetic Ion Channels: Design, Characterization and Biomedical Applications

Dan Yang

Department of Chemistry, The University of Hong Kong, Hong Kong, China

Ion transport across membranes is one of the most important biological processes of all living cells. Ion channel proteins that selectively regulate ion flows are involved in many physiological processes ranging from neuronal signaling, muscle contraction, and cardiovascular function to immune response. Dysfunction of ion channels has been associated with many severe human diseases such as cystic fibrosis, asthma, hypertension, epilepsy and myocardial infarction. Therefore, developing drugs that modulate the functions of ion channels or regulate ion transport across cell membranes have received significant attentions in pharmaceutical industry. Each year over US$6 billion are generated from the sales of drugs associated with ion channel functions. Most of those drugs affect the functions of natural calcium, sodium or potassium channels through direct binding. In this talk, I will report our recent discovery of small molecules that self-assemble into synthetic ion channels that transport small anions or cations across biological membranes and their potential biomedical applications. These synthetic ion channels can mediate ion flow across plasma membranes of living cells with remarkably high efficiency, independent of natural ion channels. They are easy to synthesize and their pharmacological properties can be readily modified for therapeutic applications. Explorations on their potential biomedical applications will also be presented.

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장소: 일산KINTEX

발표코드: **KCS-2**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 09:35, 좌장: 박승범

Protein Structural Dynamics Visualized by Time-resolved X-ray Crystallography and Liquidography (Solution Scattering)

이효철

한국과학기술원(KAIST) 화학과

The principle, experimental technique, data analysis, and applications of time-resolved X-ray crystallography and liquidography (solution scattering) to study spatiotemporal reaction dynamics of proteins in single crystals and solutions will be presented. 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, and all the atomic positions in a protein can be tracked during their biological function. However time-resolved Crystallography has been limited to a few model systems with reversible photocycles due to the stringent prerequisites such as highly-ordered and radiation-resistant single crystals and crystal packing constraints might hinder biologically relevant motions. 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 demonstrate tracking of protein’s structural changes in solution using TRXL. By providing insights into the structural dynamics of proteins functioning in their natural environment, TRXL complements and extends results obtained with time-resolved spectroscopy and X-ray crystallography.[1] Y. O. Jung et al., Nat. Chem., in press.[2] K. H. Kim et al., J. Am. Chem. Soc., 2012, 134, 7001.[3] H. Ihee, Acc. Chem. Res., 2009, 42, 356.[4] M. Cammarata, et al., Nat. Methods, 2008, 5, 881.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS-3**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박승범

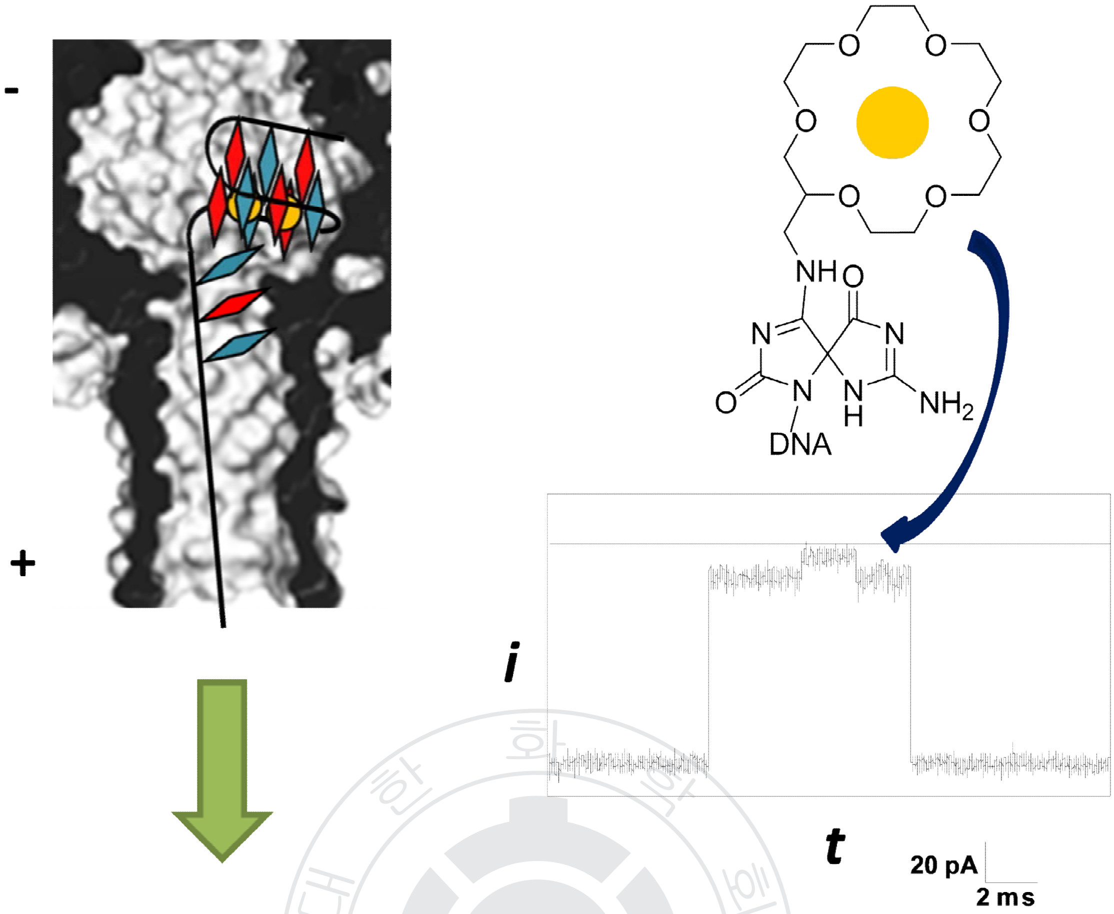
Single-Molecule Analysis of DNA Modifications with a Protein Nanopore

Aaron M. Fleming Na An Cynthia J. Burrows

Department of Chemistry, University of Utah, Salt Lake City, Utah, USA

DNA sequencing by the majority of next-generation methods relies on PCR amplification of the original genomic material with consequent loss of all information regarding base modifications that may have arisen due to epigenetic or DNA damaging events. We are particularly interested in locating sites of guanine oxidation due to oxidative stress; such lesions are thought to be particularly common in the guanine-rich G-quadruplex structures of telomeric sequences as well as in certain promoter regions of the genome. In this work, we examine a single-molecule method that involves electrophoretic translocation of single-stranded DNA through the protein ion channel alpha-hemolysin. Specific electrical signatures are observed for various folded states of the human telomeric G-quadruplex, and the kinetics of unfolding are affected by the presence of oxidized Gs. In addition, G oxidation sites can be chemically functionalized with markers that alter the current signature, providing a direct read of the location of a modified base in the sequence.

Figure 1. G-Quadruplexes are electrophoretically drawn into the alpha-hemolysin ion channel and interact with the vestibule before translocating through the nanopore. Sites of G oxidation are tagged with a crown ether to produce characteristic electrical signatures while single molecules containing DNA damage translocate through the 1.4 nm constriction.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일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS-4**
발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR
발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: Eusebio Juaristi

Chemistry and Targeting Therapies with Polymeric micelle carriers

Masayuki Yokoyama Koichi Shiraishi

Medical Engineering Laboratory, The Jikei University School of Medicine, Tokyo105-8461, Japan

A polymeric micelle is a macromolecular assembly that forms typically from AB type of block copolymers and that has a spherical inner core and an outer shell as shown in Figure 1. Polymeric micelle carriers have been actively studied for targeting of anti-cancer drugs to solid tumors. Since polymeric micelles can be formed through various cohesive interactions such as hydrophobic and ionic interactions, various chemical species including hydrophobic organic compounds and metal ions can be incorporated into polymeric micelles. Therefore, polymeric micelle carriers can deliver both contrast agents for diagnosis and drugs for chemotherapy.In this paper, we like to talk on two topics of the polymeric micelle carrier systems. First, we like to show contrast agent targeting to two therapeutic sites, solid tumors and brain ischemic stroke sites. Secondary, we talk on immunological responses to multiple injections of polymeric micelle carriers, since these immunological issues are more important in non-cytotoxic contrast agent targeting than in targeting of cytotoxic anti-cancer drugs. (The immunological responses are greatly suppressed by injections of cytotoxic drugs.) An immunological response, accelerated blood clearance (ABC) phenomenon, is well known for PEG-coated liposomes. Our polymeric micelle carriers also possess PEG as the outer shell. Since the ABC phenomenon greatly influences targeting functions of carrier systems, studies on polymeric micelles' ABC phenomenon are of great importance. Interestingly, the polymeric micelles showed no or low ABC phenomenon. This is a clear contrast to PEG-coated liposomes that strongly exhibit the ABC phenomenon. This interesting difference in the ABC phenomenon behaviors is considered to result from differences in chemical structures of the interface between PEG and the other component. This fact stresses on an importance of chemistry in biomedical applications.

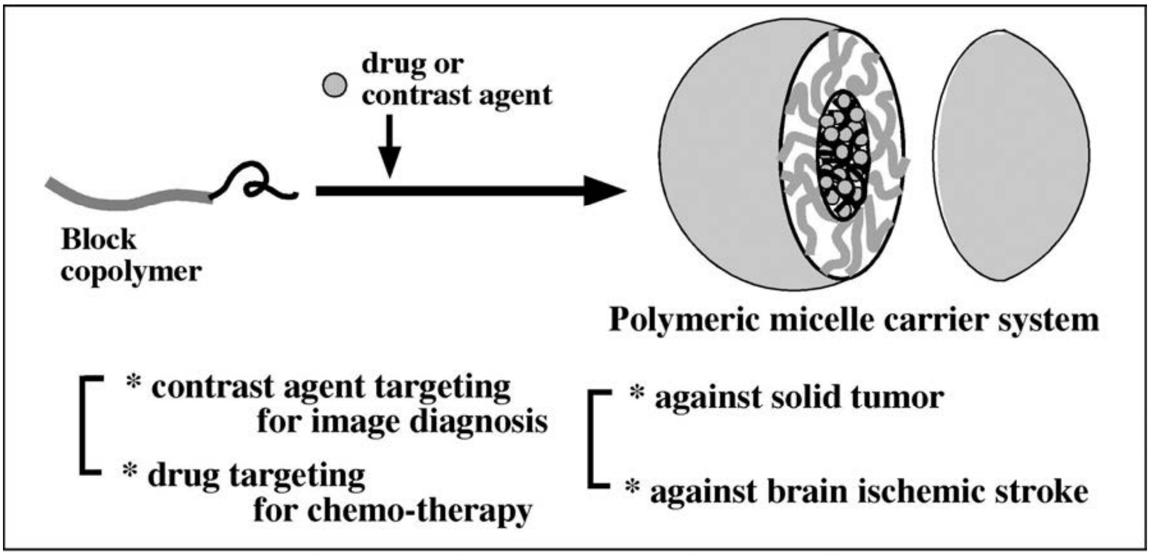


Figure 1. Theranostics with polymeric micelle carrier system.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS-5**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: Eusebio Juaristi

Organic Chemistry at the Edge of Biology: Taming Cell Behavior with Light Responsive Molecules

David Lawrence

Departments of Chemistry, Chemical Biology & Medicinal Chemistry, and Pharmacology, The University of North Carolina at Chapel Hill, Chapel Hill, NC USA

Biological systems are characterized by a level of spatial and temporal organization that often lies beyond the grasp of present day methods. Light-modulated bioreagents can be introduced into cells in an inactive form and subsequently “switched on” using light, thereby allowing the investigator to probe, perturb, or sample biological phenomena at a time and/or place of his/her own choosing. I will describe the challenges associated with the design, synthesis, and use of light-responsive bioreagents, the scope and limitations associated with the instrumentation required for their application, and a few recent examples used to scrutinize the secrets of cell signaling and behavior.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS-6**
발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: Michael Green

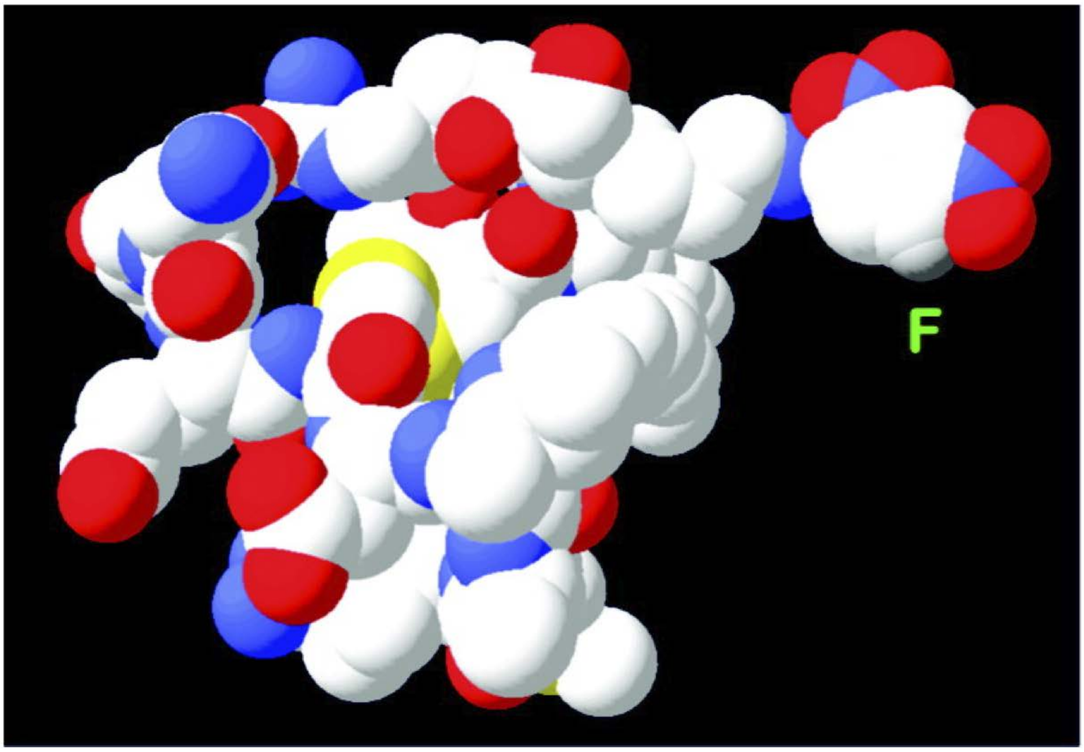
Covalent approaches to targeting cancer

Heather E. Beck Bernadette V. Marquez[1] Tololupe Aweda[1] Claude Meares

Chemistry Department, University of California, Davis, California USA [1]Mallinckrodt Institute of Radiology, Washington University, St. Louis, Missouri USA

Vascular endothelial growth factor (VEGF) is a small, dimeric protein important for angiogenesis, the formation of new blood vessels. The elegant phage-display studies of Fairbrother and co-workers led to peptide ligands that blocked the receptor binding of VEGF, but with approximately micromolar dissociation constants, which are much weaker than the nano- to picomolar dissociation constants of acceptable drugs. While not a widely used design concept, a ligand that binds irreversibly to its target has several potential advantages over such weakly binding reversible ligands. For reversible binding, the concentration of free ligand must be larger than the dissociation constant in order for the target to be >50% occupied; for a covalent ligand, under ideal conditions the target could be titrated with equimolar ligand. Once tagged, the target is permanently inactivated, an outcome qualitatively different from reversible binding. To create a site on a weakly binding peptide ligand that would carry a covalent labeling reagent, we replaced a residue that does not change the peptide's affinity for VEGF, but is located within reach of a lysine side chain on the protein. We will describe the interaction of reactively tagged peptides with VEGF, including recent studies in vivo in animal models, with particular focus on a nitroaryl fluoride reagent (see figure).

Fig.1. Marquez et al., Reactive peptide for inhibiting VEGF. *Bioconjugate Chem.*, 2012, *23* (5), pp 1080?1089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일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS-7**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: Michael Green

Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry

남원우

이화여자대학교 화학과

Dioxygen is essential in life processes, and enzymes activate dioxygen to carry out a variety of biological reactions. One primary goal in biomimetic research is to elucidate structures of reactive intermediates and mechanistic details of dioxygen activation and oxygenation reactions occurring at the active sites of enzymes, by utilizing synthetic metal-oxygen complexes. A growing class of metal-oxygen complexes, such as metal?superoxo, ?peroxo, ?hydroperoxo, and ?oxo species, have been isolated, characterized spectroscopically, and investigated in various oxygenation reactions. During the past decade, we have been studying the chemical and physical properties of various reactive intermediates in oxygenation reactions, such as high-valent iron(IV)- and manganes(V)-oxo complexes of heme and non-heme ligands in oxo-transfer and C-H activation reactions, non-heme metal-peroxo complexes in nucleophilic reactions, and non-heme metal-superoxo complexes in electrophilic reactions. The effects of supporting and axial ligands on structural and spectroscopic properties and reactivities of metal-oxygen adducts have been extensively investigated as well. In this presentation, I will present our recent results on the reactivities of various metal-oxygen intermediates in electrophilic and nucleophilic oxidation reactions. The synthesis and structural and spectroscopic characterization of mononuclear nonheme metal-dioxygen intermediates will be discussed as well.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS-8**
발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: Michael Green

Genome Editing in Cells and Organisms with TALENs and RNA-Guided ENdonucleases (RGENs)

김진수

서울대학교 화학부

Genome engineering that allows targeted mutagenesis in higher eukaryotic cells and organisms is broadly useful in biology, biotechnology, and medicine. Zinc finger nucleases (ZFNs) and transcription activator-like effector nucleases (TALENs) are powerful and versatile tools of genome editing, which are made by fusing custom-engineered DNA-binding zinc finger arrays and TALE arrays, respectively, to the *Fok*I nuclease domain. We optimized the TALEN architecture to improve the efficiency and specificity and developed a high-throughput Golden-Gate cloning system to assemble TALEN plasmid in a genomic scale. We used these TALENs to establish single- and double-gene knockout cells in which NF-κB signaling pathways were disrupted. Compared to siRNA-treated cells, these cell lines showed unambiguous suppression of signal transduction. We also used both ZFNs and TALENs to induce site-specific mutations in mice, zebrafish, and other animals.

In addition, we developed a novel genome editing technology based on RNA-guided endonucleases (RGENs). Cas9 is a sequence-specific endonuclease in type II CRISPR/Cas systems, which confer prokaryotes with adaptive immunity against invading phages and plasmids. Cas9 recognizes and cleaves target DNA sequences complementary to small synthetic guide RNAs embedded in this protein, generating site-specific DNA double-strand breaks *in vitro* and in human cells, whose spontaneous repair induces targeted genome modifications at high frequencies. Unlike ZFNs and TALENs, RGENs are customized without any cloning step, making them a broadly useful, scalable and expeditious platform for genome editing in cells and organisms.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS-9**
발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 남좌민

Coil Library-based Residue-specific Protein Force Fields

Yundong Wu

School of Chemical Biology and Biotechnology, Peking University Shenzhen Graduate School, Shenzhen, China, and College of Chemistry, Peking University, Beijing China

Simulations of Protein structures and dynamics using protein force fields play an important role in understanding the biological functions of proteins. Despite several decades' intensive efforts, the development of accurate protein force fields remains as a major challenge. We recently demonstrated that it is important to simultaneously consider the intrinsic backbone conformation and side-chain rotamers of amino acid residues, which can be obtained by statistical analysis of local conformational distributions ($\varphi,\psi,\chi1$) of a protein coil library.[1] We further developed a very efficient method to incorporate these local conformational features into protein force fields by developing amino acid-specific torsional parameters.[2-4] We have used such strategies to obtain improved OPLS-AA/C and AMBER/C force fields.[5] These force fields can better reproduce experimental NMR J coupling constants of short peptides and full length amyloid-β peptides Aβ40 and Aβ42. They can fold a series of proteins, and even give reasonably good folding transition temperatures of these proteins. *The research is supported by the National Natural Science Foundation of China (21133002 and 21203004), and the Shenzhen Peacock Program (KQTD201103).*

References:

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4.Wan, C. K.; Han, W.; Wu, Y.-D. *J. Chem. Theor. Comput.* 2012, *8,* 300-313.
5.Jiang, F.；Zhou, C.-Y.; Wu, Y.-D. *Phys. Chem. Chem. Phys.* 2013, *15,* 3413-3428.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS-10**

발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR

발표종류: 심포지엄, 발표일시: 목 16:25, 좌장: 남좌민

Glycan Microarrays for Rapid Analysis of Glycan-mediated Binding Events

신인재

연세대학교 화학과

Carbohydrates compose a large group of biomolecules with diverse structures and are found largely in the form of glycoconjugates inside or on the surface of cells. These glycan substances participate in many important cellular processes, such as cell adhesion, signaling and trafficking, through interactions with proteins. In addition, glycan-mediated biomolecular interactions also play key roles in various pathological processes. As a consequence, understanding the molecular basis of glycan-protein interactions provides deep insights into glycan-mediated biological processes. Conventional approaches have been employed to evaluate glycan-protein recognition events over past decades. Although successfully applied for studying these biomolecular interactions, the conventional techniques are labor intensive and often require large amounts of carbohydrate samples. As a high-throughput analytic tool for glycan-protein interactions, carbohydrate microarrays have been developed. The notable advantage of the carbohydrate microarray-based technology is this technology allows for simultaneous analysis of a number of glycan-protein interactions using small amount of carbohydrate samples. The carbohydrate microarrays have been applied for biological and biomedical research. In this presentation, I will discuss our recent advance in glycan microarrays for studying carbohydrate-mediated biological processes.

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장소: 일산KINTEX
발표코드: **KCS-11**
발표분야: [KCS-ACR joint Symposium] International Frontier Scientists Symposium on "Impact of Chemistry on Biology" hosted by KAST and co-organized by KCS & ACR
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 남좌민

New Plasmonic Tools for Biology

<u>Richard P. Van Duyne</u>

Department of Chemistry, Northwestern University, Evanston, IL 60201

During the last few years, there has been an explosion of interest and activity in the field of plasmonics. The goal of plasmonics is to control and manipulate light on the nanometer length scale using the properties of the collective electronic excitations in noble metal films or nanoparticles, known as surface plasmons. An improved understanding of the interactions between adsorbed molecules and plasmonic nanostructures (i.e., molecular plasmonics) is having a significant impact in a number of research areas. These include surface-enhanced Raman spectroscopy (SERS), localized surface plasmon resonance (LSPR) spectroscopy, sub-wavelength optical microscopy, and nanolithography.In the first part of this lecture, I will provide some background material on the basic physical concepts underlying molecular plasmonics with an emphasis on SERS and LSPR spectroscopy. Next, I will turn to the area of single particle surface enhanced Raman spectroscopy (SPSERS). In this section I will provide some answers for several fundamental questions such as: (1) what is the largest possible enhancement factor (EF) and (2) what nanostructure produces the largest EF. Our approach to answering these questions involved the development of new tools using single nanoparticle SERS and single nanoparticle LSPR spectroscopy spatially correlated with high resolution transmission electron microscopy (HRTEM). In the second part of this lecture, I will present recent results on using high resolution LSPR spectroscopy to detect molecular binding events, protein conformation changes, and gas sensing. This will be followed by a discussion of the development of new instrumentation for high throughput plasmonic biosensing and the study of the transport dynamics of plasmonic nanoparticles using super-resolution plasmon microscopy. I will conclude this lecture with an recent work to develop a generally applicable SERS biosensor platform that will operate in human blood and/or be interfaced with a microfluidics device.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **IND.O-1**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김보혜

Dehydration of butanols and ethanol with mesoporous SAPO-34 molecular sieves.

전종원 정성화*

경북대학교 화학과

Microwave assisted hydrothermal synthesis of micro & mesoporous SAPO-34 molecular sieves has been reported. Tetraethylammonium hydroxide (TEAOH) and carbon black were used as templating materials for micro & mesoporous SAPO-34, respectively. The obtained molecular sieves were characterized with X-ray, scanning electron microscope, adsorption/desorption of nitrogen, temperature programmed desorption of ammonia and so on. By increasing the content of the carbon black template in the synthesis, the mesopore volume increased. Dehydration of alcohols (butanols & ethanol) that are recently produced from biomass was carried out with the synthesized SAPO-34 molecular sieves, and the lifetime of the catalysts for the dehydration reaction increased as the mesoporosity increased (or as the content of the carbon black in the synthesis increased). Moreover, the performance of the microporous catalyst synthesized with microwave was better than that of the catalyst obtained with conventional electric heating. The relative performance of the catalytic dehydration may be explained by the mesoporosity (obtained with the carbon black template) and the crystal size (microwave vs. conventional electric synthesis). Therefore, it may be assumed that the fine particles of mesoporous SAPO-34 were obtained by microwave irradiation and used as an efficient acid catalyst over the dehydration of alcohols.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **IND.O-2**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 김보혜

Electrochemical behavior of porous carbon nanofibers developed from polyacrylonitrile/graphene solutions containing zinc chloride

김소연 김보혜[1,*] 양갑승[2,*] 우희권[3]

전남대학교 신화학소재공학과 [1]대구대학교 과학교육학부 [2]전남대학교 고분자 섬유 시스템공학과 [3]전남대학교 화학과

Graphene-embedded porous and smaller fibrous carbon nanofibers (CNFs) were prepared by a simple electrospinning method with the help of zinc chloride ($ZnCl_2$), and their electrochemical properties as supercapacitor electrodes were investigated. The CNFs were characterized as having a large specific surface area of up to 520 m^2g^{-1}, mesopore volume fraction up to 35%, and high electrical conductivity (over 0.45 Scm^{-1}) and exhibited a gravimetric capacitance of 148 Fg^{-1} and energy densities of 9.2-20.0 $Whkg^{-1}$ over a power density range of 400-30,000 Wkg^{-1} in 6 M potassium hydroxide electrolyte. The introduction of $ZnCl_2$ and graphene into the polyacrylonitrile (PAN) solution induced suitable micropores to accommodate many ions for high capacitance and mesopores for smooth ion transfer. Therefore, the cooperation of micro- and mesopores in the CNF electrode materials synergistically improves the performance of electrochemical double-layer capacitors (EDLCs) because these materials have a high rate capability, high capacitance, and long cycling life.

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장소: 일산KINTEX
발표코드: **IND.O-3**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 김보혜

Towards highly active nanostructures: Twinning, core-shell, and lattice mismatch

윤지선 **nguyentienkhi** 이광렬*

고려대학교 화학과

Structure-dependent catalytic property of nanoparticles has been one of major research thrusts of nanoscience and technology. Nanostructural features with high surface-to-volume ratio and high surface energy are particularly useful for catalysis application. Most notable recent accomplishments in this field are the preparation of high energy faceted nanocrystals and the formation of dendritic nanostructures for high surface area and stability under catalysis. Concave nanoframes are also suggested as catalytically useful high surface area nanostructures. Nanoparticles are designed to possess to have high energy structural features such as steps and kinks; twinning boundaries are particularly useful in creating these features. Also, core-shell nanoparticles have been prepared, where the surface energy is altered by the presence of the core with a different composition, thus creating intrinsic lattice mismatch between the core and the shell, leading to higher catalytic activity.In this seminar, I will describe various current approaches to improve the catalytic activity of nanoparticles and their implications for future research.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **IND.O-4**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 김보혜

Studies of Functional Surface Chemistry of Graphene: Characterization and Application

양지은 신현석*

울산과학기술대학교(UNIST) 에너지공학부

We modify the reduced graphene oxide(rGO) surface with electron donors or accepters. Functionalized rGO brings about the change of electronic properties. It is significant that functionalized rGO can cause the different properties following the change of charge transport. To investigate electrical properties of graphene , field-effect transistor (FET) device should be fabricated. The fabrication process of rGO FET devices includes the deposition of rGO on a SiO2 wafer and then photolithography or e-beam lithography. However, the process is complicated and, requires exquisite skill. Therefore, an easy and systematic approach to fabricate rGO FET devices is proposed, which utilizes electrostatic attraction between electrodes and rGO sheets. Negatively and positively charged rGO sheets are functionalized with carboxylic acid and amine groups, respectively. The FET of amine-functionalized rGO exhibits n-doping effect. The FET devices fabricated by this method show high mobility of carriers.

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장소: 일산KINTEX

발표코드: **IND.O-5**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김보혜

카보란 기반 새로운 광 전기적 특성의 유기전자소재

위경량 강상욱*

고려대학교 소재화학과

세가지 구조이성질체(ortho-, meta-, 그리고 para-)를 가지고 있고, 뛰어난 화학적 물리적 안정성을 가지는 카보란 물질을 기반으로 새로운 형태의 청색인광 OLED 용 호스트 물질을 개발하였다. 세가지 이성질체는 모두 카보란을 중심으로 광특성이 뛰어난 두개의 카바졸이 치환되어 있으며, bis[4-(N-carbazolyl)phenyl] carboranes (o-Cb, m-Cb, 그리고 p-Cb)으로 명명된다. 카보란의 특성을 규명하기 위하여 카보란 위치에 벤젠을 도입하여 물리적 특성을 서로 비교하였고, 그 결과 구조이성질체에 따라 o-Cb < m-Cb < p-Cb 순서로 경향성 있는 열적 안정성과 전하 이동도를 가진다는 것을 증명 할 수가 있었다. 그 중 o-Cb 물질을 제외하고 m-Cb 와 p-Cb 가 청색인광 호스트 물질에 적합한 특성을 보여 주고 있으며, 특히 p-Cb 는 높은 삼중항 에너지(T1 = 3.1 eV)와 뛰어난 열적 안정성(Tg = 164 °C) 뿐만 아니라 1.1 × 10?3 cm2/(V s)의 뛰어난 정공 이동도를 가지는 것을 실험적으로 확인 하였다. 또한 분자계산을 통하여 카보란 물질이 분자내에서 어떤 전자적 역할을 하는지 확인 하였고, 그 결과 기존에 알려진 청색인광용 호스트 물질에서는 완전하지 않았던 삼중항 에너지가 완전히 한곳에만 감금되어 있음을 확인함으로써 기존 물질들 보다 카보란 기반 물질이 뛰어난 특성을 가지는 것을 이론적으로 증명하였다. 이 결과들을 바탕으로 p-Cb 물질을 청색인광 소자에 적용하였고, 단순 소자구조에서 15.3%의 높은 외부양자효율을 얻을 수가 있었다.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **IND.O-6**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 김보혜

Synthetic approaches for CO_2 conversion using amine/epoxide in the presence of active catalyst system

김용진 오승근

한국생산기술연구원 그린공정소재연구그룹

Synthesis of carbamates, disubstituted ureas, and isocyanates is of great importance since they are used as important intermediates for the synthesis of polyurethanes. Among them, the direct synthesis of disubstituted urea from the reaction of CO_2 and amine has attracted much attention because it makes the process more efficient and safe compared to the conventional one that employ oxidative carbonylation of amines using explosive CO/O_2 mixture gas. Herein we provide the facile synthetic methodologies for the synthesis of disubstituted ureas, isocyanates from the reaction of CO_2 with epoxide and amines in the presence of active catalyst system using various strategic approaches.

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장소: 일산KINTEX
발표코드: **INOR.O-1**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 분과기념강연, 발표일시: 금 10:00, 좌장: 이민형

From Supramolecular Gels To Organic-Inorganic Hybrid Silica-Based Nanomaterials

정종화

경상대학교 화학과

Very recently, the combination of nanomaterials used as solid supports and supramolecular concepts has led to the development of hybrid materials with improved functionalities. The “hetero-supramolecular” materials can bridge the gaps separating molecular chemistry, materials science and nanotechnology. Recent examples include enhanced recognition and sensing using molecules on preorganized surfaces, the reversible building of nanometer-sized networks and 3D architectures, as well as biomimetic and gated chemistry in the hybrid nanomaterials for the development of advanced functional protocols in three-dimensional frameworks.

My group focused on the development over the past 7 years of organic-inorganic hybrid silica nanomaterials that can selectively detect and separate specific guest molecules. In this conference, I will present new types of organic?inorganic hybrid nanomaterials for use in biological and environmental applications that were developed in our research laboratory for the selective detection and separation of specific guest molecules.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-2**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 분과기념강연, 발표일시: 금 10:35, 좌장: 이민형

Photochemical and Electrochemical Regeneration of Nicotinamide Cofactors Using Metal Complexes/Nanoparticles and Carbon Dioxide Reduction

김진홍

이화여자대학교 화학·나노과학과

The sunlight used by plants to make biological fuels through photosynthesis is harvested by light-collecting antennas. These chromophores transfer excitation energy to reaction centers where it is converted to electrochemical potebtial energy via photoinduced electron transfer. An organometallic rhodium complex has been frequently employed as an efficient catalyst for hydride transfer during chemical and electrochemical formation of NADH to selectively reduce NAD^+. Several electrochemical NADH regeneration systems have been reported using Rh catalysts to study electron transfer phenomena. Here, we present a novel, simple system that employs only Pt nanoparticles (PtNPs) for the efficient photochemical generation of NADH. This system first demonstrated that PtNPs can be used in the visible light-driven photogeneration of NADH without an additional chromophore in the presence of a sacrificial electron donor, and can directly perform the catalysis of the NAD^+ reduction in the absence of another homogeneous heavy-metal catalyst in aqueous media. A visible light-driven photocatalytic system for the generation of NADH from aqueous protons was examined using molecular cobaloxime catalyst. Introduction of an electron-donating or electron-withdrawing substituent in the para position of the pyridine changed the rate constant and affected the conversion efficiency. In addition, the reduction of CO_2 was carried out in the presence of formate dehydrogenase using the NADH photochemically generated using cobaloxime. Bulk electrolysis of NAD^+ carried out with a Rh catalyst in the absence and presence of platinum nanoparticles (PtNPs) generates enzymatically active 1,4-NADH. Functionalized ITO electrodes are used to regenerate NADH using a rhodium catalyst electrochemically in a buffer solution. Amino- and mercapto-functionalized electrodes featured higher activity and stability for electrocatalytic generation of NADH than a bare ITO electrode.

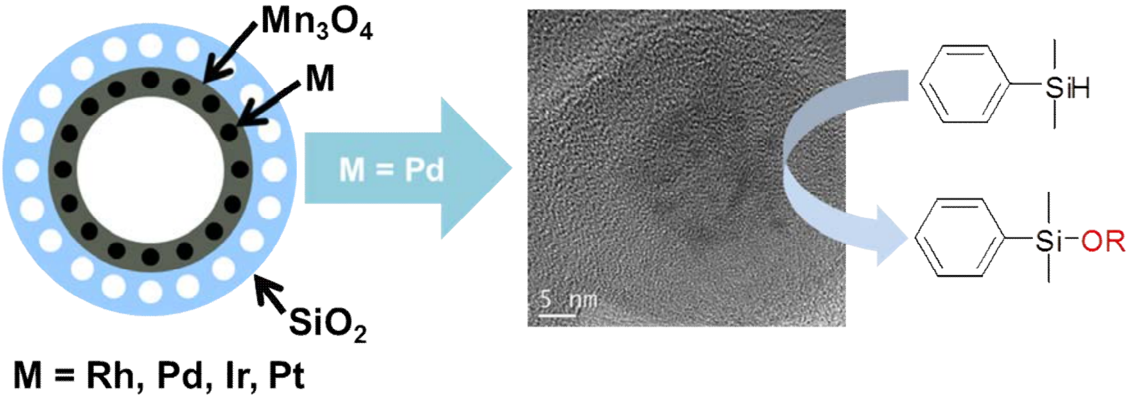
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR.O-3**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 이준승

Fabrication of Hollow Silica Nanoparticles with Catalytically Functionalized Interior Surfaces : Nanoreactor Frameworks for the Selective Catalytic Reactions

김수민 이인수*

포항공과대학교 화학과

Hollow nanoparticles, having a protected interior cavity suitable for selectively encapsulating molecules, are attractive candidates as nanoreactors which efficiently and selectively catalyze various organic reactions. For the further development of nanoreactor with enhanced selectivity, it is demanded to devise the new method of deferentially functionalizing hollow interior, which allows the molecular recognition and chemical reaction to occur only inside the hollow shell. In this presentation, I'll discuss the fabrication of nanoreactor framework consisting of a hollow silica nanoshell and a functionalized interior surface with Lewis acidic manganese and their employment in selectively catalyzing the cyanosilylation reactions of aromatic aldehydes. I will also present the study to further decorate the interior surface of the hollow silica nanoreactor with catalytically more useful metal nanocrystals, including Pd, Pt, Rh, Ir, and Pd/Pt alloy nanocrystals, through employing the galvanic replacement reaction between manganese oxide surface and metal ions in the solution. Furthermore, I will demonstrate the efficient and selective catalytic performance of the functionalized silica nanoreators with novel metal nanoparticles in the silane alcoholysis reactions.


Mn$_3$O$_4$
M
SiO$_2$
M = Rh, Pd, Ir, Pt
M = Pd
5 nm
SiH
Si–OR

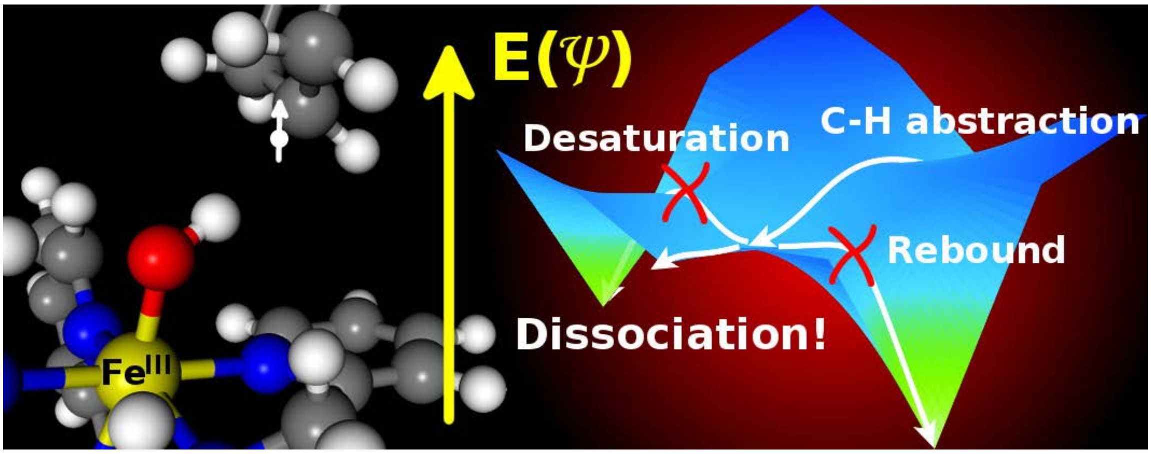
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR.O-4**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 이준승

Density Functional Theory Calculations on the Structure and Reactivities of Synthetic Nonheme Metal-Oxygen Compounds

CHO KYUNG BIN MICHAEL Sason Shaik[1] 남원우[2,*]

이화여자대학교 바이오융합과학과 [1]The Hebrew University of Jerusalem and The Lise Meitner-Minerva Center of Computational Quantum Chemistry [2]이화여자대학교 화학과

Heme metal-oxygen utilizing catalysts (M=O, M-OO, M-OOH, M-HOOH) are found in many enzymes in Nature, such as cytochrome P450, horse radish peroxidase and nitric oxide synthase, just to name a few. There are also examples of nonheme metal-oxygen utilizing enzymes, such as naphthalene dioxygenase, homoprotocatechuate 2,3-dioxygenase and taurine:alfa-ketoglutarate dioxygenase. These compounds catalyze common and essential reactions such as hydroxylation, epoxidation, desaturation and sulfoxidation. A given approach to understand the fundamentals of the reactions these compounds catalyze is to synthesize model systems. Our lab routinely produces and investigates the reactivities of such compounds, and this talk will give some examples of the theoretical calculations done in this area, in order to gain more insights than just experiments only could give. This talk will be given in English.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR.O-5**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 이준승

Controlling nanometer-sized interior gap in plasmonic gold nanoprobes

오정욱 남좌민*

서울대학교 화학부

A tremendous amount of research has been devoted to the development of unique nanostructures for the various applications such as colorimetric biosensors, photonic devices, molecular rulers, surface-enhanced Raman scattering (SERS). All the applications are related to the plasmonic coupling of nanostrutures in a very small region (i.e. below several nm). Although the nanometer-sized gap confers to the highly enhanced optical signal, especially SERS, the elaborate control in ~nm sized range with high precision and reliability is very difficult. We developed gold nanobridged nanogap particles (AuNNPs) that generates a highly stable and reproducible SERS signal. AuNNPs are synthesized from DNA modified gold nanoparticles as core particles. It is very interesting that DNA plays a crucial role to the formation of ~1 nm interior hollow gap. DNA strand has four different bases and is apt to control the length and other modification in DNA molecule, then it is suitable for the manipulation of nano-sized distance. We will discuss the synthetic strategies and the formation mechanism of AuNNP and the role of DNA.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR.O-6**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 이준승

Magnetic switch for apoptosis signaling

유동원 천진우

연세대학교 화학과

Cellular signaling is critical for controlling a number of cellular activities, such as differentiation, growth, and death. Recent advance in magnetic technology is opening up new possibilities of highly sophisticated regulation of cellular signaling in remote and noninvasive manner. Magnetic techniques using magnetic nanoparticles are uniquely advantageous due to the benign relationship between magnetic fields and biological systems; magnetic fields have no penetration depth limit and deleterious impact on biological environments. When coupled with magnetic nanoparticles, magnetic fields are transformed into other forms of energy, such as heat and mechanical force. Moreover, the generated force is so gentle (in the femtonewton range) that rheological and cytoskeletal properties of biological system are not disturbed. Consequently, it has distinctive benefits for in vivo application. This talk will focus on magnetic switches for apoptosis signaling by using heat and mechanical force and their in vivo feasibility. Detailed experimental results and possible applications will also be discussed.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS1.O-1**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 임상현

Observation of a single diffusing molecule in a sub-diffraction-limit volume by ALEX-FRET and STED nanoscopy

김남두 권지웅[1] 임영빈[1] 김성근[*]

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

With the combination of super-resolution nanoscopy and single-molecule spectroscopy, we were able to detect a single molecule in a tightly confined volume 50-times smaller than the diffraction-limited confocal volume by switching off the fluorophores with stimulated emission depletion (STED). We demonstrated the feasibility of this new technique for a ssDNA (30 bp) dual-labeled by ATTO 647N and DY-510XL. Alternating laser excitation (ALEX) FRET between two dyes was acquired under both confocal and STED conditions. With this new technique, we were able to observe a single diffusing DNA molecule at up to 5 nM concentration, which is 100 times higher than in typical single-molecule measurements.

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발표코드: **PHYS1.O-2**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 임상현

Two-dimensional LIBS of LPG and electrolytic oxy-hydrogen flames

이석환 여재익*

서울대학교 기계항공공학부

The 2-dimensional mapping of chemical species information is achieved by LIBS (laser-induced breakdown spectroscopy) in LPG and EOH flames, while the optical emission spectroscopy (OES) is used for validation of the LIBS results. The base LIBS signals, which are averaged from measurements at 320-nm to 350-nm wavelengths, describe the density information of a flame. The C_2 /base LIBS signal ratio provides the concentration of fuel, while CN/base signal provides the rate of dissociation of carbonic fuel. The H/base signal represents the concentration of fuel and water product, and the H/O signal represents the fuel/air equivalence ratio. The distributions of molecule species such as OH, C_2 , and H_2O, obtained from OES are compared with the mapping via the LIBS for validation. The OES distributions of C_2 and H_2O are similar to the LIBS results of CN/(O+N) and H/O, respectively. H/O and CN/(O+N) LIBS results provide fuel and air equivalence ratios. Thus, we demonstrate first time use of the 2-D LIBS for providing key combustion information, aside from the OES approach, such as density, atomic and molecular chemical concentration, and fuel/air equivalence ratio.

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발표코드: **PHYS1.O-3**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 임상현

Application of single-molecule spectroscopy for investigating the disease mechanism of Parkinson's disease.

김재열 최봉규[1] 신 연균[2,*] 이남기[3,*]

포항공과대학교 물리학과 [1]포항공과대학교 I-BIO/시스템생명공학부 [2]Department of Biochemistry, Biophysics & Molecular Biology, Iowa State University, USA [3]포항공과대학교 시스템생명공학부/물리학

Parkinson’s disease is one of the popular neurodegenerative diseases, which has two characteristic/pathological features; the formation of Lewy bodies and selective death of dopaminergic neurons. Since α-Synuclein is a major component of Lewy bodies and its familial mutations induce Parkinson’s disease, previous studies suggested that the oligomeric or protofibril forms of α-Synuclein induce the Parkinson’s disease. However, the molecular mechanisms of the toxic function of the oligomers still remain unclear. Here, we show that α-Synuclein oligomers efficiently inhibit neuronal SNARE-mediated vesicle fusion [1]. To prove the detailed mechanism of the oligomers’ toxicity, we applied a single-molecule spectroscopy, alternating-laser excitation (ALEX) [2]. From this single-molecule measurement, we found that α-Synuclein oligomers directly bind one of the SNARE proteins, which blocks neurotransmitter release in neurons. We also applied fluorescence correlation spectroscopy (FCS) measurements to investigate vesicle clustering mechanism by the oligomers. Our results provide a potential mechanism of Parkinson’s disease. (Reference)[1] B.-K. Choi*, M.-G. Choi*, J.-Y. Kim* et al., “Large α-Synuclein oligomers inhibit neuronal SNARE-mediated vesicle docking”, PNAS (in press). *These authors contributed equally to this study[2] J.-Y. Kim et al., “Solution single-vesicle assay reveals PIP2-mediated sequential actions of synaptotagmin-1 on SNAREs”, EMBO J. 31, 2144-2155 (2012)

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS1.O-4**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 임상현

Ultraviolet-ultraviolet hole burning spectroscopy of ions in a Paul trap

최창민 김남준*

충북대학교 화학과

We have developed a new technique of ultraviolet-ultraviolet (UV-UV) hole burning (HB) spectroscopy applicable to ions stored in a Paul trap. Due to the difficulty in distinguishing the ions produced by the pump laser pulse from those by the probe, UV-UV HB spectroscopy has never been applied to ions in an ion trap. However, we found that some photofragment ions do not get trapped but escape from the ion trap right after the irradiation of the pump pulse and thus can be detected separately from those produced by the probe pulse. Using this HB technique we successfully obtained the conformation-specific electronic spectra of dibenzo-18-crown-6 complexes with alkali metal cations (M+-DB18C6, M=K, Rb, and Cs). We also investigated the ejection process of photofragment ions from a Paul trap. We measured the dependences of the ejection time of the M+ ions on the rf amplitude, time delay between the laser and the extraction direct current (DC) pulse, and buffer gas pressure inside the QIT. We suggest that the photofragment ions undergo unstable oscillatory motion upon their generation in the QIT due to their larger values of the Mathieu parameter qz than that of the stability boundary. The fragment ions increase their oscillation amplitudes by taking up energy from the rf field and are eventually ejected out of the QIT. The lower limits of the qz values necessary for the escape of K+, Rb+, and Cs+ ions from the QIT are determined to be ~1.7.

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장소: 일산KINTEX
발표코드: **PHYS1.O-5**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 임상현

Single-Molecule Photophysical Properties of Pi-Expanded Macrocyclic Oligothiophenes

양재성 김동호*

연세대학교 화학과

Functional oligothiophenes have attracted comprehensive interest in the field of materials sciences and have been advanced to be among the most frequently used π-conjugated materials. Thiophenes are ideal building blocks in transition metal-catalyzed cross-coupling reaction that serves as a basis for the synthesis of most conjugated π-systems. They therefore provide enormous potential of structural variation which allows tuning of the electronic properties in a wide range. Furthermore, the high polarizability of sulfur atoms in thiophene rings leads to a stabilization of the conjugated chain and to excellent charge transport properties, which are one of the most crucial assets for applications in organic and molecular electronics. The traditional linear oligothiophenes suffer from undesired perturbing end effects on the conjugated chain. To circumvent this problem, in recent years, a multitude of size- and shape-persistent macrocyclic oligothiophenes has been developed and characterized. These macrocycles have the distinct advantage to ideally combine an infinite defect free π-conjugated chain of an idealized polymer with the advantages of a structurally well-defined oligomer, but excluding perturbing end effects. In this regard, we have prepared a series of macrocyclic oligothiophens, 5T-N (N = 2, 3, 4, 5, and 6), consisting of 2,5-thienylene, ethynylene, and vinylene units. Single-molecule photophysical properties of 5T-N have been explored with the single-molecule fluorescence detection techniques to reveal size dependency of their properties.

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발표코드: **PHYS1.O-6**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 임상현

Giant oscillating molecular dipoles generated by static electric fields and ultrashort laser pulses

장보영* 신석민 **Ignacio Sola[1]**

서울대학교 화학부 [1]Universidad Complutense de Madrid, SPAIN

The dynamics of molecular properties is always associated to the quantum superpositions of Hamiltonian eigenstates. While the nuclear wave function encodes the molecular entity, given by the shape or the geometry, the electronic distribution is responsible for the chemical properties. The correlation between electronic and nuclear motions generally manifest as smooth changes of the electronic distribution with respect to changes in the nuclear coordinates, which is the result of the different time scales of electronic and nuclear motions, i.e., of the widespread validity of the Born-Oppenheimer approximation. To date, most of the studied dynamical processes in molecules involve superposition of vibrational states belonging to the same electronic state. in the present work, we use ultrashort laser pulses to prepare wave packets containing a quantum superposition of both electronic and nuclear degrees of freedom, such that the motion of both electrons and nuclei is highly correlated and occurs in the time-scale of the nuclear motion. We use the molecular hydrogen ion as benchmark. We show that we can create large oscillating dipole moments, typically of the order of 20-40 debyes, whose amplitude and period can be controlled by means of a strong static electric field. This has potential applications in controlling the reactivity of a molecule, which is greatly influenced by the electronic density, and in generating electromagnetic radiation of specific frequencies.

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발표코드: **PHYS1.O-7**
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 임상현

Spectroscopic Identification of Benzyl-type Radicals by Corona Discharge of 2-Chloro-4-Fluorotoluene

윤영욱 채상열[1] 이상국

부산대학교 화학과 [1](주)엔지텍 연구개발팀

Transient species such as molecular ions and radicals have long believed to play an important role as reaction intermediates in chemical reaction. The vibronically excited but jet-cooled benzyl-type radical was generated from the precursor 2-chloro-4-fluorotoluene seeded in a large amount of carrier gas helium using a pinhole-type glass nozzle in a technique of corona excited supersonic expansion. From an analysis of the visible vibronic emission spectrum observed, we found the evidence of the formation of the 2-chloro-4-fluorobenzyl as well as 4-fluorobenzyl radicals. A possible pathway for the formation of these benzyl-type radicals is proposed. Also, the electronic energy in the D1 → D0 transition and the vibrational mode frequencies of the 2-chloro-4-fluorobenzyl radical in the D0 state were accurately determined, for the first time, by comparison with ab initio calculations and the known vibrational data of the precursor.

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장소: 일산KINTEX

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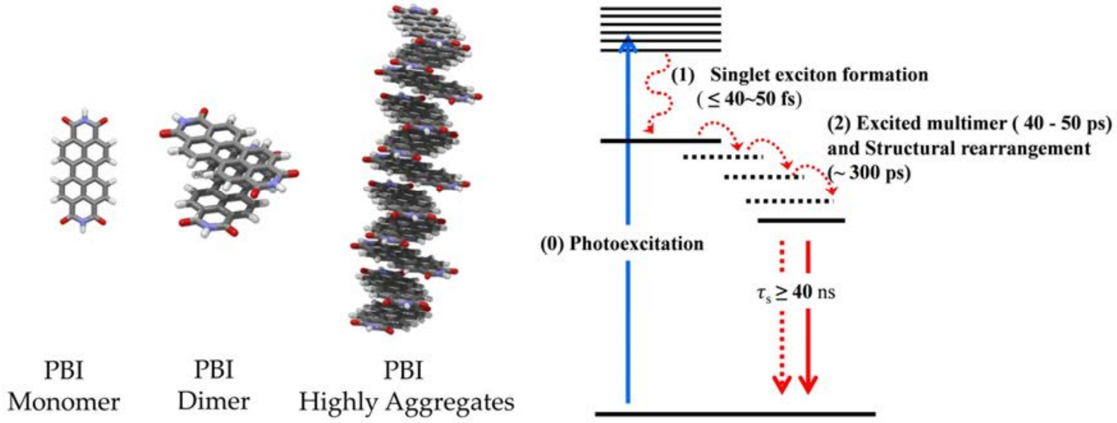
Exciton Delocalization and Dynamics in Helical π-stacks of Self-assembled Perylene Bisimides

임종민 김동호*

연세대학교 화학과

We have explored the exciton dynamics and excited-species formation processes in columnar helical aggregates of planar PBI dyes by various spectroscopic techniques such as time correlated single photon counting and femtosecond pump?probe measurements with anisotropy changes. The outcome of this study is that photogenerated excitons in helically stacked PBI dyes experience complicated relaxation processes that involve excited-state interactions such as exciton delocalization and excimer formation. The comparative study revealed that the excited-state interactions in the large-sized helically stacked aggregates extend beyond two PBI units, leading to a final excimer trap state within ~50 ps. Although in competition with this relaxation path into the excimeric trap state, exciton diffusion has been revealed by exciton?exciton annihilation processes, occurring at high excitation power. We can conclude that the exciton diffusion can reach a length of about 10 monomer units. This result shows that columnar PBI stacks might still be useful for optoelectronic applications if the relaxation process leading to excimer traps is prevented, e.g. by structural modifications of the molecules.


PBI
Monomer
PBI
Dimer
PBI
Highly Aggregates
(1) Singlet exciton formation
(≤ 40~50 fs)
(2) Excited multimer (40 - 50 ps)
and Structural rearrangement
(~ 300 ps)
(0) Photoexcitation
τ_s ≥ 40 ns

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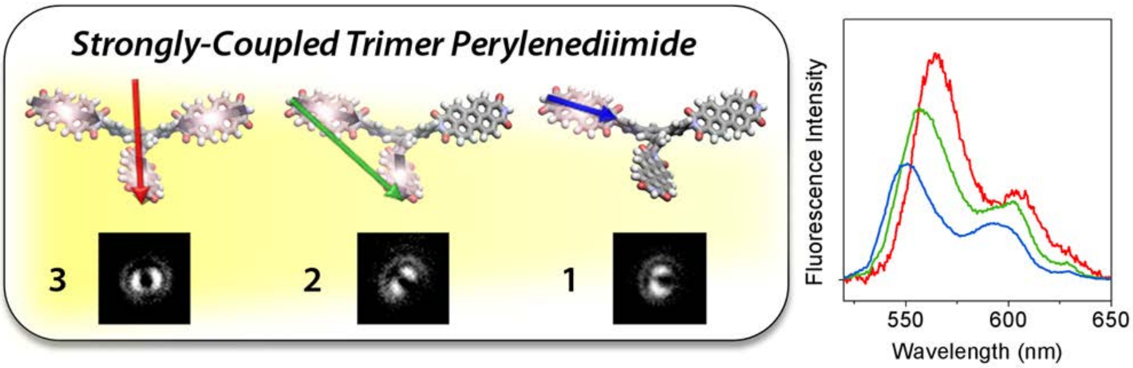
발표분야: General Oral Presentation (I)
발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 임상현

Excitonic Coupling in Linear and Trefoil Trimer Perylenediimide Molecules Probed by Single-Molecule Spectroscopy

유혜진 김동호*

연세대학교 화학과

Perylenediimide (PDI) molecules are promising building blocks for photophysical studies of electronic interactions within multichromophore arrays. Such PDI arrays are important materials for the fabrication of molecular nano-devices such as organic light emitting diodes, organic semiconductors and biosensors because of their high photostability, chemical and physical inertness, electron affinity and high tinctorial strength over the entire visible spectrum. In this work, PDIs have been organized into linear (L3) and trefoil (T3) trimer molecules and investigated by single-molecule fluorescence microscopy to probe the relationship between molecular structures and interchromophoric electronic interactions. We have found a broad distribution of coupling strengths in both L3 and T3, and hence strong/weak coupling between PDI units by monitoring spectral peak shifts in single-molecule fluorescence spectra upon sequential photobleaching of each constituent chromophore. In addition, we have used a wide-field defocused imaging technique to resolve heterogeneities in molecular structures of L3 and T3 embedded in a PMMA polymer matrix. A systematic comparison between the two sets of experimental results allowed us to infer the correlation between intermolecular interactions and molecular structures. Our results show how control of the PDI intermolecular interactions using suitable multichromophoric structures may serve to guide single-molecule device design.


Strongly-Coupled Trimer Perylenediimide
3
2
1
Fluorescence Intensity
550
600
650
Wavelength (nm)

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발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 엄성현

Aptamer-mediated SERS Intensity Amplification

김남훈 Seung Joon Lee[1] Martin Moskovits[1,*]

포항공과대학교 화학과 [1]University of California, Santa Barbara, USA

A strategy for amplified SERS-based sensing using apatmers is described. The system is designed so that the aptamer’s conformatiuonal change following its interaction with one or two molecule leverages the position of a gold nanoparticle carrying 100 or more reporter molecules whose SERS intensities are altered as a result. This is illustrated using a bifunctional adenosine-sensitive aptamer which was used to create a SERS hot spot between a bulk Au surface or 80 nm Au nanoparticle (AuNP) and an 20 nm AuNP attached to the aptamer via a biotin-avidin linkage. The 20 nm AuNP was decorated with the Raman reporter (4-aminobenzenethiol). Introducing the target into the buffer in which this system is immersed increased the reporter’s SERS signal by a factor of ~3.5. In-situ atomic force microscopy (AFM) confirmed the fact that the mean height of the AuNP-bearing aptamer decreased by ~5.6 nm consistent with the observed SERS intensity change. The introduction of uridine, guanine, and cytidine produce no significant effect either on the SERS spectrum or the topographic AFM image.

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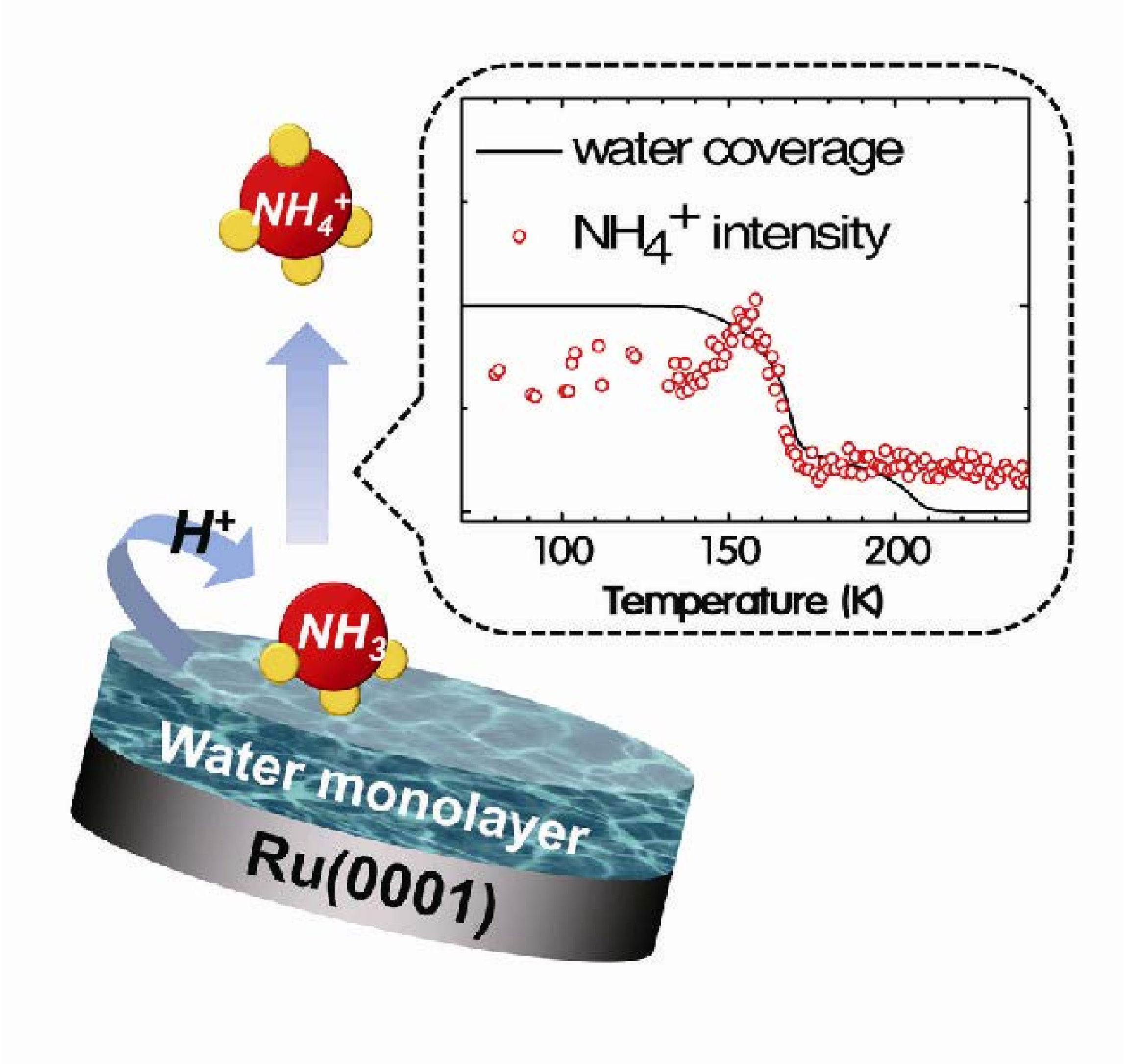
Unusual Acidity of Water Monolayer on Ru(0001)

김영순 강헌*

서울대학교 화학부

Understanding the intrinsic acid-base properties of adsorbed water on solid surfaces is fundamentally important to heterogeneous catalysis, corrosion, and electrochemistry. We studied the acid-base properties of adsorbed water on a Ru(0001) surface, a system which has become a case study example for the interaction of water with metal surfaces. The study shows that the water monolayer on a Ru(0001) surface is anomalously acidic compared to bulk water. The observation was made by conducting ammonia adsorption experiments and various surface spectroscopic measurements for adsorbed water on Ru(0001) at temperature of 80-240 K. The water molecules in the first intact H_2O monolayer spontaneously release a proton to ammonia adsorbates to produce ammonium ions. Such proton transfer, however, does not occur for H_2O in a thick ice film surface or for a mixed adsorption monolayer comprising H_2O, OH, and H.


NH4+
H+
NH3
Water monolayer
Ru(0001)
water coverage
NH4+ intensity
100
150
200
Temperature (K)

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발표분야: General Oral Presentation (II)
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 엄성현

Mutation Effects on the β2-microglobulin Fibril Formation: Molecular Dynamics Simulations and Solvation Thermodynamics Analyses

홍주연 함시현*

숙명여자대학교 화학과

β2-microglobulin (β2-m) is a major component of amyloid fibrils deposited in patients suffering from dialysis-related amyloidosis. Several mutants of β2-m have been investigated to understand the amyloid fibrillogenesis since the wild-type β2-m does not form amyloid fibril at physiological conditions. Recently, D76N and D59P mutants have been studied that are thermodynamically unstable and exhibit enhanced aggregation while W60C mutant is more stable and less prone to aggregate than wild type. However, the reason why these mutants show distinct fibril formation tendency remains elusive. Here, we carried out molecular dynamics simulations and solvation thermodynamics analyses on D76N, D59P, and W60C variants to understand mutation effects on amyloid fibril formation. We propose that the hydration status of a specific aspartic acid (D76) plays a leading role in controlling the β2-m fibril formation based on detailed analyses on atomic-level structures and solvation thermodynamics quantity changes caused by mutation.

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발표분야: General Oral Presentation (II)
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Studying Abnormality in Density Functional Theory

김민철 이상현 **Kieron Burke**[1] 심은지[*]

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

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

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발표코드: **PHYS2.O-5**

발표분야: General Oral Presentation (II)

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 엄성현

Single-turn helices in protein loops: protein dynamics controlled by small fragments

이동선 석차옥*

서울대학교 화학부

It is evident that protein function is deeply related with protein structure. Proteins in the physiological condition are not static but dynamic, and protein dynamics is also related with protein function. In this presentation, we show that short single-turn helices located in the middle of protein loops play roles related to protein dynamics by computational mutation and anisotropic network model analysis. Single-turn helices are frequently found in protein loops, but the role of the short segments in loops has not been understood clearly. If a loop containing a helical segment simply connects nearby secondary structure elements, the helix would disappear during evolution because shorter loops can play such a role more effectively. Abundance of such helical segments in protein loops implies that they may play functional roles in addition to structural roles. We observed that the single-turn helices form specific interaction networks in protein structures which cannot be attained by simple loop structures. We found that single-turn helices are involved not only in locally correlated network by structural perturbation method but also in global dynamics by anisotropic network model analysis. Structures and dynamics of wild-type loops and mutant loops with deletions in single-turn helices were analyzed in detail for several proteins. These results suggest that the small fragments of single-turn helices in protein loops play important roles in protein function by affecting protein dynamics.

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Seemingly Fickian but Heterogeneous Dynamics of Colloids

김정민 성봉준* Chanjoong Kim[1]

서강대학교 화학과 [1]Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, USA

Colloids in solution undergo a Brownian motion, which has been taken for granted for a century. For such colloids, the probability distribution of particle displacement (PDPD) is Gaussian, and the mean-squared displacement (MSD) is linear with time (Einstein's relation). Recent studies, however, revealed that the PDPD of nano-particles in entangled actin showed exponential tail with Gaussian central part instead of being Gaussian at all length scales. More interestingly, the exponential tail of PDPD appeared while MSD was still linear with time t, which requires refreshing insight on the colloid dynamics in complex systems. In this work, we present molecular dynamics simulations for heterogeneous dynamics of two-dimensional (2D) colloids. Unlike three-dimensions there is no long-range translational order for 2D crystals, and the celebrated Kosterlitz-Thouless-Halperin-Nelson-Young theory predicts two transitions in 2D melting with an intermediate phase, the hexatic phase between isotropic liquids and solids. We identify all three phases by investigating the orientational order, and study colloid dynamics in each phase. Interestingly, near solid-hexatic transition PDPD shows oscillatory behavior between central Gaussian part and exponential tail. Even though near translational relaxation time intermediate scattering function completely decays (entering Fickian regime), the oscillatory part persists until 12 times longer than translational relaxation time. In other words, 2D colloids exhibit seemingly Fickian but significantly heterogeneous dynamics, which is an extreme case of heterogeneous dynamics. We construct a kinetic map and elucidate such an anomalous behavior of PDPD of 2D colloids.

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발표분야: General Oral Presentation (II)
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 엄성현

Three-Dimensional Network of Single-walled Carbon Nanotubes for Microfluidic Applications

서정은 조석진 조용덕[1] 이수범 박미경 오은결 이해원*

한양대학교 화학과 [1]한양대학교 나노융합과학과

Filtration and capture in microfluidic systems are becoming increasingly important in a variety of biomedical and environmental, applications. The on-chip filtration is able to handle small amounts of liquid and analyte, and it increases also detection efficiency via sorting of analyte. Here, we leveraged these 3D network of SWNTs to develop a new type of microfluidic filtration platforms. The 3D network of SWNTs have hierarchical structures comprised of interconnected SWNTs between Si pillars in microfluidic channels. The CNTs were coaxially coated with Al2O3 by atomic layer deposition(ALD) to prevent CNTs from aggregation in microfluidic chips. The physicochemical properties of the 3D network of CNTs can be readily tuned by using ALD to form and engineer functional coatings on the hierarchical structures. As demonstrated in the filtering of PS nanoparticles, these types of functional hierarchical 3D structures offer new opportunities to develop novel filtration systems. And, for the extension of this approach to biomaterial assays, the networks coated with Al2O3 were silanized to functionalize with biotin. The Al2O3 coated 3D networks were used for nanoparticles filtration and streptavidin capturing. Expecally, this 3D network of SWNTs can enhance signal intensity dramatically in very diluted solution.These results will provide a robust multifuncitonal platform for a variety of biomedical and environmental applications.

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발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 엄성현

Real-time observation of water diffusion under graphene

이대웅 류순민*

경희대학교 응용화학과

나노 크기의 공간에서의 물질의 이동은 표면의 환경에 의해 영향을 받을 수 있다. 소수성 그래핀과 친수성 실리콘 기판 사이의 계면에서의 물의 확산은 호기심을 자극할 뿐만 아니라 그래핀 소자의 특성을 좌우하는 전하도핑(charge doping) 현상을 이해하는데 중요한 모델이 된다. 본 연구에서는 라만 분광법과 원자 힘 현미경을 사용하여 그래핀/SiO_2 계면 사이의 물의 확산 현상과 그에 따른 정공 밀도 변화를 탐구하였다. 열처리 된 그래핀은 기판과의 상호 작용에 의해 높은 밀도의 정공(electron hole)으로 도핑 되어 있으며, 이를 물에 담지 하였다. 본 실험에서는 이차원 라만 분광법을 통해 물 속에 담겨진 그래핀의 정공 밀도의 공간적인 분포를 확산 시간에 따라 조사하였다. 물의 확산은 시료에 따라 수 시간에서 수 일의 시간대에 걸쳐 그래핀 가장자리에서 중앙으로 이루어진다는 사실을 확인하였다. 또한 물의 계면 확산으로 인하여 전하 밀도가 감소한다는 사실은 열처리 된 그래핀의 정공 도핑을 유발하는 산소가 계면에 존재한다는 것을 증명한다.

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발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 엄성현

Oxidant-Resistant Silver Nanodots for Imaging and Ratiometric Luminescence Detection

박순영 **Junhua Yu**[1,*]

서울대학교 사범대학교/화학교육과 [1]*서울대학교 화학교육과*

ssDNA encapsulated silver nanodots are very promising material thanks to their small size, outstanding brightness and great photostability under both one- and two-photon excitation. Although exact emissive mechanisms and structures of ssDNA silver nanodots are still under debate, they are considered as most significant candidates for in vivo bioimaging with their excellent characteristics. Here, we have found out novel properties which could be used for detecting living cell induced reactive oxygen species (ROS) with our ssDNA encapsulated silver nanodots. Originally very bright red emissive ssDNA silver nanodots can shift their main emission range the blue in the presence of oxidizing agents. As this bright, simple and smart turn-on method, we can ratiometrically detect specific reactive oxygen species. Moreover, we will show some important clues of ssDNA silver nanodots' structures and emissive mechanisms from these oxidized properties.

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Optical Probing of Electronic Interaction between Graphene and Hexagonal Boron Nitride (hBN)

안광현 고택영 류순민*

경희대학교 응용화학과

Even weak van der Waals (vdW) adhesion between two-dimensional solids may perturb their various materials properties owing to their low dimensionality. Although the electronic structure of graphene has been predicted to be modified by the vdW interaction with other materials, its optical characterization has not been successful. In this report, we demonstrate that Raman spectroscopy can be utilized to detect a few % decrease in the Fermi velocity (v_F) of graphene caused by the vdW interaction with underlying hexagonal boron nitride (hBN). Our study also establishes Raman spectroscopic analysis which enables separation of the effects by the vdW interaction from those by mechanical strain or extra charge carriers. The analysis reveals that spectral features of graphene on hBN are mainly affected by change in vF and mechanical strain, but not by charge doping unlike graphene supported on SiO2 substrates. Graphene on hBN was also found to be less susceptible to thermally induced hole doping.

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발표코드: **ANAL.O-1**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김주훈

Non-linear feature extraction methods in spectroscopic analysis for classification & quantification

이상욱 이혜선[1] 정회일*

한양대학교 화학과 [1]포항공과대학교 산업경영공학과

Non-linear feature extraction methods, neighborhood preserving embedding (NPE) and supervised-NPE (SNPE), were evaluated for vibrational spectroscopic classification and quantification. The motivation was to utilize the NPE and SNPE’s capability of capturing non-linear spectral behaviors by simultaneously preserving local relationships in order that minute spectral differences among classes or concentrations would be effectively recognized. NPE and SNPE derive an optimal embedding feature such that the local neighborhood structure can be preserved in reduced spaces (variables). The spectral data were represented into several new variables through NPE and SNPE, and also by using the principal component analysis (PCA). Then, the feature-extracted variables were subsequently classified into a few groups by using both k-nearest neighbor (k-NN) and support vector machine (SVM). Also, for quantitative analysis, multiple linear regression models were developed using the feature-extracted variables through NPE, SNPE and PCA. Finally, the resulting classification accuracies and standard error of prediction (SEP) were compared each other.

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발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 김주훈

Label-Free Detection of Enriched Biomarkers from Human Serum Using Magnetic Gold Microshells and Mass Spectrometry

권승용 정택동*

서울대학교 화학부

A rapid and sensitive detection as well as quantification of peptides and proteins from complex biological samples is of importance for disease diagnosis. Such disease-associated macromolecules, existing in very low levels in biological samples, relate their concentration with the degree of disease progression. To monitor the level of peptides and proteins, matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) has been used owing to its high sensitivity (< fmol) and time-saving properties with a wide detection range of molecular mass. However, MALDI-TOF MS always suffers from interferences of a variety of highly abundant peptides, proteins, salts, and other contaminants when detecting target molecules with extremely low concentration (~nM) directly from complex biosamples. As such, preseparation and enrichment of proteins are essential for the detection of these low abundant proteins prior to MS analysis. Herein, we demonstrate fast isolation and efficient immunoaffinity enrichment of proteins from complicated biological samples using magnetic gold microshells and application to MALDI-TOF MS.

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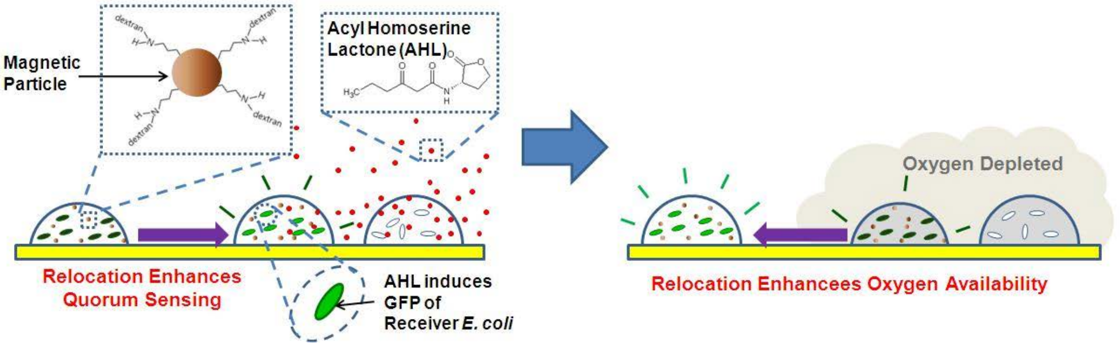
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 김주훈

Productive Chemical Interaction Between a Bacteria Micro-colony Couple is Enhanced by Periodic Relocation

변창규 **Shuichi Takayama**[1,*]

울산과학기술대학교(UNIST) 나노생명화학공학부 [1]*University of Michigan- Ann Arbor*

A unique culture environment that mimics the chemically open characteristic of natural bacteria habitats but with user-defined spatio-temporal control and microscope visualization of bacteria micro-colonies is realized through use of an aqueous two phase system (ATPS). The ATPS required is formulated with high molecular weight dextran (DEX) and poly(ethylene glycol) (PEG) dissolved in cell culture media. DEX-phase droplets formed within a bulk PEG-phase stably partition and confine bacteria within it while small molecules diffuse across the DEX-PEG boundary. The bacteria-containing DEX droplets can also be magnetically relocated, without droplet breakup or loss of its bacterial content, when DEX-conjugated magnetic particles are included. Using this dynamic bacteria micro-culture system, we subjected a chemically-interacting two-colony synthetic bacterial community to different types of colony relocation scenarios and studied their quorum sensing responses as measured by green fluorescent protein (GFP) expression. We found that decreasing the distance between the two interacting micro-colonies increased GFP expression due to increased inter-colony chemical communication but with upper limits. Periodic relocation of the chemical signal receiver colony, however, increased GFP expression beyond these typical bounds predicted by quorum sensing concepts alone by maintaining inter-colony chemical communication while also relieving the receiver colony from short-range inhibitory effects of resource depletion. In addition to providing insights on the effect of bacteria relocation, the magnetic droplet manipulation should be useful for a variety of bioanalysis applications where selective partitioning and separations at the microscale in fully aqueous conditions are needed.


Magnetic Particle
dextran
Acyl Homoserine Lactone (AHL)
Oxygen Depleted
Relocation Enhances Quorum Sensing
AHL induces GFP of Receiver *E. coli*
Relocation Enhancees Oxygen Availability

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 임재민

Study of the role of common HPLC solvents in APPI process by combining Experimental MS data and Quantum Mechanical Calculation

AHMED ARIF 최철호[1] 김성환[1]

경북대학교 Chemistry [1]경북대학교 화학과

Liquid chromatography coupled to mass spectrometry (LC-MS) has become one of the most important analytical tools for modern scientific and industrial researches. Ionization process is most important for LC-MS analysis due to its significant influence on the quality of LC-MS data. Atmospheric pressure photo ionization (APPI) is a powerful technique for analysis of polycyclic aromatic compounds (PAH) and analysis of PAH is very important to study environmental substance and crude oils. In previous studies, it has been reported that toluene, (Ahmed, A. Anal. Chem. 2012, 84, 1146-1151) especially methyl hydrogen of toluene (Ahmed, A. J. Am. Soc. Mass Spectrom. 2012, in press) is the source H+ for APPI when only toluene was used as a solvent. Moreover, methanol acts as a proton source when it exists as a co-solvent with toluene. The combination of MS data and quantum mechanical calculations has shown that size-dependent reactivity of methanol clusters ((CH3OH)n, n=1 ~ 8) is an important factor that helps determine the sensitivity of (+) APPI MS analyses.However, there still remain many questions unanswered. For example, the source of H+ when common solvents such as H2O and CH3CN coexist with toluene is not known. It has been observed that water and acetonitrile can significantly affect APPI-MS signal intensity. However, the mechanism by which water and acetonitrile are involved in APPI has not been fully understood yet. In this study, APPI mechanism, especially, the source of H+ during the generation of protonated PAH compounds were studied for toluene-water and toluene-acetonitrile mixture by combination of quantum mechanical calculation and mass spectrometry analysis.

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Novel gas chromatography-electrospray ionization/orbitrap mass spectrometry (GC-ESI/HRMS) for ionization and analysis of steroids

차은주 이재익*

한국과학기술연구원(KIST) 도핑콘트롤센터

Anabolic steroids are extensively abused to improve performance in sports. Gas chromatography-electron impact ionization/mass spectrometry (GC-EI/MS) method has been generally used for the detection of steroids. But conventional methods using the GC-EI/MS have technical bottleneck such as the hard ionization of electron impact ion source. Recently, even though the analytical methods using liquid chromatography-electrospray ionization/tandem mass spectrometry (LC-ESI/MS/MS) have been developed, the LC-ESI/MS/MS methods have also several bottlenecks such as the simultaneous ionization in single ion source and the chromatographic separation. Therefore, in this study, the novel gas chromatography-electrospray ionization/orbitrap mass spectrometry (GC-ESI/HRMS) instrument system was developed to overcome these bottlenecks by combining the GC and ESI source, and applied to the analysis of steroids. GC and ESI source were interfaced by homemade heated column transfer line and the distance, angle, spray solvent, acid modifier and ion source parameters such as gas, temperature and voltage were optimized to improve the ionization efficiency. After the extraction from spiked urine sample, 86 anabolic agents (64 exogenous substances and 22 endogenous substances) were converted into trimethylsilyl (TMS) derivatives and analyzed by GC-ESI/HRMS to demonstrate the sensitivity, selectivity, ionization effect of TMS-derivatives and chromatographic resolution. The results revealed that the present GC-ESI/HRMS system and analytical method are suitable for identification of anabolic steroids in human urine for doping control.* This research project was supported by the Sports Promotion Fund of Seoul Olympic Sports Promotion Foundation from Ministry of Culture, Sports and Tourism

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발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 임재민

Profiling of Oxidized Phospholipids in Lipoproteins from Human Plasma by FlFFF & nanoflowLC ESI-MS-MS

이주용 문명희* 임상수 변슬기

연세대학교 화학과

Oxidized low density lipoproteins (Ox-LDL), defined as oxidatively-modified LDLs in the blood by enzymatic or non-enzymatic oxidation of phospholipids, has an important role in the development of age-related vascular disease, such as atherosclerosis. Oxidation of LDL is a complex process caused by enzymatic or non-enzymatic reactions and primarily occurs in unsaturated fatty acid chains of phospholipids (PL) contained in LDLs. For the characterization of Ox-LDLs at molecular level, oxidation patterns of oxidized PL products were systematically examined with standard PL molecules by the formation of bilayer vesicles of each standard, followed by oxidation of PL vesicles using a Cu2+ solution. in this study, nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry was utilized for the separation and structural characterization of complicated Ox-PL mixtures, including long chain products with hydroxylation or hydroperoxylation at an unsaturated acyl chain, and short chain products from the cleavage of unsaturated fatty acyl chains to form lysophospholipids (LPL) or the truncation of an acyl chain into a shorter chain terminated with aldehyde or carboxylic acid. Oxidative modification was applied to LDL standard materials, and nLC-ESI-MSn analysis of the extracted PL mixtures resulted in the identification of 276 PLs, including 139 Ox-PL species. Examination of the identified PL species from the standard LDL before and after oxidation supported that the location of an acyl chain of LPL can be exchanged between the sn-1 and -2 positions when another acyl chain is cleaved during oxidation and the polar head group of PL molecules can be dissociated to form PA molecules that result in the formation of various Ox-PA products.

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발표분야: Oral Presentation of Young Biochemists
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OASL1 inhibits translation of the type I interferon?regulating transcription factor IRF7

이명섭

연세대학교 생화학과

The production of type I interferon is essential for viral clearance but is kept under tight control to avoid unnecessary tissue damage from hyperinflammatory responses. Here we found that the 2’-5’-oligoadenylate synthetase-like 1 (OASL1) inhibited translation of IRF7, the master transcription factor for type I interferon, and thus negatively regulated the production of type I interferon during viral infection. OASL1 inhibited the translation of IRF7 mRNA by binding to the 5’ untranslated region (UTR) of IRF7 and possibly by inhibiting the scanning of the 43S preinitiation complex along the message. Oasl1$^{-/-}$ mice were resistant to viral infection because of the greater abundance of type I interferon, which suggests that OASL1 could be a potential therapeutic target for boosting the production of type I interferon during viral infection.

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발표코드: **BIO.O-2**

발표분야: Oral Presentation of Young Biochemists

발표종류: 구두발표, 발표일시: 금 10:25, 좌장: 이연

Designed Nanobiomaterials for Therapeutic Growth Factor and Cell Delivery

김재윤

성균관대학교 화학공학부

Nanoparticles and hydrogels with designed physical and chemical properties can exhibit unique characteristics which have high potentials to overcome various problems in current clinical approaches to treat diseases. This presentation will introduce our recent study in the application of designed nanobiomaterials for therapeutic growth factor and cell delivery. Targeted delivery of gold nanoparticles conjugated with angiogenic growth factor to ischemic tissues resulted in recovery of blood perfusion through enhanced angiogenesis. Transplantation of designed alginate capsule-in-capsules containing pancreatic islets and nanoparticle contrast agents allowed immunoprotected insulin-producing cell delivery and multimodal imaging. Active ferrogels that can be remotely controlled by a magnetic field was fabricated to deliver various biological agents including anticancer drug, DNA, growth factor, and cells on demand.

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Probing Post-Translationally Citrullinated Sites by Br-Tagging and MALDI TOF/TOF MS

차상원

한국외국어대학교 화학과

Citrullination is a post-translational deimination of arginine residues to citrullines. This deimination reaction is catalyzed by peptidyl arginine deiminase (PAD). Since citrullination results in only 1 Da increase in mass, citullinated peptide peaks are hard to be distinguished from deamidated peptide peaks or the isotope peaks from the control peptides. Therefore, covalent labeling techniques on citrulline residues were usually employed to investigate citrullinated sites by MS. Here, we present the novel citrulline-labeling strategy with 4-bromophenylglyoxal (BPG) for the determination of the citrullination site in bottom-up and top-down ways by MALDI TOF/TOF MS. Under the acidic condition (pH

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발표분야: Oral Presentation of Young Biochemists
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Fluorescence Phenomic Screening Shed Light on the Origin of Cancer Cell-Line

이준석

한국과학기술연구원(KIST) 분자인지연구센터

A principal challenge for functional genomics is to identify genotypes that are associated with a specific phenotype. Recent advances in gene expression profiling and next-generation sequencing (NGS) technology have driven significant improve- ments in high-throughput genotyping. However, unlike the well established genotyping platforms, there is no standard quantitative methods for phenotyping yet. We envisioned that a fluorescent probe library would have great potential to identify a set of universal phenomic parameters due to their uniform phenotypic readout (fluorescence signal), and structural diversity at the molecular level. We applied 557 fluorescent library compounds to NCI's 60 human cancer cell-lines (NCI-60) to generate a systematic fluorescence phenotypic profiling data. By the kinetic fluorescence intensity analysis, we successfully discriminated the organ origin of all the 60 cell-lines.

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Proteomic Mapping of Sub-Organellar Proteome in Living Cells via Spatially-Restricted Enzymatic Tagging

이현우

울산과학기술대학교(UNIST) 나노생명화학공학부

Microscopy and mass spectrometry (MS) are complementary techniques: the former provides spatiotemporal information in living cells, but only for a handful of recombinant proteins, while the latter can detect thousands of endogenous proteins simultaneously, but only in lysed samples. In this presentation, I will introduce a new technology that combines these strengths by offering spatially- and temporally-resolved proteomic maps of endogenous proteins within living cells. The method relies on a genetically-targetable peroxidase enzyme that biotinylates nearby proteins, which are subsequently purified and identified by MS.

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Challenges in Genome-scale Genetic Engineering for Microbial Biochemical Production

방두희

연세대학교 화학과

A highly efficient method for genetically engineering bacteria will be presented. The efficiency gains make it possible to rapidly produce custom bacteria in which entire metabolic pathways have been redesigned for genetic studies or biotechnological applications. One of the most effective ways to introduce many genetic changes is multiplex automated genome engineering (MAGE), in which short stretches of DNA are inserted one at a time into a bacterial chromosome over many iterations. The process is automated but is limited to very short changes?typically up to three bases of DNA sequence at any given location?and requires a lot of instrumentation. We greatly improved on the efficiency of MAGE by selecting for changes at the site of interest and for an antibiotic resistance marker nearby. This co-selection enables them to insert 20 DNA bases at each site and increases the chances of producing multiple changes in each iteration. Using co-selection MAGE (Cos-MAGE), we altered the promoters of 12 genes in the same metabolic pathway in only 4 days, enhancing production of the industrially relevant dye indigo. The improved efficiency also makes it feasible for smaller laboratories lacking robotics to carry out genome-scale engineering.

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발표코드: **ORGN.O-1**

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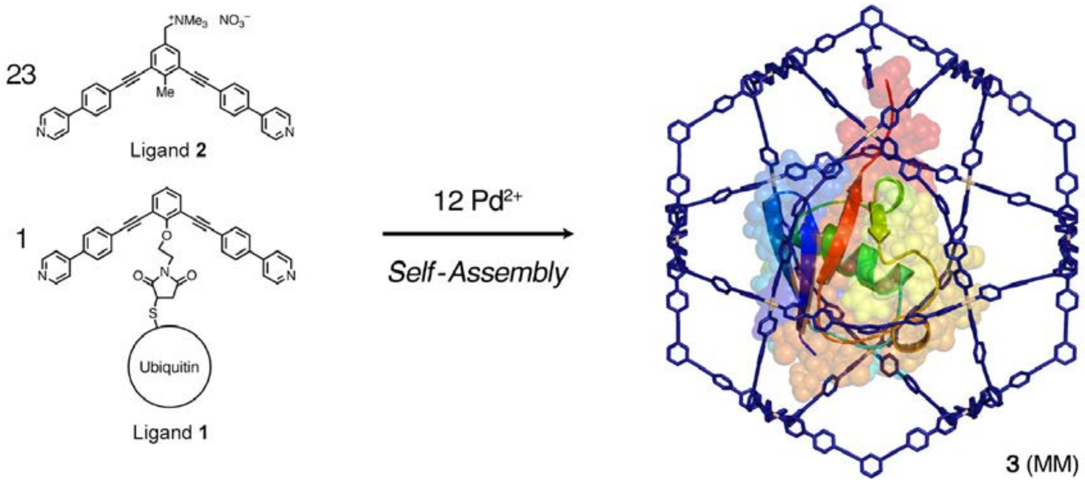
Protein Encapsulation within Synthetic Molecular Hosts

FUJITADAISHI

포항공과대학교 첨단재료과학부

Protein encapsulation has long attracted many chemists and biologists because of its potential to control the structure and functions of proteins, but has been a daunting challenge because of their sensitive nature and incommensurably larger size as compared with common synthetic hosts. Here, we report the encapsulation of a small protein, ubiquitin, within giant coordination cages. The protein was attached to one bidentate ligand (L) (**1**) and, upon addition ofPd(II) ions (M) and additional ligands (**2**), $M_{12}L_{24}$ coordination nanocages self-assembled around the protein (**3**). Due to the well-defined host framework, the protein-encapsulated structure could be well analyzed by NMR spectroscopy, ultracentrifugation, and X-ray crystallography.We demonstrated that ubiquitin (roughly 4 nm in diameter) was fully encapsulated within the 6.3 nm coordination sphere.



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Dynamic Kinetic Resolution of Secondary Alcohols with Ionic-Surfactant Coated Burkholderia cepacia Lipase

이주석 박재욱* 김만주*

포항공과대학교 화학과

We have developed a highly active enzyme by coating Burkholderia cepacia lipase with an ionic surfactant for use in DKR. With this ionic-surfactant-coated Burkholderia cepacia lipase (ISCBCL), we were able to achieve the highly enantioselective DKR of a wide range of secondary alcohols previously unexplored. Different secondary alcohols were tested as the substrate of ISCBCL to see its substrate scope and enantioselectivity in KR and DKR . In most cases, good yields and high enantiomeric excesses were obtained[1,2]

Acknowledgement
This work was supported by the National Research Foundation of Korea (KRF-2007-511-C00031 and 2009-0074357)

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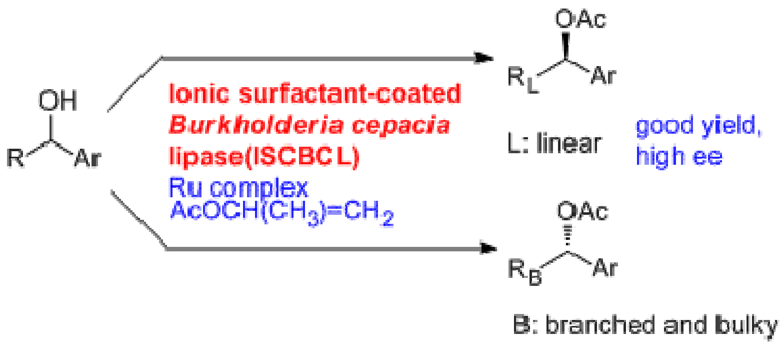
2. H. Kim, Y. K. Choi, J. Lee, E. Lee, J. Park, M-J. Kim, Angew. Chem. Int. Ed. 2011, 50, 10944


OH
R
Ar
Ionic surfactant-coated
Burkholderia cepacia
lipase(ISCBCL)
Ru complex
$AcOCH(CH_3)=CH_2$
OAc
R_L
Ar
L: linear
good yield,
high ee
OAc
R_B
Ar
B: branched and bulky

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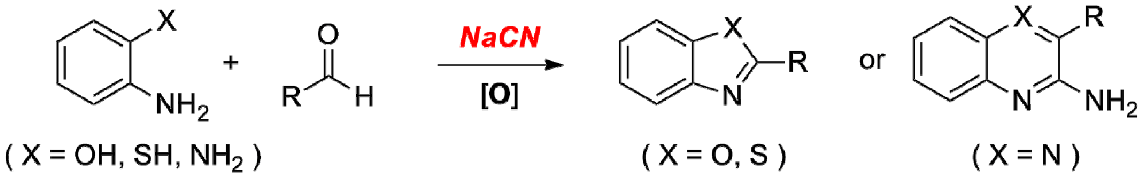
The Facile Aerobic Oxidative Cyclization for One-Pot Peperation of Benzofused Heteroaromatic Compounds

조연호 천철홍*

고려대학교 화학과

Benzofused heteroaromatic compounds such as benzoxazoles and benzothiazoles have been known as a crucial building block of therapeutic important compounds, drugs and many natural products. They have been also found in material chemical such as dyes, fluorescence and sensor. Thus, many synthetic methods have been developed to efficiently synthesize these important building blocks efficiently under mild reaction conditions. Among them, aerobic oxidative cyclization of Schiff bases derived from aniline derivative (contain X at ortho position of aniline; where X = OH, SH, NH2) with aldehydes using oxygen as the terminal oxidant has received a lot of attention. Thus, we recently developed highly efficient aerobic oxidative cyclization methods from Schiff bases in the presence of a nucleophile catalyst to afford benzofused heteroaromatic compounds. Furthermore, we have developed sequential one-pot protocols for the preparation of these important compounds without isolation of imine intermediates.



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Total syntheses of 1-deoxylycorine and lycorine

정용근 조천규*

한양대학교 화학과

Lycorine is a toxic crystalline alkaloid present in various Amaryllidaceae plant species that include Lycoris, Pancratium, Narcissus, Galanthus, Zephyranthes and Haemanthus. Arising from norbelladine in its biosynthesis, lycorine has the pyrrolo[de]phenanthridine framework that is common to many other congeneric natural compounds. It has a wide variety of important biological activities range from the inhibition of ascorbic acid biosynthesis, the prevention of cyanide-insensitive respiration to the inhibition of growth and cell division in higher plants. Similar to other Amaryllidaceae small molecule constituents, such as pancratistatin and trans-dihydronarciclasin, it has attracted much attention for its highly potent antitumor effects, both in vitro and in vivo, as well as in cancer cells that display resistance to proapoptotic stimuli. Such biological importance together with challenging chemistry of lycorine and related alkaloids have induced many synthetic studies and the generation of many structural analogs. As a part of our ongoing study exploring the utility of 3,5-dibromo-2-pyrone in target-oriented synthesis, we have envisioned the pyrrolo[de]phenanthridine skeleton of lycorine and related natural alkaloids could be rapidly constructed from the cycloadduct of 3,5-dibromo-2-pyrone with a styrene type dienophile. Present herein would be our path-finding effort that affords the eventual synthesis of 1-deoxylycorine and lycorine

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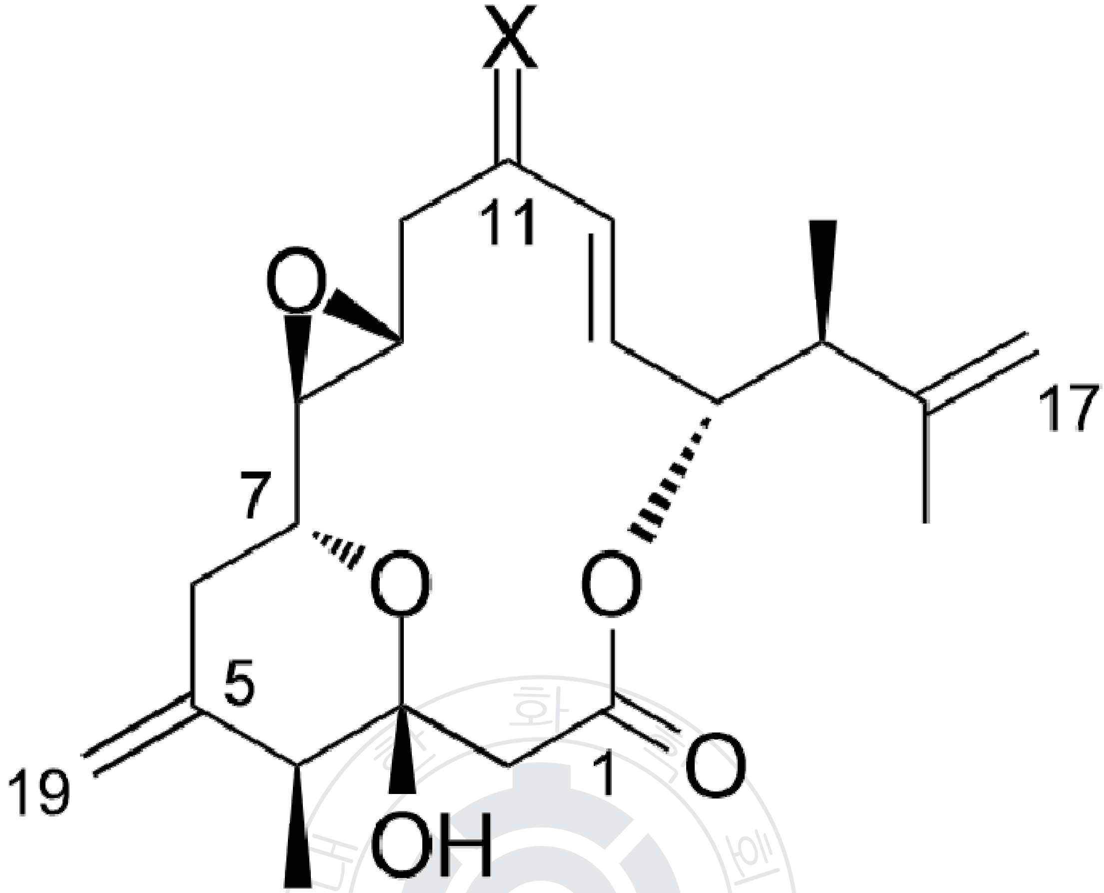
Enantioselective Total Synthesis of (-)-Amphidinolide O and (-)-Amphidinolide P

황민호 한서정[1] 이덕형*

서강대학교 화학과 [1]California Institute of Technology, U.S.A.

Kobayashi et al isolated (+)-amphidinolide O and (+)-amphidinolide P in 1995. They are fifteen-membered macrolide compounds with two exo-double bonds at C5 and C16, epoxide ring at C8-C9, trans-double bond C12-C13, two chiral methyl groups at C4 and C15 and six-membered ring bridged moiety. They have only one different functional group at C11 (carbonyl group vs. exo-methylene group). (+)-Amphidinolide O and (+)-amphidinolide P have shown in vitro cytotoxicity against murine lymphoma L1210 (IC50 = 1.7 and 3.6 ?g/mL, respectively) and human epidermoid carcinoma KB cells (IC50 = 1.6 and 5.8 ?g/mL, respectively). We report the first total synthesis of (-)-amphidinolide O and its conversion to (-)-amphidinolide.



X = O : (-)-Amphidinolide O

X = CH_2 : (-)-Amphidinolide P

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Synthesis of Indenes via Brønsted Acid Catalyzed Cyclization of 1,3-Diene Derivatives

박상준 이필호*

강원대학교 화학과

Substituted indenes can be synthesized via the Brønsted acid catalyzed cyclization of diaryl- and alkyl aryl-1,3-dienes. In this approach, treatment of symmetric or unsymmetric diaryl- and alkyl aryl-1,3-dienes with a catalytic amount of trifluoromethanesulfonic acid gives a variety of indene derivatives in good to excellent yields under mild conditions.

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Study on Divergence in the Gold(I)-Catalyzed Tandem Cyclization of 3-Silyloxy 1,6-Enynes and its Synthetic Application

김철재 이영호*

포항공과대학교 화학과

In the course of our recent study on the gold(I)-catalyzed tandem cyclization of 3-silyloxy 1,6-enynes,[1] we discovered unprecedented effects of the olefin geometry and the nature of the silyl groups on the divergence between Pinacol-terminated carbocyclization pathway vs. Claisen-terminated heterocyclization pathway. Progress on the synthesis of alkaloid natural product using this method will be also introduced.

Reference

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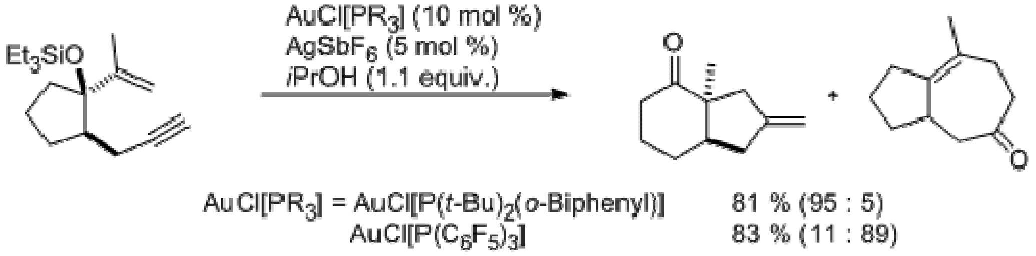

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Palladium(II) Catalyzed *ortho*-Arylation *via* Phosphate Group Directed C-H Activation

전우형 문봉진 강재효*

서강대학교 화학과

Transition metal-catalysed C-H activation is an attractive approach in aryl-aryl coupling reactions because it bypasses the use of a pre-activated aryl group such as aryl halide or aryl triflates. However, a directing group is typically required to dictate the regioselectivity of the coupling reactions. Good coordinating groups such as aldehyde, ketone, imine, ester, amide, and triazene are known to be efficient in assisting the *ortho*-C-H bond activation with high regioselectivity. In the case of phenol, temporal transformation of the phenol group into a good directing group and removal of the temporal group after the coupling reaction strategy has been generally used. Some of the examples for the temporal directing group include phenol ester, phenoxypyrimidine, phenol carbamates, and phenylphosphinite. The common feature of these directing groups is that they are highly polarizable and exhibit strong coordinating ability. While one of the convenient and efficient transformation methods for phenol masking is phosphorylation, the utility of phosphate group as an *ortho*-directing group in C-H activated aryl-aryl coupling reaction has not been reported so far, probably due to its poor coordinating abilities. In this presentation, we wish to report the first successful example of palladium catalysed *ortho*-arylation *via* phosphate group-directed C?H activation. Aryl dialkyl phosphate, which is readily available from phenol, turned out to be not only a good substrate for Pd(II) catalyzed aryl-aryl coupling reaction through *ortho*-C-H activation but also a good precursor for the consecutive C-C bond formation *via* reductive cleavage and the subsequent alkylation of the resulting aryl anion.

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MEDI.O-1**

발표분야: Oral Presentation for Young Medicinal Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 금교창

Discovery of novel hydroxamate based HDAC inhibitors for anticancer chemotherapy: property based optimization for metabolic stability and pharmacokinetic profiles

이철호

연세대학교 생명공학과

Inhibition of histone deacetylases are promising approach for anticancer therapy. HDAC inhibitors are highly divergent in structure and comprise hydroxamic acids, cyclic tetrapeptides, short chain fatty acids and benzamides. Among them, hydroxamic acids strongly bind to zinc ion in the active site of HDAC. So hydroxamate based HDAC inhibitors are expected to anticancer activities but metabolic instability and poor pharmacokinetic profiles cause poor in vivo results. Based on QSAR and PK study, γ-lactam core and diverse substituents on cap group including halogen, alkyl and alkoxy groups with various carbon chain linker were suggested for better HDAC inhibition and metabolic stability. All of synthesized γ-lactam HDAC inhibitors were tested for biological and property evaluation and 8f was found that potent anticancer activity and high oral bioavailability.

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장소: 일산KINTEX

발표코드: **MEDI.O-2**

발표분야: Oral Presentation for Young Medicinal Chemists

발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 금교창

Construction of Drug-like 1,3,4-Oxadiazole and 1,3,4-Thiadiazoles by Skeletal Diversity-oriented Synthesis via Reagent-based Regioselective Cyclization

양승주 김나연 이지형 공영대*

동국대학교 화학과

Diversity-oriented synthesis is a strategy for quick access to molecule libraries with an emphasis on skeletal diversity. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In this family, 1,3,4-oxadiazoles and 1,3,4-thiadiazoles have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as anti-inflammatory, anti-microbial, anti-convulsant, anti-cancer, and anti-hypertensive. Especially, its analogues have a potent biological activity in Wnt signaling which has been considered as a key signaling pathways that regulate cell proliferation, differentiation, and morphogenesis. In this reason, we developed a regioselective, reagent-based method for the cyclization reaction of thiosemicarbzide intermediate to synthesis 1,3,4-oxadiazole and 1,3,4-thiadiazole analogues. The thiosemicarbazide intermediate were reacted with EDC.HCl in DMSO or p-TsCl, TEA in NMP to give the corresponding 2-amino-1,3,4-oxadiazoles and 2-amino-1,3,4-thiadiazoles through regioselcective cyclization processes. The regioselectivity was affected by substituent in p-TsCl mediated cyclization. It is shown in select set of thiosemicarbazide. 2-Amino-1,3,4-oxadiazole was also shown in the reaction of p-TsCl mediated cyclization. The resulting 2-amino-1,3,4-oxadiazole and 2-amino-1,3,4-thiadiazole core skeleton are functionalized with various electrophiles such as alkyl halide, acid halides, and sulfornyl chloride in high yields.

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장소: 일산KINTEX

발표코드: **MEDI.O-3**

발표분야: Oral Presentation for Young Medicinal Chemists

발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 금교창

Target identification of glucose uptake enhancer reveals a novel PPAR gamma ligand

고민섭 박승범*

서울대학교 화학부

Refining the pipeline of the hit to lead can shorten the drug discovery process. Here, we demonstrate the well-designed platform which could be a model of the phenotype-based drug discovery process. To identify the target of a new modulator of the glucose uptake, we conducted a FITGE (fluorescence difference in two-dimensional gel electrophoresis) for a small molecule that enhances the glucose uptake in myotube. We show that the target of the glucose uptake enhancer in myotube is the nuclear receptor PPAR gamma (peroxisome proliferator-activated receptor gamma). Subsequent optimization generated lead compounds having great potency to the PPAR gamma and glucose uptake in myotube. There are three PPAR subtypes (termed PPAR alpha, PPAR delta, and PPAR gamma) according to their distinct genetic profiles. Among them, PPAR gamma activation via small molecule ligands has important pharmaceutical meaning for the control of metabolic disorders, cancer and inflammation. We confirmed that the PPAR gamma can be a selective target out of the other subtypes via transactivation reporter assay. Next, we introduced carbamoyl moiety to the tail part for make enhanced fitting. Finally, we discovered PPAR gamma selective agonist with single digit nanomolar activity. Moreover, we have confirmed that chirality of the small molecules determines the transactivation activity toward PPAR gamma , whereas the binding affinity and inhibition activity to the Cdk5 (cyclin-dependent kinase 5) mediated phosphorylation of the PPAR gamma at serine 273 is comparable for each stereoisomers. Thus, using a novel platform of the phenotype-based drug discovery process, this study has identified a new small-molecule modulator of glucose uptake targeting the PPAR gamma .

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장소: 일산KINTEX
발표코드: **MEDI.O-4**
발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 금교창

Preparation and pharmacological evaluation of potent new small molecule inhibitors against Hepatitis C virus.

<u>염수연</u> 강순방[1] 정낙철[2] 금교창[3]

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

Hepatitis C virus belongs to the hepacivirus genus and Flaviviridae family as a single-positive-stranded RNA virus. Infection of hepatitis C virus leads chronic liver disease such as liver failure, cirrhosis, hepatocellular carcinoma, and death. Hepatitis c virus RNA consists of structural proteins and non-structural proteins. Especially, non-structural proteins (NS2-NS5) duplicate hepatitis c virus. For this reason, it was focused on hepatitis c targeting. But, current standard of anti viral therapy is only the combination of pegylated interferon-? with ribavirin (Peg-IFN/RBV). So, to development anti-HCV drug is settled urgently. The several potent lead compounds were designed and synthesized as the treatment of hepatitis C. Among them, a lead compound KK6042 showed potent anti-proliferative activity against HCV cell lines with sub-nanomolar EC50. These compounds exhibited good human microsomal stability and displayed similar inhibition of major human CYP enzymes compared to reference compound BMS-790052. Furthermore, there was no evidence of its toxic effect in the hERG, cytotoxicity, and Ames test. Especially KK6042 showed excellent PK profile with high AUC and Cmax. Optimized compounds (KKK6065 and 6066) also displayed good inhibition value against HCV at 125 nM, and now these compounds are further tested on EC50. Therefore, we’ll discuss the structure-activity relationship.

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발표코드: **MEDI.O-5**
발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 금교창

N-Biphenylylmethyl-alkanamides with arypiperazines as 5-HT7 Antagonists

김영재 추현아[1,*]

과학기술연합대학원대학교(UST) 의약및약품화학 [1]한국과학기술연구원(KIST) 생명보건본부

5-HT7 receptor knockout animal studies have provided demonstrative proofs that 5-HT7 receptor is engaged in the pathomechanism of depression. Thus, 5-HT7 receptor is potentially a good target for treatment of depression. Based on the previously reported 5-HT7 receptor ligands with a quinazolinone scaffold, N-biphenylmethyl-arylpiperazinylalkanamide derivatives were designed and synthesized. Total 45 compounds were synthesized and binding affinities of these synthesized compounds to the 5-HT7 receptor and other receptors were evaluated. Most of the compounds showed very good binding affinities and behaved as antagonists resulting from functional assay. Among them, the compounds 1.19 and 1.23 were considered as potent 5-HT7 receptor antagonists (Ki = 14.0 and 22.0 nM, respectively) which were endowed with selectivity over other subtype serotonin receptors. In in vivo animal study, some synthesized compounds have antidepressant-like activity in the forced swimming test in mice.

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

Molecular modeling studies on structural requirement and underlying mechanism of pyrimidoazepine analogs for 5-HT2C receptor activation

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한국과학기술연구원(KIST) 뇌의약연구단 [1]고려대학교 세종캠퍼스 생명정보공학과 [2]고려대학교 생명정보공학과 [3]한국과학기술연구원(KIST) 생체과학연구본부

5-HT2C receptors, one of the members of aminergic G-protein coupled receptor families, are potential target for anti-obesity agents. Our pyrimidoazepine analogues that we designed and synthesized for targeting this receptor displayed agonistic or antagonistic functional activities on varying the substituents, which in turn will cause different therapeutic effects. Computational approaches, such as classification using Bayesian algorithm and recursive partitioning, a molecular docking to the homology model, and molecular dynamics simulations were adopted to reveal structural basis of these moieties to different functional activities, and underlying mechanism of how the receptor changes their conformations upon structural changes of bound ligands. The classification models revealed that aniline moiety of analogues was the determinant for functional activity of 5-HT2C receptor. The docking studies of these compounds using homology model of 5-HT2C receptor demonstrated that agonistic or antagonistic activities of ligands were attributable to the loss of broad van der Waals interactions between hydrophobic features of ligands and hydrophobic residues in TM3 and TM5, which confirmed our results of classification models. Further molecular dynamics simulation of 5-HT2C receptor homology model bound to agonists and antagonists clearly showed different conformational changes, which were measured by “ionic lock” stability at the bottom of TM3 and TM6. Our molecular modeling study identified the molecular features that were associated with different functional activities of 5-HT2C receptor, and substantiated that they actually changed the receptor conformation, which has taken a closer look at the underlying mechanism of 5-HT2C receptor activation.

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발표코드: **MEDI.O-7**
발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 금교창

Structure-activity relationships of antitubercular salicylanilides consistentwith disruption of the proton gradient via proton shuttling

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A series of salicylanilides was synthesized based on a high-throughput screening hit against Mycobacteriumtuberculosis. A free phenolic hydroxyl on the salicylic acid moeity is required for activity, and thestructure-activity relationship of the aniline ring is largely driven by the presence of electron withdrawinggroups. We synthesized 94 analogs exploring substitutions of both rings and the linker region in thisseries and we have identified multiple compounds with low micromolar potency. Unfortunately, cytotoxicityin a murine macrophage cell line trends with antimicrobial activity, suggesting a similar mechanismof action. We propose that salicylanilides function as proton shuttles that kill cells by destroying the cellularproton gradient, limiting their utility as potential therapeutics.

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장소: 일산KINTEX
발표코드: **MAT.O-1**
발표분야: Current Topics in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 송창식

Multifuctional and All-inorganic Nanocrystals;Synthesis, Properties, and Application

이종수

대구경북과학기술원(DGIST) 에너지시스템공학

Nanoparticles of different metals, semiconductors and magnetic materials can self-assemble from colloidal solutions into long range ordered periodic structures (superlattices). Multicomponent nanostructures and superlattices are the most interesting class of electronic materials because novel unexpected properties can originate from the cross-talk between quantum confined components with different functionalities. This is a new area of nanomaterial research, and is virtually unexplored. In particular, core-shell morphology maximizes the interaction between the components and provides convenient platform for studying exciton-plasmon interactions and electronic coupling between metal and semiconductor at the nanoscale. Colloidal nanocrystals are considered promising building blocks for electronic and optoelectronic devices. Potentially, they can combine the advantages of crystalline inorganic semiconductors with size-tunable electronic structure and inexpensive solution-based device fabrication. However, the insulating nature of the surface ligands used for nanocrystal synthesis typically results in the poor electronic coupling between individual nanocrystals. In an attempt to address this fundamental problem, we demonstrated that molecular metal chalcogenide complexes can serve as versatile ligands for a broad range of inorganic nanomaterials. This new class of nanocrystal colloids provides a set of advantages such as all-inorganic design and diverse compositional tunability for both nanocrystal and ligand constituents. We observed electron mobility of >15 cm^2/Vs in arrays of CdSe nanocrystals capped with metal chalcogenide Zintl ions. We demonstrate the power of this approach on several examples of prospective thermoelectric and photovoltaic materials.

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발표코드: **MAT.O-2**
발표분야: Current Topics in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 송창식

Mussel-inspired Catecholamine Polymers Nano/Bio/Energy Technologies

이해신

한국과학기술원(KAIST) 화학과

This presentation will cover recent development of technologies inspired by marine mussels particularly catecholamine. Catecholamines are rationally designed polymers and small molecules inspired be the amino acid sequence of the adhesive proteins found in mussels, which functionalizes virtually any material surfaces. After the first demonstration of material-independent surface chemistry (1), they have been utilized superhydrophobic surface modification (2), water-collecting devices (2), energy-free microfluidics (3), and adhesive materials for Li-ion batteries (4). Other nanobio applications such as material-independent hydoxyapatite crystal growth (5), block copolymer lithography on virtually any material surface (6), carbon nanotube fiber composites (7), and surface-driven gene delivery (8) will be presented.References1) Haeshin Lee et al. Science 2007, 318, 4262) Sung Min Kang et al. Angew. Chemie. Int. Ed. 2010, 49, 9401 3) Inseong You et al. Angew. Chemie. Int. Ed. 2012, 51, 6126 4) Sung Ming Kang et al. Chem. Mater. 2012, 24, 34815) S. H. Ku et al. Biomaterials 2010, 31, 25356) Bong Hoon Kim et al. Adv. Mater. 2011, 23, 56187) S. Ryu et al. Adv. Mater. 2011, 23, 19718) E. Kim et al. Angew. Chemie. Int. Ed. 2012, 51, 5598

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장소: 일산KINTEX

발표코드: **MAT.O-3**

발표분야: Current Topics in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 송창식

Graphitic Carbon Synthesis & Assembly

김상욱

한국과학기술원(KAIST) 신소재공학과

Carbon nanotubes and graphene have outstanding materials properties, including high electrical conductivity, superior mechanical properties, extremely large surface area and mechanical flexibility. Nevertheless, the directed assembly of those carbon materials into three-dimensionally patterned architectures has been a longstanding technological challenge for their ultimate utilization. This presentation will introduce our recent progress in the tailored assembly of carbon nanotubes and graphene into three-dimensional architectures employing self-assembly principles. Carbon nanotubes and graphene can be assembled into macroporous films, or hollow nanotubes, via directed assembly from solvent dispersion. This approach is cost-effective and beneficial for large-scale assembly, but pre-requests stable dispersion in a solvent medium. Directed growth from nanopatterned catalyst array is another promising approach, which enables the control of the morphology and properties of graphitic materials as well as their assembly. In addition, aforementioned two approaches can be synergistically integrated to generate carbon hybrid assembly consisting of vertical carbon nanotubes grown on flexible graphene films. Tailored assembly relying on scalable self-assembly principles offer viable and mass-producible routes towards the ultimate utilization of graphitic carbon materials in composites, nanoelectronics, displays, sensors, energy storage/conversion, and so on, including future flexible devices.

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장소: 일산KINTEX
발표코드: **MAT.O-4**
발표분야: Current Topics in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 박성진

π-Conjugated Polymers and Carbon Nanotubes for Molecular Actuators, Sensors, and Novel Conduits

송창식

성균관대학교 화학과

Electronic properties of π-electronic materials, such as π-conjugated polymers and carbon nanotubes, depend on π-electrons; we can tune their bandgaps and electron/hole transfer rates through modifying π-electrons' energy levels. Molecular design and synthesis play a huge role in controlling such π-electrons. If those π-electronic systems are coupled to well-designed molecular structures, we may create novel functions or properties. I will discuss how new properties emerge in π-electronic materials, especially by designs at the molecular level, in the context of molecular (polymer) actuators, sensors, and energy-related materials. In the first part, I will propose novel molecular structures for π-conjugated polymer actuators, and discuss their synthesis and interesting properties. In the second part, single-walled carbon nanotubes, another π-electronic material, will be modified for sensing a biologically important species, harvesting photo-energies, and discovering a novel phenomenon (thermopower wave).

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장소: 일산KINTEX

발표코드: **MAT.O-5**

발표분야: Current Topics in Materials Chemistry

발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 박성진

Photoelectrochemical Hydrogen Production from Metal Catlyst on Silicon

황성필

명지대학교 화학과

Silicon is earth-abundant, relatively low-cost semiconductor material that is most widely used incurrent photovoltaics and electronics with vast knowledge base and infrastructure. Owing to recent advance innanotechnology on silicon material, various nanostructures of silicon including nanoporous silicon, macroporous silicon, textured silicon, silicon nanowire, and silicon nanoparticles have been fabricated and applied to photoluminescence, sensors, drug delivery and so on. Each nanostructure has unique properties came from its large surface area and quantum size effect such as modulation in energy band and surface-enhanced Raman spectrum.Photoelectrochemical hydrogen generation at Silicon/electrolyte interface has been studied fordecades. Although hydrogen evolution produced by water reduction from solar energy is favorable owing to the position of conduction band edge position, kinetics of hydrogen evolution reaction on silicon is slow leading to research efforts. Herein we present the study of various nanostructure of metallic catalyst on silicon fabricated by recently developed nanotechnology and their photoelectrochemical study for hydrogen generation.

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장소: 일산KINTEX
발표코드: **EDEC.O-1**
발표분야: New Trends in Chemistry Education
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 유미현

실험 중심 과학 수업에 대한 초등학생들의 인식

구아라 임희준*

경인교육대학교 과학교육과

이 연구에서는 과학이라는 교과를 처음 접하는 3 학년 학생들이 다양한 과학 실험 도구를 사용하는 혼합물윌 분리 단원의 실험 활동을 통해 겪는 어려움을 조사하여 분석하였다. 실험 활동에 영향을 끼치는 요인을 크게 실험 활동 외적인 요인과 내적인 요인으로 나누어, 외적인 요인으로는 실험 환경 및 실험 도구, 교육과정 속의 실험 활동으로 살펴보고 실험 활동 내적인 요인으로는 실험 내용적인 요인, 실험 활동 중 상호 작용으로 나누어 실험 활동의 어려움을 분석하였다. 이를 위해 파주시에 위치한 한 초등학교 3 학년 학생들을 대상으로 과학 수업을 실시하고, 설문지 및 과학 일기, 심층 면담을 실시하였다. 본 연구에서 학생들이 어려움을 겪는 실험 활동 내적인 요인으로는 과학실의 실험 도구 및 실험 환경의 준비가 잘 이루어지지 않았다는 점이다. 그리고 과학실 교육이 처음인 만큼 교육 과정 속에서 실험 도구를 접해보고 다루어 보는 기회와 시간을 제공하는 과학실 교육이 필요한 것으로 나타났다. 또한 혼합물의 분리 단원에서 '두부 만들기'는 이번 개정 교육과정에서 4 학년 과정에 있는 실험 내용이 3 학년 과정으로 들어오면서 3 학년 수준의 학생들에게 교사가 혼자 지도하기에는 많은 어려움이 있는 것으로 나타났다. 실험 활동 외적인 요인으로는 실험 내용적인 면에서 실험이 너무 간단하여 흥미를 잃은 학생들이 나타났고 실험을 통한 과학적인 내용 파악보다는 실험 과정을 요리와 같이 느끼는 학생들이 보였다. 실험 활동 중 상호 작용면에서는 모둠원간의 협동이 잘 안되는 점, 실험 활동에서 교사가 도와주지 않은 점에서 어려움을 겪은 것으로 나타났다. 3 학년 학생들은 과학실에서 겪는 모든 활동이 처음이므로 학생들에게 실험하는 과정과 방법에 대한 안내와 지도, 발달 단계에 맞는 실험 활동이 제공되어 처음 과학을 접하는 학생들이 흥미를 잃지 않고 효과적인 과학 수업이 될 수 있도록 학교와 교사의 꾸준한 노력이 필요하겠다.

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과학 수업 구조와 내용 분석을 통한 초등 교사의 신념과 교수 실제 사이의 관계

임희준

경인교육대학교 과학교육과

학생을 가르치는 교사가 갖고 있는 신념은 수업 과정에서 표출되기 때문에 교사의 신념에 대한 연구는 매우 중요하다. 또한 동일한 교육과정과 교과서를 사용하는 초등학교에서 교실 수업의 실제는 교사에 따라 상이하다. 본 연구는 초등학교 과학 수업에서 교사의 과학 및 과학 학습에 대한 신념이 교수 실제와 어떤 관계가 있는지를 알아보고자 하였다. 이를 위하여 초등학교 5 학년 교사 4 명을 대상으로 교사의 과학 및 과학 학습에 대한 신념을 알아보고, 수업 후 반구조화된 면담을 실시하여 과학 교육의 목적, 과학 수업에서 교사의 역할, 학생의 역할, 교사가 사용하는 교수-학습 방법 등에 대한 교사의 인식을 조사하였다. 그리고 교사의 신념과 교수 실제 사이의 관계를 알아보기 위하여 2 차시의 과학 수업을 녹화/녹음하였다. 녹화/녹음한 자료를 이용하여 수업시간 분석과 수업구조 분석을 실시하였고, 교과내용 측면, 수업방법 측면, 학습환경 측면에서 수업의 내용을 질적으로 분석하였다.연구 결과는 다음과 같다. 첫째, 교사의 과학 학습 신념에 따라 수업 진행 방식과 수업의 구조에 차이를 보였다. 수업시간 분석 결과, 과학 및 과학 학습에 대한 신념에서 전통적 관점을 보인 A 교사와 B 교사는 대부분의 수업을 교사설명 위주로 진행하였다. 반면에 과학 및 과학 학습에 대한 신념에서 현대적이고 구성주의적 관점을 보인 C 교사와 D 교사는 교사설명, 학생활동, 상호작용, 문제풀이, 기타 활동 등에 시간을 고르게 분산하고 있었고, 다양한 방법으로 수업을 진행하고 있었다.둘째, 과학 및 과학 학습에 대한 신념에서 전통적 관점을 보인 A 교사는 교수 실제에서 교과서 중심의 설명식 수업을 진행하였다. 반면에 상대적으로 현대적이고 구성주의적인 신념을 보인 C 교사와 D 교사는 교수 실제에서 교과서 내용을 재구성하고 다양한 교수 방법과 전략이 활용되는

수업을 진행하였다. 그러나 리커트 검사에서는 전통적 관점을 보였고, 개방형 설문에서는 현대적이고 구성주의적 관점을 보인 B 교사는 교수 실제에서는 교사의 일방적인 설명식 수업을 하고 있었다.초등 교사의 과학 및 과학 학습에 대한 신념에는 교사간에 차이가 있었으며, 이러한 신념의 차이는 대체적으로 과학 수업의 실제와도 관련이 깊은 것을 나타났다. 그러나 학교와 교사의 물리적, 심리적 환경에 의해 신념이 제대로 발현되지 않는 경우도 있음을 알 수 있었다. 교사 신념의 다양한 측면에 대한 연구와 교사의 교수 실제에 영향을 미치는 다른 변인들에 대한 지속적인 연구가 필요할 것으로 생각된다.

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화학에서 초중학교 학생들의 능력 비교

최원호

순천대학교 화학교육과

학생들의 수준별 능력을 파악하는 것은 교수학습 방향을 설계하는데 도움이 된다.본 연구에서는 초등학교 화학 영역에서 수준별 특징을 조사하며, 중학교 수준과 어떤 차이가 있는지 분석하고자 한다. 상위 학교급인 중학교 수준과 비교하여 초등학교 학생들의 화학 영역에서 능력을 파악하는 것은 한 학교급만을 조사할 때보다 학생들에 관한 정보를 더 구조화하여 이해할 수 있다.

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발산적 가설 설정활동에서 창의적 사고기법의 활용이 학생들의 창의적 문제해결력 신장에 미치는 효과

박지은 강순희*

이화여자대학교 과학교육과

이 연구는 대학교 일반화학실험 수업에서 자유연상법, 속성열거법, 브레인라이팅 등의 창의적 사고기법을 활용하는 것이 학생들의 창의적 문제해결력의 신장에 어떤 효과가 있는지를 알아보기 위한 것이다. 과학에서의 문제해결은 탐구의 과정이라고 할 수 있다. 특히, 가설설정은 문제 해결의 핵심적인 과정으로 알려져 있다. 가설설정에서의 발산적 사고를 촉진하기 위하여 통제반에는 다양한 가설을 설정해보도록 직접적으로 지시하는 수업을 시행하였다. 또한 실험반에서는 직접적 지시와 더불어 창의적 사고기법을 추가로 활용하였다. 한 학기동안 대학교 1 학년 학생들을 대상으로 수업을 시행한 후, 이 수업이 학생들의 창의적 사고력, 비판적 사고력과 창의적 인성에 미치는 효과를 알아보았다. 그 결과 학생들의 창의적 사고력, 비판적 사고력, 창의적 인성에는 유의미한 효과가 나타나지 않았다(p

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발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 여상인

대학 교육에서 반성적 실천의 사례: 교수의 자서전적 연구

한재영

충북대학교 사범대학 화학교육과

교육에서 반성은 가르침의 과정과 배움의 과정에 모두 필요하다. 반성은 외부로부터의 평가나 피드백이 아닌 내부로부터의 되돌아봄을 강조한다. 가르치는 사람은 반성을 통해 자신의 교수 행위를 평가하고 수정할 수 있으며, 배우는 사람은 반성을 통해 자신이 학습한 내용이나 과정을 되짚어보고 학습의 효과를 높일 수 있다. 이중 교사의 반성과 그를 통한 실천의 개선은 ‘반성적 실천’의 개념으로 널리 알려져 있으며, 이것은 교사의 전문성을 이루는 중요한 요소가 된다. 즉 예비 교사는 자신의 전공 교과의 내용을 학습할 뿐 아니라 끊임없이 반성을 하며 개선해 나가는 능력을 키워야 한다. 따라서 사범대학 교수는 반성적 실천을 강조하고 그러한 예시를 보여줄 필요가 있다. 이 발표에서는 예비 과학 교사를 가르치고, 과학 교육 연구를 하며, 사범대학 구성원으로써 봉사를 하고, 한 가정의 가장인 연구자 자신이 자서전적 연구를 통해 본인의 삶을 반성하고 개선해 나가는 사례를 발표한다. 자서전적 연구에서 찾아낸 ‘나’의 모습을 제시하고, 그 모습이 어떻게 변해가고 있는지 이야기하면서, 연구와 교육과 삶의 접점을 공유해 보고자 한다. (이 연구는 2009 년 정부(교육과학기술부)의 재원으로 한국연구재단의 지원을 받아 수행된 연구임(NRF-2009-327-B00652))

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지역일반고등학교 학생들의 융복합 과학교육을 위한 과학기술특성화대학의 역할(실제 사례를 중심으로)

김성균

대구경북과학기술원(DGIST) 기초학부

현재 국내의 R&E 프로그램 등 고등학생들을 위한 연구과제 교육프로그램은 영재고, 과학고, 과학중점고 등 특성화고교를 중심으로 이루어지고 있어 지역의 일반계 고등학생의 경우 이러한 과학교육 프로그램의 수혜에서 소외되어 있는 것이 사실이다. 더구나 일선 고등학교에서 실험 등 실습교육은 물론 이론교육에서 조차 입시 선택 교과의 문제등으로 인해 편향적으로 이루어 지고 있는 실정이다. 이런 현실을 감안할 때 과학에 큰 관심은 있으나 현실적, 환경적인 문제로 인해 실습교육을 접하기 어려운 지역의 일반계 고등학생들을 위한 교육프로그램이 기획되어야 할 것으로 여겨진다. 이런 관점에서 볼 때 실험 인프라가 잘 갖추어진 지역의 과학특성화대학의 역할이 매우 중요하다고 할 수 있다. 본 발표에서는 DGIST 에서 지역일반고등학교와 함께 진행한 "창의경영수업"사례와 미국 캘리포니아주립대학에서 진행하고 있는 고교생 과학교육캠프인 COSMOS 프로그램의 사례를 소개하고자 한다.

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산의 세기 비교, 이온화도와 이온화 상수가 호환되지 않는 문제에 대한 교과서 내용 및 화학교사의 인식 분석

백성혜 전민철*

한국교원대학교 화학교육과

연구에서는 중등학교 화학 교사 50 명을 대상으로 강산의 평준화 효과, 이온화도와 이온화 상수에 대한 이해 정도를 알아보고, 개념 형성의 주된 근거가 무엇인지를 설문과 면담을 통하여 알아보았다. 그리고 교수요목기의 교과서부터 2009 개정 교육과정 화학Ⅱ 교과서의 서술 내용을 외국 교과서, 일반화학, 분석화학 및 유기화학 등 대학 교재, 화학 자료집 등의 서술 내용과 비교 분석하고, 과학사적 관점에서 서술내용의 전제 조건을 분석함으로서 산의 이온화도와 이온화 상수가 호환되지 않는 문제에 대한 교사의 인식의 차이를 찾고자 하였다. 연구 결과, 대부분의 화학 교사들은 강산의 이온화도와 이온화 상수 값이 호환되지 않는 현상에 대해 혼란스러워 하고 있었으며, 수용액 속에서 나타나는 강산의 평준화 효과를 이해하지 못하고 산의 세기를 비교하는 모습을 보이고 있었다. 교사들은 교과서에 제시된 강산의 이온화도와 이온화 상수 값을 별다른 비판적 사고를 거치지 않고 수용하고 있었다. 강산은 H3O+보다 산의 세기가 크므로 그 종류와 무관하게 물 속에서 평준화 효과에 의해 산의 세기가 같아진다. 또한 교과서에 제시되는 산의 이온화도와 이온화 상수가 호환되는 관계를 과학사적 관점에서 살펴보면 약산(약전해질)의 묽은 용액에만 적용될 수 있다. 이러한 결과로부터 화학 교사들이 산의 개념에 대해 올바른 인식을 가지기 위해서는 화학 교과서의 내용에 대해 비판적인 시각에서 사고하고 설명 상의 오류를 찾을 수 있는 능력을 길러 줄 수 있는 교사교육이 필요함을 알 수 있다.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

High Ambipolar Mobilities in OFETs and High Efficiency in OSCs Based on Dithienothiophene and Diketopyrrolopyrole

김인복 김동유[1,*]

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

Donor-acceptor type conjugated polymer, PDTDP, containing dithienothiophene (DTT) and diketopyrrolopyrrole (DPP) was synthesized by stille polycondensation. The polymer showed small optical band gap of 1.44 and 1.42 eV in solution and film and HOMO level of 5.09 eV. The change in crystallinity and morphology of the polymer were investigated with the various annealing temperatures through XRD and AFM. The OFETs in all annealing condition exhibited hole and electron mobilities, the highest values with μh = 1.63 and μe = 0.41 cm^2?V^{-1}?s^{-1} at 250 ^{o}C. According to the ambipolar characteristics, the polymer complementary inverters were fabricated and showed the output voltage gain over 25. PDTDP fabricated from blends with PC$_{71}$BM also exhibited good performance in PSCs with a power conversion efficiency (PCE) of 4.45 %, a open-circuit voltage (V$_{OC}$) of 0.67 V, a short-circuit current density (J$_{SC}$) of 10.8 mA?cm^{-2}, and a fill factor (FF) of 0.62 under AM 1.5G irradiation. The PCE was enhanced by improving the morphology between the polymer:PC$_{71}$BM and increasing both hole and electron mobilities using 1, 8-diiodooctane (DIO) as a processing additive in its active layer system.

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

Phosphorescent Polynorbornene Copolymer with Iridium(III) and Triarylborane Side Groups

김태원 이민형*

울산대학교 화학과

Vinyl addition copolymerization of functionalized norbornene monomers using Pd(II) catalyst efficiently produced phosphorescent polynorbornene copolymers containing side-chain iridium(III) and triarylborane moieties (P1-P3). The catalytic system provides high-molecular-weight copolymers with a controlled incorporation of monomers. While the solution UV/vis absorption and PL spectra show two bands ascribable to each side group in the copolymer, the PL spectra of film exhibit a single band originating from iridium moiety. Details of synthesis and photophysical properties of copolymers will be discussed along with fluoride sensing property.

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

Chitosan-Hematin conjugates: A Novel Horseradish Peroxidase-mimicking Biocatalyst for Adhesive Catechol-functionalized Polymer Hydrogels

류지현 이해신[1,*]

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Cross-linking methods are important to fabricate polymer-based hydrogels for its applications in biomedical fields because of the effect on the mechanical properties such as mechanical strength, stability, and adhesion force. Herein, we reported a small molecular catalyst immobilized chitosan conjugates, chitosan-g-hematin for facilitating catechol-catechol / catechol-amine cross-linkings to rapidly form chitosan hydrogels. Hematin oxidizes catechols mimicking the biological role of oxidoreductase. Chitosan oligosaccharide was grafted with multiple hematin groups for the purpose of obtaining a biocompatible, stable and water-soluble biocatalyst for in situ gelling hydrogels. Chitosan-g-hematin catalyst showed improved solubility in physiological conditions compared to unmodified hematin, and the conjugated hematin exhibited excellent catalytic properties to form chitosan-catechol hydrogels within 5 minutes. In addition, chitosan-g-hematin had excellent cell viability in vitro under the experimental conditions (0.01 %) which can induce robust crosslinking of hydrogel. These biocatalyst-based catechol-functionalized chitosan hydrogels showed increase of adhesion force (33.6 ± 5.9 kPa) with rapid gelling property compared to untreated catechol-functionalized chitosan (4.2 ± 0.5 kPa) on mouse subcutaneous tissues. Furthermore, other catechol-functionalized polymers (hyaluronic acid and poly(vinyl alcohol)) with a chitosan-g-hematin biocatalyst were also showed gratefully enhanced adhesion force compared to untreated catechol-functionalized polymers. This hematin-conjugated chitosan oligosaccharide was useful to fabricate the catechol-functionalized polymer hydrogels with controlled physicochemical properties such as adhesion force, mechanical strength, and gelation time.

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장소: 일산KINTEX
발표코드: **POLY.P-4**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Mussel Cuticle Cohesion-mimicking Catechol-functionalized Chitosan Hydrogels for Biomedical Applications

류지현 이해신[1,*]

한국과학기술원(KAIST) 나노과학기술대학원 [1]한국과학기술원(KAIST) 화학과

Blue marine mussel (Mytilus edulis) byssal threads are covered with granular morphology cuticles, which are cross-linked by both covalent bonds and metal coordination bonds. Bio-inspired by byssal cuticle chemistry, the covalent bonded catechol-functionalized chitosan/thiolated Pluronic hydrogels and the iron-coordinated catechol-functionalized chitosan hydrogels were synthesized for hemostatic materials and tissue adhesives. The covalently crosslinked, adhesive chitosan/Pluronic injectable hydrogels with remnant catechol groups showed strong adhesiveness to soft tissues and mucous layers, and also demonstrated superior hemostatic properties. The iron-mediated chitosan hydrogels showed instant crosslinking and strong adhesion forces, and also exhibited adhesive properties between soft tissues and poly(caprolactone) films. These chitosan-based hydrogels are expected to be usefully exploited for injectable drug delivery depots, tissue engineering hydrogels, tissue adhesives, and anti-bleeding materials.

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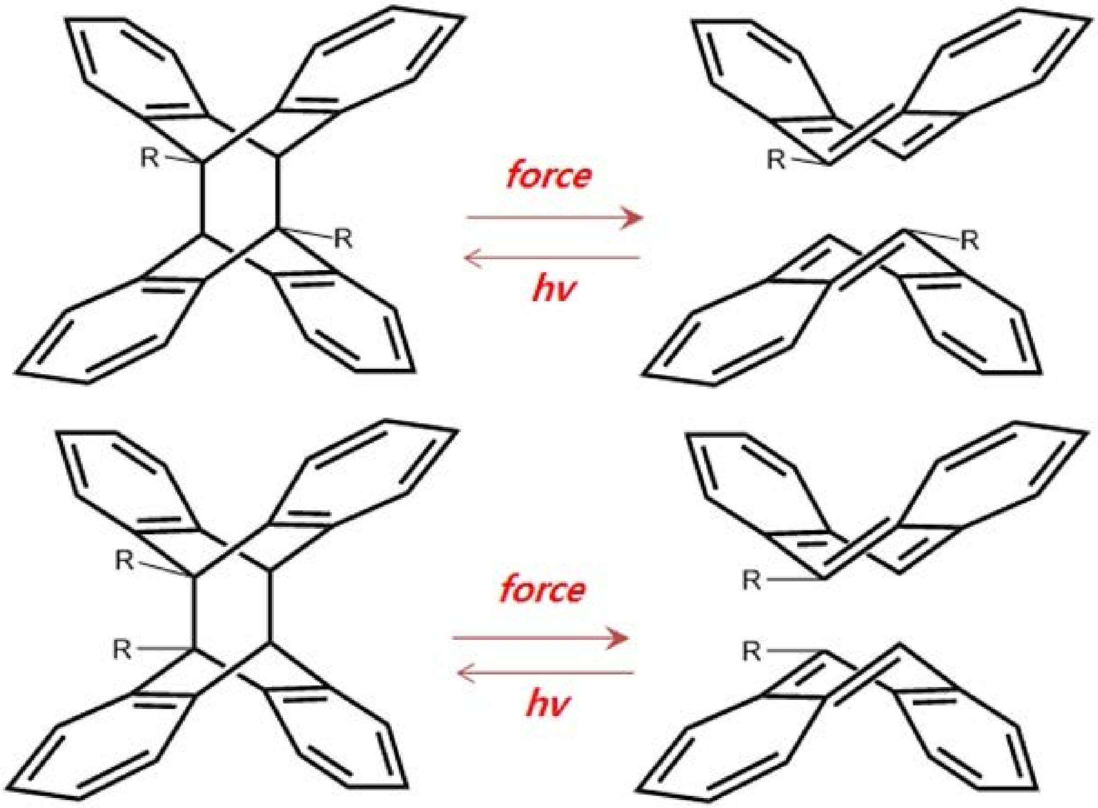
발표코드: **POLY.P-5**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Mechanochemistry of Anthracene Photodimer-Linked Polymers

박민아 정찬문

연세대학교 화학과

In the past years, several studies have demonstrated that macroscopic mechanical forces can be harnessed at the molecular level, creating a new tool for the organic and materials chemist. The field of mechanochemistry touches on materials chemistry from the point of view of each of its principle progenitors with potential utility in areas ranging from stoichiometric reactivity and catalysis to stress-responsive, self-healing, and self-assessing polymers. The object of this study is to synthesize two types of anthracene photodimer-linked polymers and investigate the mechanism of the mechanical reactivity for the polymers. One mechanophore-containing polymer is prepared by step-growth polymerization with anthracenecarboxylic acid dimer and polycaprolactone diol. The polymer contains similar number of the mechanophore and polymer units. The other polymer synthesis uses single electron transfer living radical polymerization (SET-LRP), a kind of chain-growth polymerization, to place a mechanophore unit near the center of polymer backbone. Next, the mechanochemical behavior of the polymers is investigated by ultrasound irrdiation. The decomposition mechanism of anthracene dimer unit is studied. The obtained results are compared with those of thermal and photochemical behavior of the mechanophore linked polymers. A cyclooctane ring decomposition caused by mechanical forces has not been reported. In the study, mechanochemical behavior of the polymers is investigated by nuclear magnetic resonance spectroscopy (NMR), Fourier transform infrared spectroscopy (FT-IR), UV/Vis spectroscopy, fluorescence spectroscopy, and gel permeation chromatography.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일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY.P-6**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Emissive Properties of Vinyl-type Polynorbornene Copolymer with Side-Chain Iridium(III) Emitters and Carbazole Hosts for Highly Efficient PhOLEDs

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울산대학교 화학과 [1]한국과학기술원(KAIST) 화학 [2]한국과학기술원(KAIST) 화학과

Vinyl addition copolymerization of norbornene monomers using a Pd(II) catalyst in combination with 1-octene chain transfer agent efficiently produces well-defined soluble polynorbornene copolymers bearing side-chain $(C^{\wedge}N)_2\mathrm{Ir}(O^{\wedge}O)$ emitters and 9,9'>-(1,3-phenylene)bis-9H-carbazole (mCP) or 9,9'-1,1'-biphenyl)-4,4'-diylbis-9H-carbazole (CBP) host moieties. The catalytic system provides high-molecular-weight copolymers with a controlled incorporation of monomers. Among the solution-processed devices fabricated based on a single emissive layer comprising the blue-, green-, and red-phosphorescent copolymers (PBn, PGn, and PRn, n = 1-4) with various concentrations of emitters (1.7-13.9 mol%-Ir), the devices based on PB4 (10.5 mol%-Ir), PG2 (5.5 mol%-Ir), and PR4 (13.9 mol%-Ir) display the best performances with maximum power efficiencies of 12.9, 25.6, and 3.3 lm/W and maximum external quantum efficiencies of 8.8, 13.3, and 5.1%, respectively, for each color. Details of synthesis and characterization of copolymers and their emissive properties in PhOLEDs will be discussed.

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

3,4-Disubstituted polyalkylthiophenes for high-performance thin-film transistors and photovoltaics

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한국철도기술연구원 에코시스템연구실 [1]경북대학교 자연대/화학과 [2]Stanford University

Poly(3-hexylthiophene) (P3HT) has been the most commonly used organic semiconductor for organic solar cells due to a high absorption and good charge transport. The high charge carrier mobility of P3HT has permitted the solar cells to be made thicker (~220nm) than most other polymer-fullerene devices. Conjugated polymers with (mostly) planar backbones are often considered as optimal for organic-based electronic devices. We systematically impose synthetically-tailored twists within the conjugated backbones of a family of polythiophenes and examine their influence on charge carrier mobilities and bulk heterojunction (BHJ) solar cells. We demonstrate that poly(3,4-dialkyl-terthiophenes) (P34ATs) have a comparable transistor mobility and greater environmental stability (less degradation of on/off ratio) than regioregular poly(3-alkylthiophenes) (P3ATs). This suggests that a strong π-π stacking is not always necessary for high charge carrier mobility and that other potential polymer packing motifs in addition to the edge-on structure (π-π stacking direction parallel to the substrate) can lead to a respectable electronic performance. The high charge carrier mobility of the hexyl and octyl-substituted P34AT has enabled a high power conversion efficiency in a polymer:fullerene bulk heterojunction photovoltaic device.

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

Up-scaled polyplex preparation using 3D microfluidic system and its application to gene delivery

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충남대학교 생화학과 [1]포항공과대학교 화학공학과

Intracellular delivery of plasmid DNA usually required to combine with a carrier system for efficient non-viral gene delivery. Negatively charged plasmid DNA can interact with positively charged polymers such as poly(amidoamine) (PAMAM) dendrimer or polyethylenimine (PEI) via electrostatic interaction and form polyplexes. These polyplexes are easy to prepare and efficiently translocate the DNA into the cytoplasm. However, typical method for preparing polyplex has limitations in inhomogeneous particle size and surface charge density. Inhomogeneous particle size and surface charge density usually led to low transfection efficiency of polyplexes. Therefore, it is important to develop a novel method that preparing well defined polyplex particles in terms of homogenized hydrodynamic size and surface charge density. Here, we present the new microfluidic approach to prepare the quality controlled polyplexes and applicated to gene delivery study. PAMAM dendrimer was used as cationic polymer and fabricated polyplex particles with pDNA using 3D microreactor and compared its physicochemical properties and transfection ability to bulk mixing method.

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

Fluoroaniline을 포함한 친수성 안의료용 렌즈 고분자의 중합 및 물리적 특성

노정원 성아영*

세한대학교 안경광학과

본 연구는 2,4-difluoroaniline 을 하이드로젤 렌즈 모노머에 첨가하였을 때 렌즈의 물성 변화를 알아보기 위해 hydrogel 렌즈의 기본 모너머인 HEMA(2-hydroxyethyl methacrylate), NVP(N - vinly pyrrolidone), MA (methacrylic acid) 및 교차결합제인 EGDMA(ethylene glycol dimethacrylate) 그리고 개시제인 AIBN(azobisisobutyronitrile)을 기본조합으로 하여 reference lens 를 먼저 공중합하였다. 또한, 이 조합을 기본으로 하여 2,4-difluoroaniline 을 약 1~10%로 첨가량을 점차 증가시켜 공중합한 후 물성 변화를 측정하고 분석하였다. 중합조건으로는 1 차 공중합 80 ℃에서 40 분, 2 차 공중합 120 ℃에서 40 분 동안 총 2 회에 걸쳐 열처리하였다. 생성된 공중합체의 물리적 특성을 측정한 결과, 평균함수율 38 ~ 41%, 굴절률 1.432 ~ 1.434, 인장강도 0.300 ~ 0.116 kgf 그리고 접촉각의 경우 77.33 ~ 66.15° 범위의 분포로 나타났다. 또한, 2,4-difluoroaniline 의 첨가량이 증가할수록 가시광선 투과율의 경우 92%에서 81%로, UV-A 는 88%에서 62%로, UV-B 는 83%에서 45%로 감소하여 자외선 차단효과가 있는 것으로 나타났다. 본 실험결과로 볼 때 생성된 공중합체는 hydrogel 렌즈의 기본적인 물성의 큰 변화를 나타내지 않으면서도 자외선 차단효과를 가지는 고분자 재료로 사용될 수 있을 것으로 판단된다.

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

Reversible Order-Order Self-Assembly Transition of a Rodlike Poly(*n*-alkyl isocyanate) in Thin Films via Selective Solvent-Annealings

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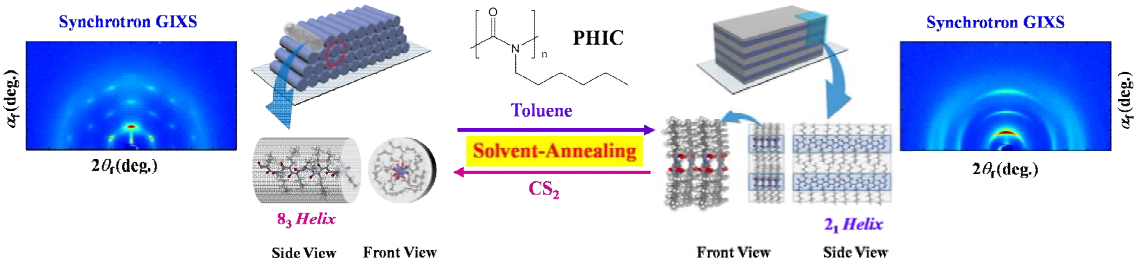
포항공과대학교 화학과 [1]동아대학교 화학과 [2]광주과학기술원(GIST) 신소재공학과, PIMS [3]포항공과대학교 첨단재료과학부

The conformational and structural details of poly(*n*-hexyl isocyanate) (PHIC) have received significant attention because of their unique stiff chain characteristics and potential applications in various fields. A well-ordered hexagonal close packing (HCP) structure of PHIC with 8/3 helical conformation was successfully demonstrated in thin films annealed selectively with carbon disulfide vapor. A well-ordered multibilayer structure of the polymer with *β*-sheet conformation was also formed in the films annealed selectively with toluene vapor. Moreover, a fully reversible transformation between these two self-assembled structures was demonstrated by consecutive annealing with carbon disulfide and toluene.



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장소: 일산KINTEX
발표코드: **POLY.P-11**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymers Bearing Zwitterionic Sulfobetaine Brushes: Correlation between Thin Film Morphology and Bacterial adherence Properties

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포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

In this study we synthesized a series of well-defined brush polymers bearing zwitterionic sulfobetaine groups. The thermal properties and phase transitions of these polymers were investigated. The polymers were found to form favorably into multi-bilayer structures, always providing hydrophilic, zwitterionic sulfobetaine end groups at the film surface. For the films, water sorption behavior was examined. In addition, surface energy components were determined for the polymer films and the bacterial cells deposited on cellulose acetate membranes. The brush polymer films were found to suppress bacterial adherence significantly. An understanding of the suppression of bacterial adherence was attempted in terms of surface energies and thermodynamics. The results collectively indicate that the sulfobetaine-containing brush polymers are suitable for use in biomedical applications that require the reduced possibility of post-operative infection.

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발표코드: **POLY.P-12**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Incorporation of Adenine into Brush Polymers: Synthesis, Structure, and Biocompatibility

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In this study, two novel brush polymers with similar structures were synthesized and explored using various analytical methods. These two DNA-mimicking polymers are poly[oxy(11-(3-(9-adeninyl)propionato)-undecanyl-1-thiomethyl)ethylene] (PECH-AP) and poly[oxy(11-(5-(9-adenylethyloxy)-4-oxopentanoato)undeca-nyl-1-thiomethyl)-ethylene] (PECH-AS). According to respective structural analyses, both polymers formed multibilayer structures; the adenine moieties at the bristle ends of each polymer were partially interdigitated together using hydrogen bonding. The study also found that the polymers were thermally stable up to 220 degrees C and that they could easily be prepared in high quality films by conventional coating processes. Though two polymers are structurally similar, PECH-AS showed higher hydrophilicity and better water sorption characteristics than PECH-AP. These differences were attributed to the chemical structures in the bristles of the polymers. Both of the adenine-rich surfaces of the polymer films showed following characteristics: selective protein adsorption, suppressed bacterial adherence, facilitated HEp-2 cell adhesion, and good biocompatibility in mice. However, PECH-AS film showed higher hydrophilicity and water sorption values than PECH-AP film, which indicates that it will perform better when designing biocompatible devices.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Polymer Containing Both Tetrathiafulvalene and Fullerene Groups

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A new polymer (6TTF-polymer) containing both electron-rich tetrathiofulvalene (TTF) and fullerene (C_{60}) was successfully synthesized via coupling reactions. The chemical architecture of 6TTF-polymer was characterized by spectroscopic techniques such as FT IR, ^1H NMR spectroscopes, its thermal behavior was monitored by DSC. Moreover, the electrochemical properties were estimated by cyclic voltammetry, photoluminescence and ultraviolet spectroscopes. The cast 6TTF-polymer films were bendable and ductile that the molecular weight was high enough. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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Phase evolution of a board-shaped tetrathiafulvalene molecule

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A symmetric tetrathiafulvalene-base molecule (symTTF11) was newly synthesized by attaching four flexible alkyl chains at the periphery of board-shaped molecule. Phase behaviors and physical properties of symTTF11 were investigated by the thermal, microscopic and scattering experimental techniques. Since the assembled symTTF11 columns were well organized in the ordered layer structures over a macroscopic domain in the columnar smectic LC phase, symTTF11 showed a good charge carrier mobility, which was about two-order of magnitude faster than that in the columnar crystalline phase. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government

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High-Molecular-Weight Aliphatic Polycarbonates by Condensation Polymerization of Diols and Dimethyl Carbonate: Synthesis, characterization and degradation

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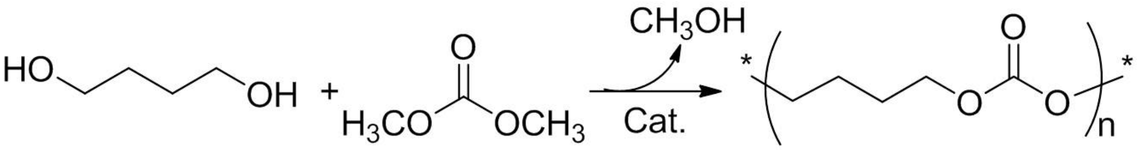
A synthetic strategy was developed for the condensation polymerization of aliphatic diols with dimethyl carbonate to produce high-molecular-weight aliphatic polycarbonates. In the first step, the oligomers were formed bearing almost equal number of hydroxyl and methyl carbonate end groups. In the second step, the condensation reaction was conducted at a high temperature (>180℃) to connect the -OH and -OC(O)OCH_3 chain ends while removing the generating methanol under a reduced pressure. Small amount of sodium alkoxide (0.02-0.5 mol%) was used as a catalyst. Using anhydrous diol was crucial to speed up the reaction rate and also to reproduce the consistent result. In the second step, the pressure was gradually reduced and the temperature was optimized in order to reduce side reactions. By this strategy, high-molecular-weight poly(1,4-butylene carbonate)s and its copolymers incorporating various other diols (2-10 mol%) were prepared with Mw, 100000-200000 in a short reaction time of total 6.5 h. This strategy was also effective in producing other high molecular weight aliphatic polycarbonates (Mw, ~200000) using 1,6-hexandiol and cyclohexane-1,4-dimethanol. When the [-OH]/[-OCH_3] ratio of the oligomers generated in the first step was deviated from ~1, it was hard to attain such a high molecular weight. After polymerization, the base catalyst was neutralized by the treatment with acryl chloride or more effectively with melamine phosphate. After quenching, the polymer showed the same level of thermal stability as the pure polymer.



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Molecular Beacon Aptamer-based ATP Detection

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Molecular beacon (MB) is an oligonucleotide, which is a hairpin shaped molecular probe labeled with a fluorophore and quencher at both termini. Due to the ATP aptamer sequence for molecular recognition element, with cationic conjugated polyelectrolytes (CPEs), molecular beacon aptamer (MBA) undergoes a conformational change via electrostatic and hydrophobic interactions. In the absence or presence of ATP, MBA make an open chain form (turn-on state; CPE-induced FRET signal) or a G-quadruplex (turn-off state; quenching), resulting in clear turn-on/-off signal (highly sensitive and selective ATP detection is possible). Here we report the CPEs-based ATP detection with modification in the stem stability in MBA. Depending on binding strength in the MBA stem part, the equilibrium between the open-chain and hairpin structures of MBA can be adjusted, resulting in fine-tuning of sensor properties.

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HMDS(hexamethyl disilazane)을 이용한 다공성 분체의 표면 개질 및 이를 통한 유기 자외선 차단제 안정화

공수성 홍원기 김동명*

한국콜마 색조화장품 연구소

자외선은 200~400nm 짧은 파장 영역대의 광선으로 비타민 D 생성, 살균작용, 음이온 생성 작용 등에 이용 되고 있으나, 인체의 피부가 노출되면 급성반응이 나타나며, 만성반응으로 심각한 질환이 발생하게 된다. 이와같은 질환은 자외선을 적절히 차단함으로써 억제 시킬 수 있으며, 여기에 이용되는 자외선 차단제는 크게 유-무기 자외선 차단제로 나뉠 수 있다. 무기 자외선 차단제는 산화아연, 이산화티탄이 이용되며, 이들은 높은 굴절률(> 2.0) 및 우수한 광안정성을 보여주며, 유기자외선 차단제는 BMDBM, OMC, BEMT 등이 주로 이용된다. 그러나 무기자외선 차단제는 백탁현상 및 사용감의 한계로 인해 제한이 있고 함량 대비 낮은 자외선 차단효과가 나타난다. 또한 유기자외선 차단제는 낮은 광안정성과 금속산화물과 착물 형성 가능성, 피부 침투 및 자극 유발등의 문제로 사용상 제한을 받고 있다. 이를 해결코자 다공성 물질을 이용한 연구가 다양하게 보고되고 있으나, 담지율이 10% 미만으로 산업에 적용하기에는 한계가 있다. 이에 본 연구에서는 HMDS(hexamethyl disilazane)를 silylation 법을 이용하여 20% 이상 담지 시키고 이를 안정화를 시켜 산업적으로 이용하고자 하였다.

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

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인제대학교 나노공학부

In this study, the scaffolds were fabricated by the solvent and non-solvent sintering and centrifugation method using poly(D,L-latic-co-glycolic acid)(PLGA) porous microparticles and hydroxyapatite(HA) which was known to help for cell movement, proliferation and differentiation of bone and cartilage. The particle sized and pore sized by the analysis using scanning electron microscopy(SEM) were 120 um and 13 um, respectively. The more amount of HA was used to prepare microparticles, the higher peak of FT-IR of 1052 cm^-1(PO4^2-) could be observed. HA-PLGA scaffold was carried out in PBS 7.4 buffer at 37.5℃. Porosity test of HA-PLGA scaffold is measured by liquid substitution method. Compressive strength of PLGA scaffolds(HA 120 mg) was 0.143Mpa. The scaffold with the larger particle sized and pore sized showed the less mechanical property, which seems to come from the lower molecule-weight of PLGA polymer. The further studied about cell proliferation and viability need to be performance to verify that the scaffolds have bone optical properties for tissue engineering.

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Flame-Retardant Treatment of Cellulose fabrics using graft copolymerization

김태경

한국화학연구원 그린화학연구단 환경자원센터

The graft copolymerization of phosphorous/nitrogen-containing acryl compounds on cellulose fabrics(cotton, rayon) was studied as function of temperature, concentration of monomer and initiator. The focus of this study was to optimize the flame retardancy finishing on cellulose fabrics with free radical grafting. Also the effect of reaction conditions on grafting parameters, i.e. grafting ratio, efficiency, conversion and add on has been examined. The characterization of this finishing was made by color measurement, IR analysis, thermo-gravimetric analysis, limited oxygen index. The results showed that the free radical grafting process onto cellulose fabrics reduced the first thermal decomposition temperature, while the amount of char residues increased compared with untreated cellulose fabrics. In case of add on 30% treated cellulose fabrics were totally unburned after combustion , which is flame retardant. This flame retardancy may occur through a condensed phase mechanism. The resulting cellulose fabrics are suitable for use as working clothes, baby clothes, curtains, towels and bedding sheets.

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Property control of LbL assembled sPPO membrane for fuel cell PEM applications

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한양대학교 유기나노공학과 [1]한양대학교 분자시스템공학과

Fuel cell membrane based on sPPO (sulfonated poly(2,6-dimethyl-1,4-phenylene oxide)) was prepared via layer-by-layer (LbL) deposition method with PDDA (poly(diallyl dimethyl ammonium chloride)). PPO has good thermal and mechanical properties, and its highly sulfonated analogs exhibit good proton conductivity but poor methanol permeability. LbL technique has advantage in control of membrane permeability. So, the sPPO with high degree of sulfonation was tried to be converted into a good membrane material by modification through LbL technique. As a result, LbL engineered sPPO membranes showed decreased methanol permeability as the number of layer increased. but still maintaining decent proton conductivity. The selectivities of all membranes were better than Nafion 117.

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Synthesis and Characterization of PLGA-PEO-PPO-PEO-PLGA Pentablock Copolymers

조은범

서울과학기술대학교 정밀화학과

We report the synthesis and characterization of PLGA-PEO-PPO-PEO-PLGA pentablock copolymers. Pluronic F68 was used a basic block copolymer and D,L-lactide and glycolide were attatched to the hydroxy end group of PEO-PPO-PEO triblock copolymer. Stannous octoate was used as a catalyst to open the cyclic lactide and glycolide molecules inside anhydrous toluene solvent. Reactants were refluxed for 1 day at 120 oC condition and precipitaed in a large amount of diethyl ether solvent. Final products were obtained by vacuuming mixtures with residual diethyl ether for 30 days. Five kinds of pentablock copolymers were characterized with 1H- and 13C- NMR and GPC (gel permeation chromatography), which show PLGA blocks were well attached and molecular weights were well controlled compared with the reactants. Thermogravimetric analysis also show the weight ratios of PLGA/(PEO+PPO).

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Morphological Analysis of Well-defined 1,3,4-Oxadiazole Brush Polymer with using Synchrotron Grazing Incidence X-ray Scattering

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포항공과대학교 첨단재료과학부 [1]포항공과대학교 화학과

In this study, quantitative structural analyses were done with novel functional brush polymer, poly(n-nonyl 4'-(5-phenyl-1,3,4-oxadiazol-2-yl)-[1,1'-biphenyl]-4-carboxy- late acrylate) (PVOXD) containing oxdiazole moieties at the end of brush side chains. The grazing incidence X-ray scattering (GIXS) measurements were done to investigate the structure within thin film and it was revealed that the layer structure, stacked along out-of-plane direction, was developed via thermal annealing process. Quantitative GIXS analyses, using GIXS formula derived previously, reveals that the layer structure was formed with 3.56 nm of long period. Also brush side chains are stacked each other to form π-π stacking of phenyl substituted oxadiazole groups. Also, in-situ GIXS measurements were done during heating and subsequent cooling, showing reversible transitions, combined with investigation of thermal properties. The melting behavior of brush side chains and breakdown of the layer structure occurred stepwise during heating. During subsequent cooling, the reverse transitions were observed and the layer structure was fully recovered reversibly.

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Construction of hierarchical structures of the tetrathiafulvalene molecule on the different length scales

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A programmed amphiphilic TTF molecule (amph-7TTF14) was newly synthesized. From the x-ray diffraction pattern of the uniaxially oriented amph-7TTF14 film, the crystal structure was identified to be a monoclinic unit cell. The face-to-face π-π interaction between TTF groups and the nanophase separation between rigid TTF groups and flexible hydrophobic alkyl and hydrophilic tri(ethylene oxide) tails were the main driving forces for the self-assembly of amph-7TTF14. Based on the experimental results, the amph-7TTF14 formed not only flat ribbons but also scrolls and helixes, in which the ribbons further aggregated to create the fibrous hierarchical structures. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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Nitric oxide delivery based on polymer as antibacterial agent

박정홍 김원종*

포항공과대학교 화학과

When methicillin-resistant *Staphylococcus aureus* (MRSA) firstly was isolated in 1961, the number of patients has been increased year by year. The patients have been frozen with fear by life-threatening infection by multi-drug resistance bacteria in hospital. Many researchers have been developed new antibiotics such as silver ion, silver nanoparticles, polymer, peptide, and so on. However, the cytotoxicity and limited application of antibiotics remained an unsolved problem. Nitric oxide (NO) has been highlighted on researchers due to its efficiently broad spectrum antibacterial activity. To delivery NO efficiently, a number of NO donors has been developed such as S-nitrosothiol, NO aspirin, nitroglycerin and N-diazeniumdiolate (NONOates). NONOates has many attentions in terms of easy synthesis and releasing in physiological condition. The successful synthesis of NO releasing material which is composed of biocompatible Pluronic F68, BPEI 1800 to support secondary amine and NONOates was verified as a good antibacterial agent against Gram-negative *Escherichia coli* (*E.coli*), Gram-positive *Staphylococcus aureus* (*S.aureus*) and MRSA. Using confocal microscopy, bactericidal ability of NO was revealed compared to control or polymer F68. Then, the destruction of bacteria membrane induced by NO was verified by TEM. In addition, F68-BPEI1800-NONOates did not show high cell cytotoxicity *in vitro* as confirmed by MTT assay. In summary, F68-BPEI1800-NONOates was demonstrated NO delivery materials with application for antibacterial activity.

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Selective Adsorption and Patterning of Halloysite Nanotubes on Si Surface

황선민 강훈구 노재근

한양대학교 화학과

Halloysite nanotubes (HNTs), a type of natural clay with nanotubular structures, are promising candidates for various applications such as controlled release, nanotemplating and catalyst carrier. HNTs also can be used as anionic materials in basic pH condition than neutral pH condition. To provide the selective adsorption region for HNTs, we modify silicon surface using poly ethyleneimine (PEI) and poly styrenesulfonate (PSS) due to its each strong positively and negatively charge. Si surface was modified by PEI, which provides the adsorption site for HNTs layers via electrostatic interactions by solution diping method. Then, the micro-patterned PSS films prepared on PDMS surface were transferred on PEI layer by stamping the micro-patterned PSS on PEI-covered Si surface. Finally, when the patterned substrate is dipped in the aqueous solution of dispersed HNTs, HNTs are selectively adsorbed on PEI layer due to electrostatic interaction with PEI layer and repulsion with PSS layer. The micro-patterned HNTs layers with high selectivity was obtained by controlling electrostatic interactions between surface and HNTs and confirmed by means of atomic force microcopy.

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Isosorbide와 polycarbonatediol를 이용한 polyurethane 합성 및 물성조사

오소연 공명선

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Polyurethane 은 diisocyanate 와 polyol 이 반응하여 생성되는 우레탄기를 분자 내에 함유하는 고분자이다. 분자내의 우레탄기는 극성 수소결합을 형성하여 특수한 물성을 부여함으로써 내약품성, 내마모성, 기계적 물성 및 내구성이 우수하여 다방면에 널리 사용되고 있다. 본 연구에서는 생체 적합성을 가지는 고탄성 폴리우레탄을 합성하기 위하여 soft segment 로서 무독성이며 내충격성 및 약산에 강한 polycarbonatediol 과 hard segment 로서 역할을 하는 1,4:3,6-dianhydro-D-sorbitol(isosorbide)을 diol 로 사용하고 hexamethylene diisocyanate (HDI)와 중축합하여 다양한 비율의 polyurethane 을 합성하였다. 두 성분의 조성에 따라서 다양한 용매에 대한 용해도, GPC 에 의한 분자량, DSC 및 TGA 등의 열분석과 인장강도 및 신장율 등의 기계적 분석을 통해 평가하였다. 또한 생분해도는 PBS 용액 내에서 진행하여 물성 변화를 조사하였다.

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Layer-by-Layer Self-Assembled Multilayer Films Comprisinga Dual Stimuli-Responsive Block Copolymer for Drug Delivery Applications

<u>김순화</u> 빈센트 홍종달*

인천대학교 화학과

Stimuli-responsive thin films and coatings combine a wide range of fundamental scientific and commercial objectives, these smart polymer films have been proposed for various applications including drugdelivery and membrane permeation mechanisms. Herein, we report on the layer-by-layer (LBL) self-assembly of dualtemperature- and light-responsive diblock copolymer poly((N-isopropylacrylamide)-b-poly(spiropyran)) (PNIPAM-b-PSP)(P6) with apolycation.The neutralpolyspiropyran (PSP) block in P6 copolymer can be isomerized to charged polymerocyanine(PMC) by UV lightirradiation.The P6unimers or micelles were included in the multilayer films through LBL self-assembly utilizing the ionic interactions between the chargedPMC block and the polycation.The LBL self-assembly of the multilayer film was characterized using UV/visible spectroscopy and ellipsometry. Furthermore, the multilayer film was utilized for the controlled release of small dye molecules from the multilayer filmin response to the solution temperature.This method showed a potential use in controlled release of model dyes in response to the external stimuli and could be a promising candidate for the application in drug delivery.

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New Stable Self-Assembling Polyoxyethylene Glycopolymers: Synthesis, Structure, and Properties.

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포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

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

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Au/Ag@CNT Nanophotocatalyst with Enhanced Light-Absorption and Transmission Ratios

변교연 이하진[1] 최원산*

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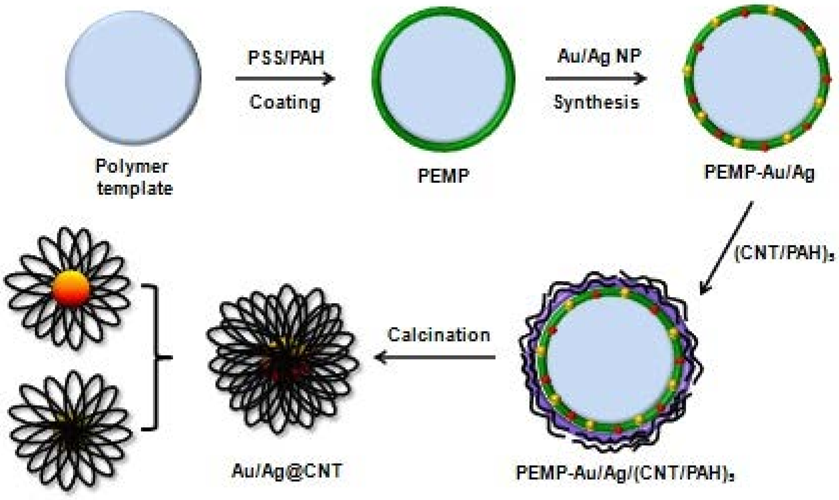
Our study demonstrates a facile approach for the synthesis of noble metal core-in-carbon nanotubes shell (Au@CNT mesh or Au/Ag@CNT mesh) structures, which can be used as catalysts or visible-light driven photocatalysts for transforming or decomposing toxic materials to desired materials. The metal@CNT structures, submicro-meter sized noble metal cores in the CNT mesh shells, were prepared by synthesizing metal nanoparticles (NPs) and then coating polyelectrolytes/CNTs on polymer colloidal particles using a layer-by-layer self-assembly technique, followed by a heat treatment. Our structures could be promising candidates for visible-light driven photocatalysts for the following reasons: i) their core structures can provide a reactive surface where noble metal can react with toxic materials; and ii) their shell structures can provide mechanical robustness against wear and tear, as well as facile mass transportation due to the mesh structure of the CNT shell. Another remarkable advantage of the Au/Ag@CNT structures is that the aggregation of cores after catalytic reaction can be avoided by shell structures. Our structures showed outstanding catalytic performance for removing or transforming unwanted materials.

Au/Ag@CNT Nanocatalysts



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Reversible Color Modulation with Grating Patterned Electroactive conjugated polymer

신해진 김은경[1,*]

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A single electroactive conjugated polymer device with gratings exhibited different colors upon application of a low external potential between -2 and 2V. Electroactive conjugated polymer, poly(3,4-propylenedioxythiophene-phenylene) (P(ProDOT-Ph)), was successfully patterned with the fast and simple micromolding in capillaries (MIMIC) process. Under the illumination of white LED light, the diffraction gratings showed various color varied from green to violet with an intermediated blue color upon application of -2 to 2V thus covering the visible spectral range (RGB) and which was not achieved with an unpatterned film. This work demonstrates how the change in the refractive index of an electroactive polymer upon application of an external potential can be exploited for electroactive functional devices. With complete reversibility and colormodulation on applying a voltage, keeping their diffracted color and intensity even after power was turned off for longer than 40 hours.

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High CO_2 uptake and selectivity by thermally-rearranged molecular networks with nano-channels

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The OMNs-TR with open channel and monolith structure was synthesized by thermal treatment of organic molecular networks (OMNs) using urea chemistry which included decomposition of urea by heat and continuing reaction of decomposed isocyanates to dimer or trimer. The synthesized OMNs-TR show improved porosity, CO_2 adsorption capacity (15 wt%), selectivity (α, 140) and repeated adsorption/desorption without change of capacity due to the open channel and hierarchical pore structure in networks and the monolithic structure prepared from inter-particles reaction. The OMNs-TR indicate also improved chemical and thermal stability (300 to 500℃) due to the cross-linked isocyanurate moieties and retain its structure under high pressure (50bar).

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Incorporation of Rice-like Nanoparticles into Inorganic Capsules and Their Multifunctional Characteristics

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A novel strategy for preventing aggregation, increasing surface area, and enhancing light-harvesting efficiency of multifunctional nanoarchitectures is introduced, and use of the synthesized multifunctional nanoarchitectures as recyclable absorbents or photocatalysts is demonstrated. Our iron oxide (IO)carriers encapsulated with multi-rice-like IO particles (IOPs) are fabricated by the synthesis of the IO carriers prepared by calcination of the IO-coated polymer particles, followed by “ship-in-bottle” synthesis of rice-like IOPs within the IO carriers. The distinctive structures of the IO carriers containing multi-rice-like IOPs prevent aggregation and contamination of the rice-like IOPs, and allow multiple reflection of light within the carriers due to a unique structure, both of which enhances photocatalytic or adsorption abilities for decomposing toxic substances or removing heavy metal ions, respectively. Our approach described here will provide a new design concept for synthesizing hierarchical nanomaterials containing multi-nanomaterials.

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Nafion과 이온성액체를 이용한 이산화탄소 분리막 연구

황용하 원종옥[*] 방호선 이정현[1] 강용수[1]

세종대학교 화학과 [1]한양대학교 에너지공학과

오늘날 지구온난화에 대한 위기의식이 고조됨에 따라 온실가스를 감축하기 위한 노력들이 진행 중이다. 이산화탄소 분리막을 이용하면 이산화탄소를 분리, 회수하는 과정에서의 비용을 줄이고 배기가스에서의 이산화탄소 배출양을 줄일 수 있다. Nafion solution 에 PVP 를 첨가하고 지지체인 polysulfone 지지막 위에 electrospinning 기법으로 직접 방사하여 nafion/PVP fiber 를 얻어냈다. polysulfone 지지체위에 nafion fiber 층을 만든 후 각각의 3 가지 이온성 액체{1-hexyl-3-methylimidazoilium bis (trifluotom ethanesulfonyl)imid([hmin][Tf_2N]), 1-hexyl-3-methylimidazoilium tetrafluoroborate([hmin][BF_4]), 1-hexyl-3-methylimidazoilium hexafluorophosphate([hmin][PF_6])}를 첨가하여 electrospun Nafion/PVP membrane 을 제조하였다. SEM 을 이용하여 Electrospun Nafion membrane 의 단면 및 fiber 의 형태를 확인 할 수 있었고 기체투과도 장치를 이용하여 막을 통과한 기체의 양을 bubble meter 를 통해 이산화탄소의 선택도를 측정하였다. 같은 방법으로 Nafion/PEO 막을 제조해서, Nafion/PVP 막과 결과를 비교연구한다.

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염료 감응 태양 전지 전해질에 도입한 photo-cross-linking 시킨 PEGDMA의 효과

<u>송홍규</u> 원종옥* 최혜리 남소래

세종대학교 화학과

기존의 액체상 전해질을 이용한 염료 감응 태양 전지의 약점인 전해질의 누수와 증발을 막기 위해 준고체상 전해질을 이용하여 염료 감응 태양 전지를 제작하였다. 이에 따른 Short-circuit photocuttent density (Jsc)와 효율의 감소를 극복하기 위해 제조가 간편하고 전도성이 높으며 flexible 하여 휴대성과 응용성이 높은 전도성 고분자 막을 이용하여 전해질 내의 이온의 이동성을 증가시켰다. 전도성 고분자 막은 poly(ethylene glycol) dimethacrylate (PEGDMA)와 Tetraethyl orthosilicate (TEOS)를 이용하여 제조한 용액을 working electrode 의 TiO_2 층에 적용한 후, UV light 를 이용하여 photo-cross-link 시켜준다. 그리고 알려진 dye sensitized solar cell 제작 방법에 따라 platinum 이 doping 된 counter electrode 와 결합하였다. 이에 따른 향상된 이온 전도도의 효과를 확인하기 위해 photovoltaic performance 의 측정을 통하여 변환 효율을 측정하고, IPCE (Incident Photon-to-electron Conversion Efficiency)를 통해 Jsc 가 증가하는 것을 확인하였다. 또한 EIS (Electrochemical Impedance Spectroscopy) 및 IMVS (Intensity Modulated Voltage Spectroscopy) 를 측정하여 염료 감응 태양 전지에 미치는 영향을 연구하였다.

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Photo-cross-link 시킨 PEGDMA를 전해질로 도입한 염료 감응 태양 전지의 성능 연구

최혜리 원종옥* 송홍규 남소래

세종대학교 화학과

액체상 염료 감응 태양전지는 높은 광전 변환 효율의 장점을 가지고 있는 반면 유기 용매를 사용하기 때문에 전해질의 누수와 휘발로 인한 문제점을 갖고 있다. 이러한 문제를 개선하기 위해 Photo-cross-link 시킨 poly(ethylene glycol) dimethacrylate (PEGDMA)를 고체상으로 도입한 염료 감응 태양전지를 제작하였다. 이온 전도성을 갖는 PEGDMA 에 flexible 한 성질을 갖도록 methoxy poly(ethylene glycol) monomethacrylate (PEGMA)를 섞어서 고분자 용액을 제조하였다. TiO2 가 코팅된 working electrode 에 dye solution 을 dipping 하고 제조한 고분자 용액을 도포 한 후 UV light 를 조사하여 photo-cross-link 시켜주었다. 그 다음으로는 잘 알려진 염료 감응 태양전지 제작 방법에 따라 platinum 이 코팅된 counter electrode 를 결합하여 cell 을 제작하였다. 이온 전도성이 우수한 고분자가 charge transfer 효과를 증대시킬 것으로 기대하고 이에 따른 효과를 확인해 보았다. photovoltaic performance 의 측정을 통해 향상된 변환 효율을 측정하고, IPCE (Incident Photon-to-electron Conversion Efficiency)를 통해 Jsc 의 증대를 확인하였다. 또한 EIS (Electrochemical Impedance Spectroscopy)를 측정하여 고체상의 PEGDMA 가 액체상 염료 감응 태양전지의 단점을 보완하면서 전해질 내에서 charge transfer 를 증가 시킨다는 것을 확인하였다.

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photo-cross-linking 조건에 따른 PEO젤의 특성연구.

남소래 원종옥* 박성진

세종대학교 화학과

제조가 간편하고 전도성이 높으며 flexible 하여 휴대와 응용성이 높은 전도성 고분자 막을 개발하기 위하여 photo-cross-linking 이 가능한 poly(ethylene glycol) dimethacrylate (PEGDMA)와 methoxy poly(ethylene glycol) monomethacrylate (PEGMA)를 이용한 PEO 젤을 제작하였다. PEGDMA 는 이중결합을 2 개 가지고 있어 cross-linking 시킬 수 있고 이중결합을 1 개 가지고 있는 PEGMA 를 섞어주면 flexible 하게 만들 수 있어 전도성을 좋게 만들 수 있다는 장점을 가지고 있다. 또한 이 PEO 젤은 Li-ion battery, DSSC 용 전해질, 올레핀 촉진수송 분리막 등 여러 고분자 전해질로 응용 할 수 있다. 이 PEGDMA 와 PEGMA, photoinitiator 로 2,2-Dimethoxy-2-phenyl-acetonphenone (DMPA)를 섞어 용액을 만든 후 352nm 의 UV 로 radiation 하여 막을 만든다. UV 를 radiation 한 시간, photoinitiator 의 양, PEGDMA 와 PEGMA 의 비율 등을 바꾸어 전해질을 제조해 이온 전도도에 미치는 영향을 연구한다.

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Cu-organic frameworks를 포함한 CO_2 촉진수송 분리막 연구.

최지영 원종옥* 김하영[1] 김영미[2] 이정현[3] 강용수[3]

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최근 대기중의 CO_2 양의 증가로 인하여 지구 온난화가 문제로 대두되고 있다. 이러한 문제로 인하여 CO_2 선택성을 가진 carrier 를 함유한 촉진수송 분리막을 제작하였다. 전이금속인 Copper 와 에스테르계열인 Disodium glutarate (glu)와 bis(4-pyridyl)기를 가진 1,2-bis(4-pyridyl)ethane (bpa), 4,4'-trimethylenedipyridine (bpp)를 이용하여 Cu-OF 를 합성하였다. 합성한 power 구조를 XRD 를 이용하여 crystal 형태의 Cu-OF 와의 구조를 비교하였고 Cu-OF 의 powder 사이즈를 조절하여 사이즈 효과를 확인하였다. Matrix 인 poly(2-ethyl-2-oxazoline) (POZ)와 섞어 Polysulfon support membrane 에 코팅하여 복합막을 제조하였다. Matrix 와 Cu-OF 와의 상호작용을 확인하기 위하여 분리막의 단면을 SEM 측정하였고, XRD 를 측정하여 bragg's low 를 이용해 d 값을 계산하여 비교해 보았다. Cu-OF 의 gas sorption 을 B.E.T 로 측정하고 흡착정도를 확인하고 분리막의 기체선택도를 측정하였다.

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Nafion112-poly(pyrrole) membrane에 대한 물성 연구

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Nafion?은 poly(tetra-fluoroethylene)의 골격에 술폰산기를 도입한 폴리머로서, Polymer Electrolyte Fuel Cell (PEFC)에 쓰이고 있는 대표적인 이온전도성을 가진 분리막이다. 이 분리막은 열적으로 안정되고 내약품성이 높으며 프로톤 전도성이 있으므로 고분자 전해질, 이온교환막으로서 이용된다. 여기에 경제적으로 저렴하고, 가공성과 열적 안정성이 뛰어난 poly(pyrrole)을 중합시킴으로써 프로톤 이동과 전자의 이동이 용이해진 분리막을 제조하였다.이 분리막을 제조하기 위해서 Du pont 사의 Na^+-form 인 Nafion112 막으로부터 H^+-form 의 Nafion 막을 얻어내기 위하여 과산화수소수와 황산을 이용하여 전처리 과정을 수행한다. 이 때 얻어진 H^+-form 의 Nafion112 막에 전기전도성 고분자인 poly(pyrrole)을 도입하여, 산화된 poly(pyrrole)의 양전하가 Nafion112 막의 설폰기를 카운터이온으로 받아들여 Nafion-poly(pyrrole) 분리막을 얻는다. 이렇게 새로 얻은 이온전도성과 전기전도성을 모두 가진 Nafion-poly(pyrrole) 분리막의 물리화학적 특성을 알아보기 위하여 TGA, FT-IR, 전기전도도를 측정하였다. 추가적으로 Nafion-poly(pyrrole) 분리막에 은나노입자를 도입하였을 때, 은나노입자가 기체투과도에 미치는 영향을 알아보았다.

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Preparation and synthesis of novel acceptor-donor-acceptor (A-D-A) type conjugated small molecules for organic photovoltaic (OPV) cells

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Photovoltaic devices generate useful electric energy from sun light through multiple steps of energy conversion processes. Among them, organic photovontaic (OPV) devices offer a cost-effective approach to future renewable energy sources. However, there are still problems to accomplish high power conversion efficiencies (PCE) in OPVs because of the incompatibility between the spectra of the organic materials used in active layer and the solar spectrum. To overcome this absorption limitation, synthesizing new low band gap materials is essential to improve PCE of organic solar cells. To this purpose, three low band gap molecules consist of triphenylamine dimer donor (D) unit and benzothiadiazole-based electron-accepting (A) unit alternative structure were newly designed and synthesized as a modified donor material for OPV cells.

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실리콘 기반의 봉지재를 이용한 백색 LED의 encapsulation 연구

김미리 김상훈 김진권[1,*] **PIAO LONGHAI**[*]

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LED 봉지재는 외부로부터 LED 칩을 보호하고 전기적으로 절연시켜주며 빛을 투과시켜 외부로 빛을 방출시키는 기능을 수행한다. 현재 LED 봉지재의 종류는 epoxy 와 silicon 두 가지가 있다. Epoxy 봉지재는 굴절률이 높고 가격이 저렴하다는 장점을 가지고 있지만, 자외선에 대한 내성이 낮고 고온에서 황변현상이 일어나 투과율이 저하되어 수명이 짧은 단점을 가지고 있다. Silicon 봉지재는 투명도가 좋고 자외선에 대한 내성이 강하며 열, 빛, 화학 물질에 대한 내구성이 높고 난연성이 우수하여 수명이 길다. 하지만 가격이 비싸고 굴절률이 낮은 단점이 있다. 본 연구에서는 고 굴절 투명 나노 입자, 실리콘 기반 봉지재, 황색 형광체를 사용하여 LED 칩을 봉지하였다. 우선 TiO2 의 표면개질을 통해 봉지재의 굴절률을 높였고, 점도의 조절을 통해 황색 형광체를 봉지재에 안정적으로 분산될 수 있도록 하였다. 후에 LED 칩에 봉지시키고 여러 가지 경화온도에서 봉지재를 경화시켰다. 봉지한 LED 의 광학적 특성을 연구하였다.

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Corrosion protection of nanostructured silver by ultrathin polymer coating

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Noble metals are subject to chemical attack in the nanometer regime. Representatively, silver, one of the noble metals, also features highly active surface in the nanometer regime. It is well known that silver nanoparticles function as the catalyst for various chemical reactions. However, the enhanced surface activities of silver nanoparticles make them prone to corrosive deterioration. Here, the corrosion behavior of silver nanoparticles coated with a conjugated polymer layer was investigated. Specifically, electrochemical corrosion and sulfur tarnishing behaviors were examined using potentiodynamic polarization and spectrophotometric analysis, respectively.

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Characterization of Nanostructures in Blend and Copolymer films depend on Annealing Condition

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Microphase separation is normally observed in block copolymer. As the annealing condition is controlled the morphology of polymer film is changed. In this study, dPS-b-PMMA was used to investigate microphase separation in copolymer film. Blending dPS and PMMA homopolymers were also used to compare their surface nanostructures. The AFM (Atomic Force Microscopy) results indicated the surface structure and thickness of the films depended on annealing condition and solution concentration. In order to figure out lateral structure TOF-SIMS (Time-Of-Flight Secondary Ion Mass Spectrometry) was used in the negative ion mode by a Cs^+ primary ion beam, TOF-SIMS depth profiles demonstrate variations in hydrogen, deuterium, carbon, oxygen, hydrocarbons and deuterated hydrocarbons within the block copolymer to the depth.

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Development of Bulk Heterojunction Photovoltaic Cells using Fluorinated Benzothiadiazole Derivatives

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Organic photovoltaic (OPV) cells have received significant attention, because the plastic based cells have possibility of realizing flexible, portable, and economic devices for alternative energy sources. However, OPV cell efficiency is considerably lower than that of inorganic-based devices, which is a big point of weakness for actual application. Therefore, the fluorine-substituted benzothiadiazole derivatives with effective electron accepting unit were newly designed and synthesized to give the sufficient low-band gap to enhance solar cell efficiencies. In this study, we report successful application of fluorine moieties to donor-acceptor type conjugated small molecule, with modified performance in bulk-heterojunction solar cells.

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White organic light-emitting diodes with two covalently bonded fluorescent molecules

김수연 박상혁*

공주대학교 화학과

White organic light emitting diode (WOLEs) has been intensively investigated because it can be applied to full color displays and future lighting sources. In order to realize full color OLEDs with high efficiency, it is required that the luminescent molecule has high emission efficiency and the device structure for fabrication process is simple. In this respect, fluorescent molecules featuring excited state intramolecular proton transfer (ESIPT) process are promising candidates for the emitting materials due to its characteristic large Stokes' shifted emission with no self-absorption. Here, we present a modified white-light-emitting molecule based on a ESIPT molecule and a strong blue fluorophore. Prepared molecule is composed of covalently linked blue- and yellow-light-emitting moieties between which energy transfer is limited, leading to the production of intense white luminescence in solid state.

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Real-time monitoring of DNA dissociation using carbon dot-gold nanoparticle-polyethyleneimine nanohybrids.

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포항공과대학교 화학과

Monitoring of polymeric carrier/plasmid (pDNA) dissociation inside cell is one of the most important mechanisms for gene delivery to design an efficient delivery vector rationally. Even though there are many reports about mechanism study such as cellular uptake and endosomal escape, the study on the dissociation of carrier/pDNA has not been reported thoroughly. Herein, we developed a novel carrier system which can monitor the dissociation of carrier/pDNA in real-time manner, and deliver the pDNA effectively. The carrier/pDNA dissociation was monitored using carbon dot (CD) which is receiving many attention for promising alternative of quantum dot (QD) since its excellent optical properties and biocompatibility. The fluorescence of CD is quenched by Au nanoparticle when they interact with non-labeled pDNA since CD and Au surface is modified with highly cationic polymer, polyethylenimine (PEI). When the pDNA was dissociated from carrier, the fluorescence of CD recovered and this fluorescence intensity changes enabled the monitoring of dissociation. In addition, this CD/Au carrier system showed not only great transfection efficiency but also high cell viability at the optimum condition which is the prerequisite of the effective gene delivery carrier.

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Templated Synthesis of Rattle-Typed Particles and Their Application as Nanophotocatalysts

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A novel protocol for the synthesis of core@shell particles with Ag or Au/Ag core structures has been introduced, and its use as a photocatalyst for decomposing toxic materials has been demonstrated. A monometallic Ag or bimetallic Au/Ag core was incorporated into the interior of SiO2 capsules via controlled heat treatment of the metal nanoparticle/SiO2-coated polymer particles. By appropriate treatment, it was possible to transform the Ag or Au/Ag core into the Ag@AgX or Au/Ag@AgX core within the SiO2 capsules (Ag@AgX@SiO2 or Au/Ag@AgX@SiO2). This novel method for core@shell particles is useful for incorporating AgX with plasmonic materials into the capsules materials. To the best of our knowledge, synthesis and use of core@shell-typed photocatalysts have not yet been reported. The Ag@AgX@SiO2 or Au/Ag@AgX@SiO2 photocatalysts showed excellent catalytic properties for the decomposition of toxic substances.

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Dual-scale light trapping structure for highly sensitive SERS substrates

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We fabricated dual-scale diamond-shaped gold nanostructures (d-DGNs) consisting of larger scale diamond-shaped gold nanoposts (DGNs) with smaller scale gold nanoparticles via interference lithography as a highly sensitive and efficient substrate for surface enhanced Raman scattering (SERS). The periodicity and size of DGN arrays leading to enhanced plasmonic fields and light trapping are optimized by changing the beam parameter of the laser and the reactive ion etching time. Our studies reveal that the synergistic effect of combination of light trapping substrate and small gold nanoparticles which increase the dipolar plasmon feasible for highly sensitive SERS substrates.

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Pseudocapacitor electrodes based on polyaniline nanostructures

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Owing to its excellent electrical properties, polyaniline (PANI) is considered to be one of the most promising conducting polymers for future applications. Here, we demonstrate that the anisotropic growth of PANI nanostructures with different aspect ratios in the presence of the stabilizer, poly(N-vinylpyrrolidone). We further examine what factors determine the device performance when PANI nanostructures are used as the electrode-active materials for supercapacitors. The electrochemical properties of PANI nanostructure electrodes were investigated in three-electrode and two-electrode configuration. Cylic voltammetry and charge-discharge tests were carried out to examine the performance of the nanomaterial electrodes.

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Mesoporous Surface Texturing on Titania Inverse Opal Structure for Photoanode

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Titania Inverse Opal (TIO) structures have been widely used for photoanode materials. However, large dimensions in a range of a few hundred nanometers decrease surface area for active sites. To increase the surface area, we applied surface texturing step utilizing self-assembly of block copolymer templates onto the process for the fabrication of TIO structures. Surface texturing provides TIO structure a dramatic improvement in light absorption bands, as well as increased surface area. Surface textured TIO (st-TIO) structures can improve the efficiency of many energy-related devices via the excellent photo-absorption achieved by light trapping effect and increased surface area.

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Synthesis, Characterization, and Photovoltaic Properties of New Benzo[1,2-b:4,5-b’']dithiophene-based Low Bandgap Polymers

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A series of low bandgap polymers (P1 and P2) composed of benzo[1,2-b:4,5-b’']dithiophene (BDT) and diketopyrrolopyrrole (DPP) derivatives were synthesized using a Stille coupling reaction for use in organic photovoltaic devices. Electron-donating alkylthiophene vinylene side groups were incorporated into the BDT units and branched long alkyl chains were introduced to the polymer chains to increase their solubility. The polymers were well soluble in common organic solvents, such as chloroform, chlorobenzene, etc. The UV-visible absorption maxima of the P1 and P2 thin films were at 698 nm and 775nm, respectively. Intramolecular charge transfer (ICT) interactions induced a low bandgap of the polymers. The highest occupied molecular orbital (HOMO) energy levels of P1 and P2 were calculated to be -5.43 and -5.41 eV. The LUMO levels of P1 and P2 were calculated to be -4.28 and -4.37 eV, as estimated from the optical band gaps and HOMO energy levels. The deep HOMO levels may contribute to improve oxidative stability and higher open-circuit voltage (Voc). The organic photovoltaic properties of the polymers will be studied.

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Synthesis and properties of a new azo benzene containing polymer for holographic storage materials.

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Azo benzene containing polymers have been studied on past years due to the light induced anistropic effect by optical isomerization of ‘cis↔trans’ characteristic on azo benzene functional groups. Especially, by using this light induced anistropic effect of azo benzene containing polymers, many possible applications as optical information storage medium have been studied. In this study, a new azo benzene containing polymer was synthesized by direct polymerization of using the epoxy-resin monomer. Synthesized polymer was successfully characterized by organic spectroscopic methods(NMR, IR, Uv-Vis, GPC). It is expected to have the possibility of holographic recording medium application.

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Synthesis, Characterization, and properties of Conducting polymer containing aromatic heterocyclic moiety.

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광운대학교 화학과

Substitution of various functional groups on heterocyclic compound is suggested as a method to modify and to improve the electrical properties and optical properties of heterocyclic compound. The new resulting polymers are soluble in organic solvents such as THF, $CHCl_3$ and DMF. The polymers are characterized by ^1H NMR, ^{13}C NMR and FT-IR. Optical properties of the polymers are measured by UV-vis spectroscopy, PL spectroscopy. Photoluminescence of the A polymer shows 390nm and B polymer shows 530nm in $CHCl_3$. These polymers will be applied to LED as emitting material.

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Synthesis and characterization of head-to-side connected photoresponsive main-chain liquid crystalline polymers

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A photochromic azobenzene moiety based head-to-side connected main-chain liquid crystalline (LC) polymer abbreviated as PLCP was newly synthesized via ADMET polymzerization. Utilizing the combined techniques of DSC, POM and 1D WAXD, it was realized that PLCP formed a nematic (N) phase below the isotropization temperature and the N phase turned to the glassy N phase below the glass transition temperature. By using light and/or heat, we successfully demonstrated the rewritable UV-patterned PLCP film as well as the mechanical deformation of the uniaxially oriented PLCP microfiber. Due to the wireless remote controllability of reversible actuating and patterning behaviors of PLCP polymer, PLCP can be applied as a key material in optoelectronic and bio-mimetic devices.

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Elongation Properties of Carbon nanotube reinforced polymer nanofibers : Residual Solvent and Crosslinking Effects

김한수 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Electrospinning is an effective technique to form non-woven fibers with average diameters in the range of micro- to nanometers using an electrostatic force from a polymer solution.This method provides physically well-defined polymeric nanofibers, and their structures and dimension are well studied. In contrast, due to their brittleness and fragility, their mechanical properties, as polymeric molecules are confined in nanometer-scale dimension, are difficult to determine. In particular, a hint of residual solvent in the fibers weakens their macroscopic properties, e.g. tensile modulus and yield strength, dramatically. Often the reported results are controversial and condition-dependent. Questions as to whether their mechanically hardened strengths are fundamental to their confined effects in nanoscale dimension, or whether residual solvents are effectively soften the polymer matrix, are not answered. We developed a motor-controlled setup, which can measure elongation modulus of electrospun nanofibers, and the mechanical properties have been compared before and after the thermal incubation. With this method, we will further present our expanded experiments, providing the reinforcement effects of nano-composite fibers, and cross-linking effects.

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Na로 중화된 폴리(메틸 메타크릴레이트-co-메타크릴 산) 아이오노머의 형태학 연구

고광환 김영민 김준섭[1,*]

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이번 연구에서는 Poly(Methyl Methacrylate-co-Methacrylic acid) (PMMA-co-MA)Na 아이오노머에 대한 알킬 사슬의 길이가 다른 지방족 다이카복시산 염의 효과에 대해 연구하였다. 폴리(메틸 메타크릴레이트-co-메타크릴산) P(MMA-co-MAA) 공중합체는 감압증류하여 정제된 단량체(메틸 메타크릴레이트와 메타크릴산)를 과산화 벤조일을 개시제로 사용하고, tetrahydrofuran(THF)을 용매로 사용하여 약 60 ℃에서 자유 라디칼 용액 공중합에 의해 만들었다. 반응시킨 고분자 용액을 과량의 메탄올에 떨어뜨려 침전을 시킨 후, 그 침전된 고분자를 거르고 약 100℃에서 진공, 건조시켰다. 형태학 연구를 위해 X-선 회절분석기(X-ray diffraction) Rigaku 사의 XRD(D/MAX-3C)를 사용하였고, 분석 조건은 Cu target(λ=1.5406 Å)으로 관 전압 35kV, 관 전류 15mA 였으며 주사 속도는 1°/min 로 2θ 값을 2~45° 범위에서 얻었다.

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Nanocapsules as active substance carriers by organic sol-gel methods

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Nanocapsules of covalent molecular network were synthesized using sol-gel transition inside their microemulsions accompanied with solvent diffusion. The diameter distribution of the capsules was controlled by addition of surfactants. The capsules were thermally stable and solvent-resistant. We studied loading of foreign organic substances or metal nanoparticles into the capsules by varying the synthesis parameters. The size, chemical and morphological structures of the capsule were also studied using dynamic light scattering, fourier-transform infrared spectroscopy, scanning electron microscopy and transmission electron microscopy.

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친환경 가소제를 첨가한 에틸 셀룰로우스의 기계적 성질 및 형태학

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이번 연구에 사용된 친환경 가소제는 폐 지방산 조리용 오일들(식물성과 동물성 오일)로 만들어졌으며, 이 친환경 가소제(PM-200)를 에틸 셀룰로우스에 첨가하여 기계적 성질과 형태학에 대해서 조사하였다. 기계적인 성질은 TA 사의 DMA(dynamic mechanical analyzer, Q800)를 사용하였으며, 형태학은 X-선 회절분석기(X-ray diffraction)는 Rigaku 사의 XRD(D/MAX-3C)를 사용하였고, 분석 조건은 Cu target(λ=1.5406 Å)으로 관 전압 35kV, 관 전류 15mA 였으며 주사 속도는 1°/min 로 2θ 값을 2~45° 범위에서 얻었다. 다양한 함량으로 PM-200 를 넣은 에틸 셀룰로우스의 저장 탄성율을 온도의 함수로 얻었으며, 에틸 셀룰로우스의 경우, 온도가 올라감에 따라 유리상에서부터 유리전이, 고무상, 흐름으로 모듈러스 커브를 보여주었다. 모듈러스가 커브가 떨어지기 시작하는 점이 PM-200 의 양이 증가함에 따라 낮은 온도쪽으로 이동하며, 기울기가 점점 더 급격해진다.

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다양한 양이온으로 중화된 폴리스타이렌 메타크릴레이트 아이오노머의 입도 분석

박혜련 장대현[1] 이범규 김준섭[2,*]

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용액 상태에 있는 폴리(스타이렌-co-메타크릴레이트) (PSMA) 아이오노머의 다양한 상호작용과 거대 분자의 고조 사이의 관계를 이해하기 위해 입자의 크기와 분포에 대해 동적 광 산란법을 이용해 조사하였다. Na 로 중화된 PSMANa 아이오노머의 이온기 농도를 3.6, 5.5, 9.6 mol%로 달리하여 dimethylformaide(DMF)에 고분자를 녹이고 입자의 크기와 분포를 측정하였다. 3.6 mol%의 이온기를 가지고 있는 PSMA 공중합체가 만드는 입자 크기 분포를 입자의 지름에 대한 함수로 얻었으며, 2.0 x 10-2 g/mL 농도의 용액에서 얻은 피크 최고점은 입자 크기가 12 nm 에서 관찰되었다. 2.0 x 10-3 g/mL 농도의 용액에서 입자 크기는 17 nm 로 피크의 최고점 위치가 이동한다.

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Developing single-planar digital microfluidics devices based on electrowetting

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Digital microfluidic (DMF) devices being able to control a group of submicro drops of liquid actuated by electrowetting are expected to be used to alternate biological or chemical experimental tools which have been currently equipped with bulky instruments, since for DMF devices there are certain advantages such as faster mixing and easier access to the digitalized drops. In this reason, DMF should become a next popular tool for lab-on-a-chip applications. While in most studies of DMF, the double-plate (closed) devices are conventionally adopted by many researchers, the single-plate (open) devices are a little studied, mainly because unexpectedly the digitalized drops of samples are not well actuated on a single plate. In this study, by applying an oil coating method to reduce the surface tension, we developed a novel open device that was successfully enabled to manipulate smoothly the various actuations of digital drops such as translational motion, merging and oscillation. This open DMF device should be usefully utilized, if properly integrated in the specific patterned electrodes for electrowetting control, for bio-, chemical- and medical liquid samples, likewise the electronic integrated chips. In the further work, we will perform to analyze various bio-samples on our newly developed planar DMFs.

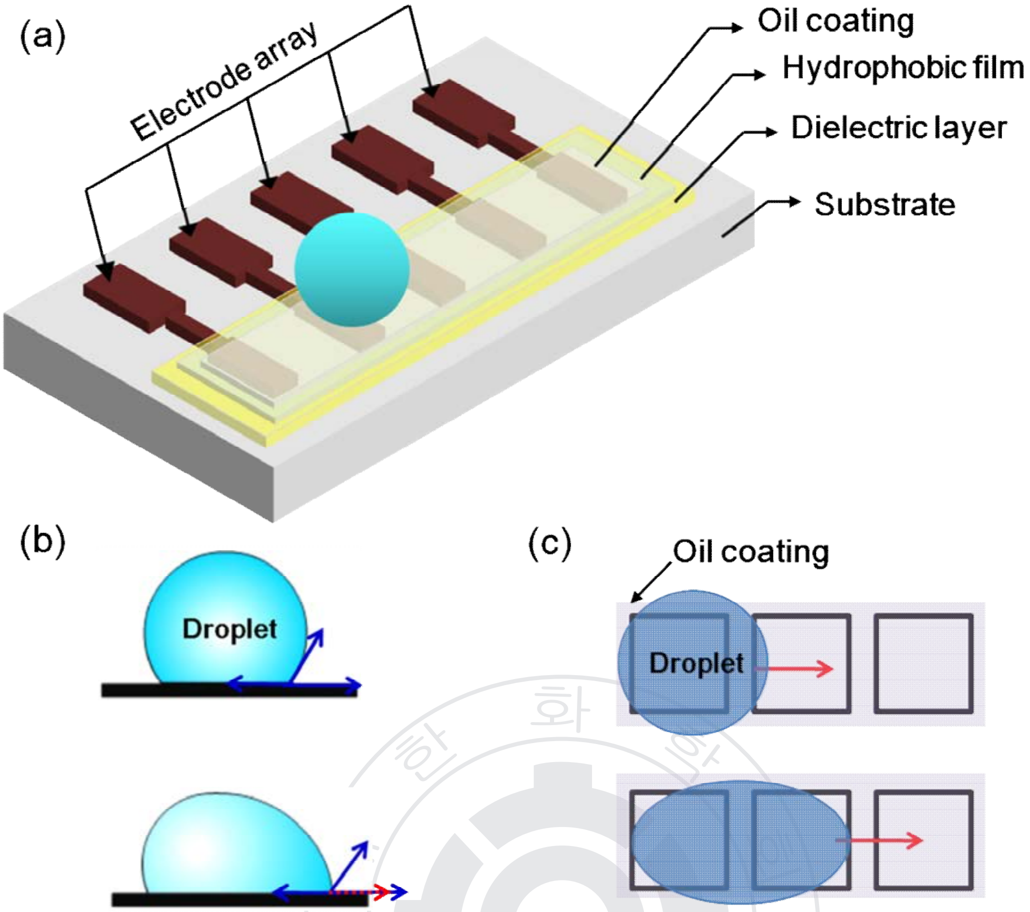

Figure 1. (a) schematic of the proposed single plate digital microfluidic device, (b) cross-sectional view of the device, (c) top view of the device

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Crown ether를 첨가한 Na로 중화된 스타이렌계 아이오노머의 회합 거동

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스타이렌계 아이오노모인 poly(styrene-co-styrenesunfonate) (PSSA)Na 와 poly(styrene-co-methacrylic acid) (PSMA)Na 에 crown ether(15-crown-5)를 첨가하여 동적 광산란을 이용하여 입자의 크기와 분포에 대해서 조사하였다. PSSA 는 Makowski 등의 방법을 이용해 술폰화 반응을 통해 얻었다. 공중합 시킨 용액을 메탄올에 떨어뜨려 침전 시킨 후, 침전 고분자를 거르고 약 100 ℃에서 진공?건조 시켰다. 중합시킨 고분자들의 산 농도(mol %)를 알아보기 위하여 일정량의 고분자 시료를 벤젠/메탄올 (9/1 v/v) 용액에 녹인 후 페놀프탈레인 지시약을 사용하여 0.05 N NaOH/메탄올 용액으로 적정하였다. 이때 적정된 PSSA 의 산 농도는 6.75 mol % 였다.

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Construction of Striped Fullerene Patterns in a Cholesteric Liquid Crystal Medium

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Fullerene-based molecule (C60RM) exhibiting a good chemical affinity to various organic compounds was newly synthesized. The large temperature dependence of C60RM solubility in a nematic liquid crystal (LC) provides us a great opportunity for studying the self-assembly and consequent pattern-formation of C60RM in an elastically anisotropic LC medium. We successfully demonstrated the striped pattern formation of the C60RM particles in the cholesteric fingerprint state. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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Surface-induced phase transition behaviors of the rod-disc liquid crystal

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Surface-induced phase transition behaviors of a rod-disc (cyanobiphenyl-triphenyl) liquid crystalline (LC) molecule (RD12) were researched by changing the surface chemistry and the physical interactions. Upon varying the width of the LC cells and their surface chemical and physical states, the RD12 phase transition behavior was rapidly changed. The nematic (N) phase of RD12 in the LC cell with a low cell gap and polyimide (PI) rubbed surface could be preserved and the crystallization of RD12 was completely suppressed. Based on the systematic experimental investigations, it was concluded that the glassy N phase was formed due to the fact that the surface anchoring force is bigger than the crystallization force. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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Macroscopically oriented Chromonic electrospun nanofiber containing the self-assembled nanocolumns

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A macroscopically oriented chromonic electrospun nanofiber with the self-assembled Sunset-Yellow FCF (H-SSY) was fabricated by the combination of electrospinning and self-assembling techniques. Based on the thermal, scattering and microscopic analyses, it was realized that H-SSY formed a glassy columnar nematic (N) phase in the PVP/H-SSY nanofiber. Utilizing the 2D WAXD and polarized FTIR results, it was realized that the nanocolumns were aligned parallel to the long axis of the nanofiber. The anisotropically oriented PVP-H-SSY nanofiber mats embedding the self-assembled nanocolumns may open new doors for the practical applications in electro-optical devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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Robust Thin Film Polarizer Fabricated from Chromonic Liquid Crystals

박민욱

전북대학교 고분자나노공학과

A robust chromonic liquid crystal (CLC) thin film polarizer was fabricated by the self-assembly of lyotropic CLCs and the photo-polymerizing processes. Their optical behaviors and molecular packing structures were investigated from using the combined techniques of microscopy, scattering and spectroscopy. To stabilize the oriented Sunset Yellow FCF (H-SY) films and to minimize the possible defects generated during and after the coating, acrylic acid was added and photo-polymerized. The polymer-stabilized H-SY films showed good mechanical and chemical stabilities without sacrificing a high polarizability. Additionally, patterned polarizers were fabricated by applying a photomask during the photo-polymerization of AA, which may open new doors for the practical applications in electro-optic devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2012K001428) of Korean government.

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One-step glass-like coating on a thermoplastic surface for microscale organic reaction

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In this study, we present a simple method to fabricate an extremely resistant coating layer inside a microchannel using bis(triethoxysilylpropyl)amine, fabricated on a polycarbonate (PC), to obtain a glass-like layer on the PC surface under room temperature condition. We examine the effect of the concentration of the bis(triethoxysilylpropyl)amine solution, curing temperature, and curing time. To confirm successful coating of the microchannel, we examine the resistance of the coated PC microchannel to several organic solvents such as toluene, ethanol, and tetrahydrofuran. As a practical application, we explore the feasibility of the coated microchannel for organic synthesis to realize faster reaction in highly cost-effective manner.

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Ethanol based thermoplastic bonding assisted by UV curing for rapid microdevice assembly

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In this study, we introduce a rapid strategy for the assembly of thermoplastic microdevice employing ethanolic solution followed by UV photocuring under ambient condition. Poly(methylmethacrylate) (PMMA) substrate was used for thermoplastic substrate for its wide applicability. To achieve robust sealing, two PMMA substrates were contacted with each other immediately after the treatment with ethanolic solution, and were illuminated under UV. Permanent sealing was realized within 1 min. Various bonding analyses were conducted by performing tensile strength measurement, high-throughput leakage test, burst test, and peel test. The highest bond strength was determined to be approximately 6.17 MPa when 90% ethanolic solution was employed, and the bonding was sufficiently robust to endure intense introduction of liquid sample whose per-minute injection volume was almost 1,200-fold higher than the total internal volume of the microchannel fabricated.

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Gene Delivery Vector using Self-Assembled Dendron-Cyclodextrin Nanotubes

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본 연구팀에서는 focal point 에 pyrene 을 도입한 amphiphilic amide dendron (2G-Py)이 수용액상에서 vesicle 형태로 self-assembly 되었다가 β-cyclodextrin(β-CD)과 inclusion complex 를 형성하게 함으로써 표면이 β-CD 로 덮여진 나노튜브로 self-assembly 되는 현상을 규명한 바 있다. 또한 나노튜브 표면에 있는 CD 의 C6 위치의 -OH 그룹을 원하는 다양한 작용기로 치환하여 다양한 기능을 갖는 나노튜브를 만들 수 있다는 것도 규명하였다. 본 연구에서는 위의 나노튜브를 이용하여 gene delivery 에 응용하고자 negative charge 를 갖는 gene 과 charge-charge interaction 을 할 수 있도록 positive charge 를 띄는 물질을 나노튜브 표면에 도입하였다. 또한 cell 에 잘 adhesion 되고 들어갈 수 있도록 arginine group 을 도입하고, 나노튜브의 dispersion stability 를 증가시키기 위하여 PEG 를 표면에 도입하였다. 이렇게 만들어진 나노튜브는 SEM, TEM 등으로 그 구조를 확인하였다. 또한, gene delivery vector 로 사용할 수 있는지 알아보기위하여 gel retardation test 를 진행하였고, transfection 이 일어나는 것을 in vitro 실험을 통해 확인하였다.

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Mesoporous Silica Nanocarriers with Stimuli-Responsive Peptide Gatekeepers for Controlled Guest Release

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본 연구에서는 MCM-41 타입의 실리카 나노입자 (SiNP, 직경 60 nm, pore 2 nm)의 pore 입구에 생체자극에 감응하는 peptide 를 gatekeeper 로 장착하여, 생체자극에 의해 guest 분자의 방출을 조절할 수 있는 delivery carrier 를 제조하였다. 본 연구에서 사용된 peptide gatekeeper 는 장시간동안 실리카 pore 에 loading 되어있는 약물의 release 를 억제할 수 있으며, peptide 의 길이에 따라 loading 되어있는 약물의 release 시간을 조절할 수 있음을 확인하였다. 또한, 특정한 생체자극에 의해 peptide gatekeeper 가 분해되어 loading 되어있는 약물을 선택적으로 release 시킬 수 있음을 확인하였다. 본 연구의 결과를 이용하여 다양한 생체자극에 감응하여 약물을 효율적으로 target site 에 전달하는 실리카 나노입자 제조를 가능하게 할 것으로 기대된다. SiNP 및 peptide 의 구조와 guest 분자의 조절방출 특성은 FTIR, HPLC, LC/MS, BET, TEM, SEM, fluorescence spectrum 등으로 규명하였다.

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Complex Formation of Amide Dendrons with Nucleic Acids and Their Transfection Efficacy

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본 연구팀에서는 amide dendron 을 이용하여 조건에 따라 다양한 형태의 self-assembled structure 를 갖는 것을 확인한 바 있다. 본 연구에서는 이러한 dendron 의 자기조립특성을 이용하여 gene delivery vector 로 사용하고자 한다. 이를 위하여 negative charge 를 띄는 gene 과 charge-charge interaction 을 통한 complex 를 효과적으로 형성하도록 덴드론의 focal point 에 positive charge 를 띄는 작용기를 도입하였다. 이렇게 합성된 덴드론의 자기조립특성을 TEM 과 SEM 을 통해 확인하였으며, 덴드론과 gene 의 효과적인 complex 형성을 gel retardation test 와 zeta potential 을 통해 확인하였다. 또한, 덴드론의 focal point 에 도입된 작용기의 종류에 따른 complex 의 형성능력과 transfection efficiency 의 변화를 규명하였다.

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Facile loading of Cu+ species over porous metal-organic frameworks (MOFs) and adsorptive desulfurization with Cu+-loaded MOFs

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경북대학교 화학과

Metal-organic frameworks (MOFs, MIL-100-Fe, iron-benzenetricarboxylate) supported with Cu+ species were obtained firstly under mild condition without high temperature calcinations. The Cu+-loaded MOFs were evaluated as efficient adsorbents for the liquid-phase adsorption of benzothiophene (BT). The effect of Cu+ loading on the adsorption kinetics and maximum adsorption capacity (Q0) for the adsorption of BT was also studied. Q0 increased with increasing copper loading up to a Cu/Fe (wt./wt.) ratio of 0.07 in Cu+-loaded-MIL-100-Fe, resulting in an increase in the Q0 by 14% compared with the virgin MIL-100-Fe without Cu+ ions. Since the surface area and pore volume decrease with the loading of copper, the increased Q0 over the Cu+-loaded MIL-100-Fe adsorbents suggests specific favorable interactions, probably by π-complexation, between Cu+ and BT.

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Fabrication of Robust Superhydrophobic Mg Surface Using Functional Molecules

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Superhydrophobic surface has become a very popular field in academic and industrial field. Superhydrophobic surfaces, such as the leaves of the lotus plant, are extremely difficult to wet and has self cleaning property. Superhydrophobic properties with a water contact angle(≥150°) and a slide angle(≤10 °) is believed to be regulated by a low surface energy material and a surface geometrical nano- and microstructure. The prepared superhydrophobic surfaces have contain limitations, such as long term and poor durability. Therefore it is required to develop a method to fabricate stable and robust supterhydrophobic surfaces. We report on a synthesis of polyacrylated triphenylene derivative and its application for fabricating a superhydrophobic surface. The coating solution was prepared by mixing polyacrylated triphenyl derivative, nano-sized silica, and photoinitiator in MC. After the plate was dried and UV cured. The surface morphology of the sample was analyzed using FE-SEM, XPS, and water contact angle was measured.

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Effect of acidity and basicity of metal-organic frameworks (MOFs) on adsorptive denitrogenation of model fuels

imteaz ahmed 정성화[*]

경북대학교 화학과

A metal-organic framework (MIL-100(Cr)) was modified to impart acidity or basicity to understand the effect of the acidity or basicity of MOFs on the adsorptive removal of nitrogen-containing compounds (NCCs) [1]. The modification was done by grafting ethylenediamine and aminomethanesulfonic acid onto coordinatively unsaturated sites of the MOF, MIL-100(Cr). The adsorptive removal of a basic quinoline or benzothiophene can be improved noticeably, especially at low concentrations, with the introduction of an acidic site; however, a basic MOF causes a severe decrease in the adsorptive performance for a basic adsorbate such as quinoline. The effect of the interaction of the base?base on adsorption was more severe or detrimental for a hard base quinoline than for a soft base benzothiophene. Functionalized MOFs show a slightly decreased adsorption for a neutral adsorbate such as indole probably because of the decreased porosity of the MOFs compared with the virgin MOF without functionalization. Moreover, a functionalized MOF (with -SO3H group) can be used several times after simple washing with acetone. It may be concluded that, the NCCs can be favorably removed by acid?base interactions between NCCs and MOFs [1, 2].References1.I. Ahmed, Z. Hasan, N.A. Khan and S. H. Jhung, Appl. Catal. B 129 (2013) 123-1292.I. Ahmed, N.A. Khan, Z. Hasan and S. H. Jhung, J. Hazard Mater http://dx.doi.org/10.1016/j.jhazmat.2013.01.024

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의료용 렌즈 고분자의 물성에 미치는 difluoropyridine의 영향

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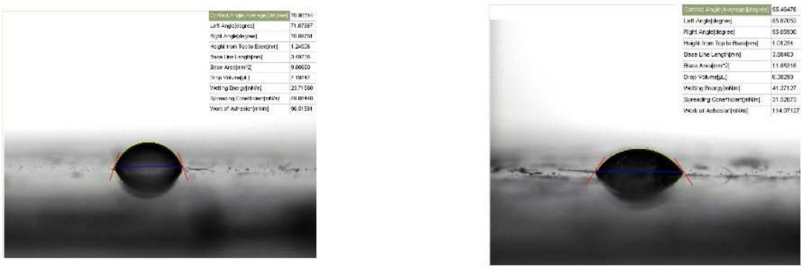
기능성이 첨가된 안 의료용 렌즈 재료의 중합을 위해 2,6-difluoropyridine 을 첨가제로 사용하여 HEMA(2-hydroxyethyl methacrylate), MMA(Methy methacrylate) 및 AA(Acrylic acid)와 교차결합제인 EGDMA(ethylene glycol dimethacrylate) 그리고 개시제인 AIBN(azovisisobutyronitrile)을 사용하여 공중합 하였다. 생성된 고분자는 무색 투명한 색을 나타내었으며, SEM 분석 결과, 전반적으로 매끄러운 표면을 유지하였다. 생성된 고분자의 물리적 특성을 측정한 결과, 굴절률 1.4350~1.4358, 함수율 37.26~36.89% 및 가시광선 투과율은 90.6~91.6%를 나타내었다. 또한, 자외선 영역의 투과율은 UV-A 87.8~87.2%, UV-B 82.0~80.8% 로 각각 나타났다. 접촉각의 경우 73.45~54.28 로 측정되어 2,6-difluoropyridine 의 비율이 증가 할수록 렌즈의 표면 습윤성이 향상되어 접촉각이 낮아지는 경향을 보였다.[Fig. 1.] 본 실험 결과를 통해 2,6-difluoropyridine 을 첨가한 콘택트렌즈는 기본적인 콘택트렌즈의 물성을 만족하였으며, 습윤성이 높은 렌즈의 재료로 사용될 수 있을 것으로 판단된다.



Contact Angle(Average)[degree]	70.98514
Left Angle[degree]	71.07567
Right Angle[degree]	70.89761
Height from Top to Base[mm]	1.24936
Base Line Length[mm]	3.49736
Base Area[mm^2]	9.60650
Drop Volume[μL]	7.19547
Wetting Energy[mN/m]	23.71590
Spreading Coefficient[mN/m]	49.08440
Work of Adhesion[mN/m]	96.61581

Contact Angle(Average)[degree]	55.46476
Left Angle[degree]	55.87052
Right Angle[degree]	55.05900
Height from Top to Base[mm]	1.01294
Base Line Length[mm]	3.88463
Base Area[mm^2]	11.85318
Drop Volume[μL]	6.38290
Wetting Energy[mN/m]	41.27127
Spreading Coefficient[mN/m]	31.52073
Work of Adhesion[mN/m]	114.07127

(a) Ref. (2,6-difluoropyridine 0%)　　(b) Sample A. (2,6-difluoropyridine 10%)

Fig. 1. Contact angle of samples
[(a): Ref. (2,6-difluoropyridine 0%)　(b) Sample A. (2,6-difluoropyridine 10%)]

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One Step Process for Fabrication of Superhydrophobic Surface by Immersion Method

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Younga Kim, Kyuchul Lee, Yonghyun Ahn*
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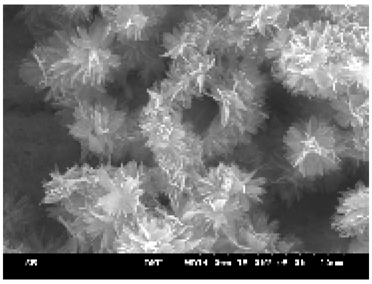
The superhydrophobicity of solid material is a key factor in industrial field. The chemical composition and nano structure of the surface are important factors for determining the property of surface. The fabrication of superhydrophobic surfaces have been required two factors. The one is to create a nano structure on the surface and the other is to coat with low surface energy material. We fabricate a superhydrophobic flower-like micro-rough surface in one step by dipping Mg plates into the solution of fluorinated alkyl silane and alkyl phosphonic acid in ethanol. Prepared rough surface morphology is like flower and the degree of roughness can be controlled by the dipping time and concentration of alkyl phosphonic acid.



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Copolymerization and ophthalmic application of poly(HEMA-co-MMA) in the presence of chloroaniline group

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HEMA, MMA, NVP, EDGMA were copolymerized with 2-, 3- and 4-chloroaniline for ophthalmic application. The physical, optical, and surface characteristics of the hydrogel ophthalmic lens copolymers were investigated to examine the usefulness as components for ophthalmic hydrogel contact lenses. The water contents and the refractive index were in the range of 34.84~36.59% and 1.434~1.441, respectively. Meanwhile, the surface wettability, contact angle ranging from 56.0 to 73.8 ° increased with increasing the addition ratio of chloroaniline. In case of 2-CA and 3-CA combination, the transmittance for UV-B was 18.8% and 11.2%, respectively. The spectral transmittance of 4-CA sample for UV-B was 3.8%, showing that the UV-B transmittance is generally very low. The polymeric materials satisfied the basic characteristics required for ophthalmic contact lenses. The polymers have excellent UV-block effect, indicating that the material can be used to fabricate high performance hydrogel ophthalmic lenses with UV blocking effect.

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Study on the adsorbent-adsorbate interactions from Cd(II) and Pb(II) adsorption on activated carbon and activated carbon fiber

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The adsorption characteristics of Cd(II) and Pb(II) in aqueous solution using granular activated carbon (GAC), activated carbon fiber (ACF), modified ACF (NaACF), and mixture of GAC and NaACF (GAC/NaACF) has been studied. The surface properties, such as morphology, surface functional group, and composition of various adsorbents were determined by using X-ray photoelectron spectroscopy (XPS) and scanning electron micrograph (SEM) measurements. The specific surface are, total pore volume, and pore size distribution were investigated by using nitrogen adsorption, Brunauer-Emmett-Teller (BET), and Barrett-Joyner-Halenda (BJH) methods. In this study, the NaACF showed high adsorption capacity and adsorption rate for the heavy metal ions, due to the improved ion-exchange capabilities by more oxygen functional groups. Moreover, the mixture of GAC and NaACF was used as adsorbent and determined the interaction of adsorbent-adsorbate in competitive two adsorbents.

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Low cost carbon fiber with multi-functions through melt-spinning of residual oil/lignin blends

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Carbon fiber is one of the most important materials to develop the eco-friendly society, to apply light weight vehicles and effective adsorbent materials. The low cost is the most important factor to expand applications. We prepared lignin-based carbon fibers (CFs) with average diameter 20 μm from melt spinning of the blends of hardwood lignin and pyrolyzed fuel oil (PFO), byproduct of naphtha cracking process (NCC). The lignin contains oxygen functional groups and the PFO does hydrocarbons of aromaticity of 0.7. The CFs spun from the miscible blend and carbonized at 800℃showed smooth surfaces with a maximum tensile strength of 1.1 GPa and a modulus of 82 GPa at 1.35% stain. The carbon fibers have 7wt% oxygen which would contribute to adsorb toxic gases with polar groups, such as formaldehyde and amine containing chemicals with fragrance. The CFs have strong potential to apply to reinforce material for carbon fiber composite and adsorbent of toxic gases at low cost.

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Visible light-induced photocatalytic activity of Ag-containing TiO_2/carbonnanofibers composites.

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In the present work, Ag-loaded TiO_2/carbon nanofiber (CNF) catalysts were prepared to study their improved photocatalytic efficiency in the visible spectrum. CNFs were chosen as a support for the TiO_2 catalyst because of their large specific surface area, pore volume, uniform microporosity, and high adsorption/desorption rates. By enhancing the photocatalytic activity of the TiO_2/CNF composites with Ag nanoparticles, the current study aims to: (i) extend the light absorption spectrum into the visible region, (ii) reduce the electron/hole pair recombination and (iii) enhance the contact time of the photocatalysts with organic pollutants, which increases the reaction efficiency as a result of the high specific surface area of the micropores. The reduction of methylene blue (MB) adsorption in an aqueous solution by the photocatalysts occurred due to the combined effects of MB adsorption in the pores of CNFs and decomposition by the photocatalysts throughout the process. The Ag-TiO_2/CNF photocatalyst degraded MB 17 times faster than the TiO_2/CNF composites with no Ag nanoparticles after 3 h under visible light illuminations.

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Thermal Si-C Coupling Reaction of Allyl Chloride with Trichlorosilane and Their Mechanistic Aspects

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Thermal Si-C coupling reaction of allyl chloride with trichlorosilane was studied without catalyst at temperatures ranging from 150 to 250℃. In this reaction, the organosilicon compounds are formed from the dehydrochlorination reaction and hydrosilylation reaction. In particular, 3-chloropropyltrichlorosilane of hydrosilylation reaction products and allyltrichlorosilane of the dehydrochlorination reaction products were obtained mainly. Except for two substances, 1,3-bis(trichlorosilyl)propane was obtained by the hydrosilylation reaction of allyltrichlorosilane. 3-chloropropyltrichlorosilane and allyltrichlorosilane compounds were competitively obtained each other in competition reaction. When the temperature is low, the 3-chloropropyltrichlorosilane were mainly produced and when the temperature is high, the allyltrichlorosilane were mainly produced. And 1,3-bis(trichlorosilyl)propane was produced through continuous hydrosilylation reactions. Compounds was analyzed by GC and GC/MSD, 1H NMR, 13C NMR, DEPT-135 NMR, 29Si NMR and FT-IR. Thermal reaction of allyl chloride with trichlorosilane gives complex products because of the above-mentioned two reactions occur competitively.In order to investigate the reaction mechanism, we calculated the energy of the unstable intermediates using the Gaussian program. Dissociation energy of trichlorosilane when decomposed the radical or ion was calculated at 298.2K. Gibbs free energy of ions and radicals are 273.77kcal/mol and 143.21kcal/mol, respectively. This energy is too high and can not happen in the experimental conditions of this paper. Gibbs Free Energy of the transition state in a reaction that produces 3a is 64.28kcal/mol. 3a is 4 membered ring transition state with Si-H and C-C double bond. And the Gibbs Free Energy of 3-chloropropyltrichlorosilane is -18.87kcal/mol. And Gibbs Free Energy of the transition state in a reaction that produces 4a is 59.75kcal/mol and the Gibbs Free Energy of allyltrichlorosilane is -13.73kcal/mol. It is considerably higher that 3-chloropropyltrichlorosilane and allyltrichlorosilane to produce the transition

state of the Gibbs free energy is 50-60kcal/mol range. Therefore, it was confirmed that the thermal reaction may occur at temperatures higher than 200℃. From this calculation, it was confirmed that the Gibbs free energy of 3-chloropropyltrichlorosilane is relatively lower and more stable.As a result of this thermal reaction, it was confirmed that hydrosilylation better than dehaloganation reaction took place.

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

Purification of PABA from synthesis in the MFB and MFB from industrial waste to available high-value green resources.

정효진 김경덕 **Dagvajantsan Oyunerd** 유영 김석찬 박규순

국민대학교 화학과

p-Xylene 을 산화시켜 DMT 를 얻는 과정에서 생기는 부산물인 MFB 혼합물을 MFB, DMT 로 분리 정제하기 위하여 acetal 반응을 이용하여 순도 높은 MFB 를 얻고 화장품에 많이 사용되는 PABA 로의 합성 후 정제를 하였다.

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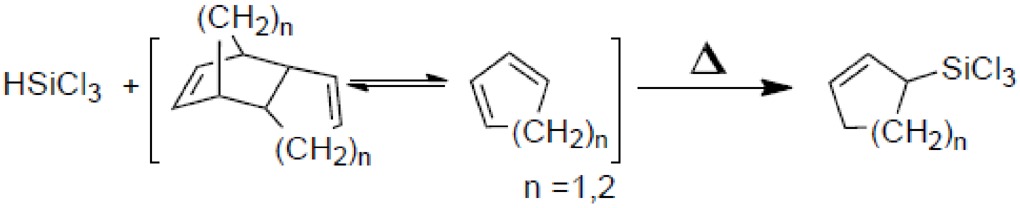
발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal reaction of cyclic alkadiene with trichlorosilane

정동의 한준수[1] 유복렬[1,*] 이광렬[2]

고려대학교 [1]한국과학기술연구원(KIST) 물질구조제어연구단 [2]고려대학교 화학과

The thermal hydrosilylation1-3 of trichlorosilane (1a) with cyclic alkadienes such as cyclopentadiene (2a), 1,3-cyclohexadiene (2b), and 1,4-cyclohexadiene (2c) were studied at temperatures ranging from 170 °C to 250 °C. In this reaction, the hydrosilylation rate increased as the reaction temperature was raised using an equimolar ratio of 1a to 2a. The reaction of 2a with 1a at 250 °C afforded 2-cyclopentenyltrichlorosilane (3a) as the major hydrosilylation product within 1 h in good yield (82%). This reaction also works when dicyclopentadiene (2a′) was used as a reactant instead of 2a. In a large scale preparation under the same conditions, 3a was obtained in 82% isolated yield. It is significant to note that 2a′ can be used for the hydrosilylation, with no requirement of a cracking step under our thermal conditions. While the reaction of cyclohexadienes with 1a under the same conditions gave a mixture of three hydrosilylation products such as 2-cyclohexenyltrichlorosilane (3b), 3-cyclohexenyltrichlorosilane (3c) and cyclohexyltrichlorosilane (5) in moderate yields, along with other unsaturated C6 components, such as benzene and cyclohexene. In the thermal reaction of cycloalkadienes with 1a, the five-membered-ring diene 2a undergoes both a hydrosilylation reaction with 1a as well as a [4+2] cycloaddition reaction, leading to the hydrosilylation product 3a in good yield. While the six-membered ring dienes, 2b and 2c, undergo four different types of reactions, including hydrosilylation, [4+2] cycloaddition, dehydrogenation, and hydrogenation in competition to give the hydrosilylation products, hexane, and benzene, respectively. The reaction rates of cyclic alkadienes under our thermal conditions increase in the following order: 2c << 2b < 2a.


HSiCl3
+
(CH2)n
(CH2)n
(CH2)n
n =1,2
Δ
SiCl3
(CH2)n

일시: 2013년 4월 17~19일(수~금) 3일간
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발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Mesophase Pitch Synthesis from FCC-DO and Carbon Fiber Preparation

이동훈 양갑승[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 고분자 섬유 시스템공학과

Pitch precursors for carbon fibers were synthesized from fluidized catalytic cracking-decant oils (FCC-DO) in the absence of catalyst. The FCC-DO was hydrogenated in the presence of tetrahydronaphthalene (THN) at elevated pressure and temperature, and then prepared carbon fibers from them. The hydrogenation reduced the viscosity of FCC-DO from 5243.0 to 483.7cP and the elemental analysis of C/H mol% of 0.98 of FCC-DO to 0.95 of hydrogenated FCC-DO. On the other hand, the aromaticity of FCC-DO increased from 0.69 to 0.90 by the hydrogenation i.e., the aromatic components stacked together became soluble in the NMR sample. The synthesized pitch showed18.3% yield on the basis of the FCC-DO and the softening point was 298.3℃. The precursor pitch was melt-spun through a circular nozzle by pressurized N_2, stabilized at 300℃, carbonized at 800℃ and finally graphitized at 2800℃. The graphitized fiber exhibited anisotropic morphological structures in cross section of the fibers.

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

Conventient Synthesis and Characterization of Antibacterial Silver Nanoparticle/Bis(*o*-phenolpropyl)silicone Composites

박재영 정현숙* 노지은[1] 우희권[1,*]

조선대학교 생명공학과 [1]전남대학교 화학과

The ready synthesis and analysis of antibacterial silver nanoparticle/bis(*o*-phenolpropyl)silicone composites have been performed. The one-pot reduction of Ag(+) salts to stable Ag(0) nanoparticles is promoted by bis(*o*-phenolpropyl)silicone [(*o*-phenolpropyl)$_2$(SiMe$_2$O)$_n$, n = 2, 3, 8, 236], polysiloxanes possessing reductive phenolic O-H bonds as end group. The transformation was accelerated by $HAuCl_4$. XRD, TEM, FE-SEM, and solid-state UV-vis analytical tools were employed to characterize the polymer nanocomposites. TEM and FE-SEM data display the formation of hybrid composites in which large numbers of spherical silver nanoparticles are dispersed throughout the silicone matrix. The size of silver nanoparticles is in the range of 10- 20 nm. XRD patterns are consistent with that for multicrystalline silver. However, in the absence of the bis(*o*-phenolpropyl)silicone, most of the silver particles undergo macroscopic coagulation, suggesting that the alcoholic silicone moieties are essential for stabilizing the metal nanoparticles.References[1] Roh, S.-H.; Lee, J.; Woo, H.-G. Advances in Organometallic Chemistry, in press.[2] Kim, B.-H.; Woo, H.-G. *Gelest Catalog*, Gelest: New Jersey, 2008; 50-57.[3] Kim, M.-H.; Woo, H.-G.; Lee, B.-G.; Kim, D.-H.; Yang, K.-S.; Kim, B.-H.; Park, Y.-J.; Ko, Y. C.; Roh, S.-H.; Sohn, H. Journal of Nanoscience and Nanotechnology 2011, *11(2)*, 1593 ? 1596.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

The development of environmental friendly biodegradable detergent

김아나 유영 김석찬

국민대학교 화학과

Useful organic solvent in the fine chemical industry causes acute symptoms such as headache, vomiting, dizziness, and shortness of breath and chronic poisoning symptoms such as memory loss, kidney disease and muscle spams. As above, organic solvents is truly needed in the fine chemical industry, but has a devastating impact on our health. In order to solve these problems, developed countries have already been developing of low toxicity and biodegradable solvents to replace conventional cleaners. Diester, Acetate, Propionates, Glycolates Lactate esters and Fatty acid esters are the typical low-toxicity solvents. The feature of these solvents are like these : they can replace aromatic and aliphatic solvent, reduce or remove non-volatile organic compounds, easily biodegradable and reduce the toxicity. But it is hard to find domestic eco-solvent, widely use alternative materials developed in foreign countries.

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

Colored Surface Finishing through Intercalation of Basic Dyes into Ion Exchangeable Silicates

<u>임종헌</u> 김태욱[1] 한양수[2,*]

딜라이트오브서피스앤컬러 품질 [1]딜라이트오브서피스앤컬러 총괄 [2](주)나노스페이스

A new color coating method on the basis of intercalation of cationic dye molecules into layer silicate was reported for the first time. At first, a water-borne type coating formulation containing layer silicate (synthetic hectorite) was prepared by mixing polyurethane and melamine resins along with the water-dispersed silicate dispersion. Such prepared primary coating solution was coated on various substrates by dipping or spray coating method, followed by drying at around ~ 100 ℃. Thermally cured primer coated specimen was then simply dipped into dye solutions from a few seconds to a few minute to intercalate dye molecules into layer silicates. After washing with water and subsequently alcohol to remove the residual colorant, the colored sample was thermally cured once again, resulted in colored surface final product. This new coloring process using intercalation offers a cost-effective and environmental-friendly coloring technology.

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

Inorganic-Organic Hybrid Hard Coating Solution Containing Colloidal Silica

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딜라이트오브서피스앤컬러 품질 [1]딜라이트오브서피스앤컬러 총괄 [2](주)나노스페이스

Water-borne type hard coating solution was prepared using organo-silanes and layer silicate nanocomposite. Intercalation of melamine and polyurethane dispersions into layered silicate resulted in synthetic resin-layer silicates nanohybrids with ordered stacking structures. Subsequent hydrolysis of silane compounds such as tetraethoxysilane, (TEOS), vinyltrimethoxysilane (VTMS) and polysiloxane in the presence of the synthetic resin-silicate hybrid dispersions produces novel waterborne inorganic-organic hybrid dispersions. In order to improve the surface hardness and glossy effect colloidal SiO2 (~12 nm) solution was also added into coating solution up to 5 wt%. The novel inorganic-organic hybrid coating solution was successfully applied for hard coating material with excellent performances in pencil hardness, solvent-resistance, film adherence and surface glossy. Extended thermal curring at 110 ℃ resulted in a great enhancement of surface hardness and solvent resistance.

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

Dehydration of butanols and ethanol with mesoporous SAPO-34 molecular sieves.

전종원 정성화[*]

경북대학교 화학과

Microwave assisted hydrothermal synthesis of micro & mesoporous SAPO-34 molecular sieves has been reported. Tetraethylammonium hydroxide (TEAOH) and carbon black were used as templating materials for micro & mesoporous SAPO-34, respectively. The obtained molecular sieves were characterized with X-ray, scanning electron microscope, adsorption/desorption of nitrogen, temperature programmed desorption of ammonia and so on. By increasing the content of the carbon black template in the synthesis, the mesopore volume increased. Dehydration of alcohols (butanols & ethanol) that are recently produced from biomass was carried out with the synthesized SAPO-34 molecular sieves, and the lifetime of the catalysts for the dehydration reaction increased as the mesoporosity increased (or as the content of the carbon black in the synthesis increased). Moreover, the performance of the microporous catalyst synthesized with microwave was better than that of the catalyst obtained with conventional electric heating. The relative performance of the catalytic dehydration may be explained by the mesoporosity (obtained with the carbon black template) and the crystal size (microwave vs. conventional electric synthesis). Therefore, it may be assumed that the fine particles of mesoporous SAPO-34 were obtained by microwave irradiation and used as an efficient acid catalyst over the dehydration of alcohols.

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

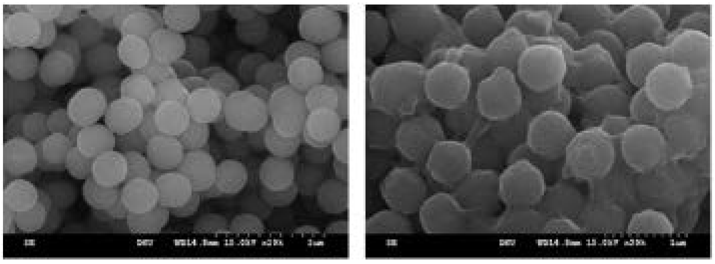
Superhydrophobic marbles fabricated by surface modification of nano-silica particles

고승철 이상미 안용현*

단국대학교 화학과

Seungcheol Go, Sangmi Lee, Yonghyun Ahn*
Dept. of Chemistry, Dankook University

Surface modification of the silica nano particles to obtain a superhydrophobic surface has been investigated during recent years. One of the superhydrophobic surface properties is a self-cleaning. A superhydrophobic surface is satisfied with a water contact angle of more than 150˚ and sliding angle of less than 10˚. The wettability of solid surfaces is controlled by both surface roughness and low surface energy material. Nano-particle size and surface coating material of silica marble create surface roughness and low energy material surface. We obtained approximate 500nm silica particles by St?ber method. Then surface of particles was coated in the solution of HFTHTMS and alkylphosphonic acid in ethanol. The superhydrophobic marbles were fabricated and characterized with with FE-SEM, XPS and FT-IR.



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발표코드: **IND.P-89**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1-alkoxydiglycerides using the 1-alkoxyglycerol

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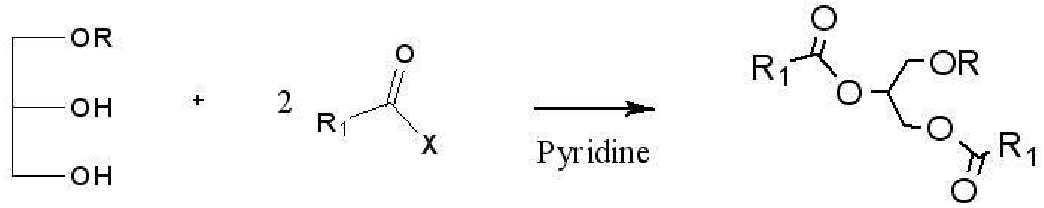
1-alkoxydiglycerides were synthesized from oleolyl derivative and 1-alkoxyglycerol. The yields of the products of oleoly derivative, stearyl, lauryl and olely, were 81.26%, 80.77%, 85.34% respectively. The products were confirmed by GC, GC/MSD, HR/MSD, IR, NMR, EA. The pour point and viscosity of the products were tested as well.

Abstract



X: -Cl, -OR'
R: Stearyl, lauryl, olely
R_1: olely

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발표코드: **IND.P-90**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dye/TiO2/Pt Hybrid Systems 에서 친수성기의 변화를 통한 가시광에서의 수소발생과 Charge-Separate 상태의 동역학

하은경 조양진[1] 위경량[1] 강상욱[1,*]

고려대학교 세종캠퍼스 소재화학과 [1]고려대학교 소재화학과

(E)-3-(5'-{4-[bis(4-R1-phenyl)amino]phenyl}-4,4'-(R2)2-2,2'-bithiophen-5-yl)-2-cyanoacrylic acid 염료를 이용하여 Dye/TiO2/Pt hybrid 광촉매 기반의 가시광에서의 수소발생에 대한 연구를 진행하였다. 수소발생의 효율은 EDTA 를 전자주개로 사용하고 λ>420 nm 파장의 빛을 조사한 수용액 상태에서 진행하였으며, 염료의 친수성은 치환체 R(MOD (R1=CH3OCH2, R2=H)?MO4D (R1=R2=CH3OCH2)>HD (R1=R2=H)>PD (R1=C3H7, R2=H))에 변화를 주었다.MOD/TiO2/Pt 의 경우, 광여기 수소발생 양자효율이 0.27±0.03 으로 나타났다. MOD 와 PD 가 TiO2 나노입자에 흡착된 투명필름을 pH3 수용액 처리 후 Transient absorption 측정을 한 결과 염료의 라디칼 양이온(Dye.+) 형태가 매우 빠르게(

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

암모니아보란을 이용한 효율적인 보라진합성 촉매 변환반응과 합성된 보라진의 질화붕소 (white graphene) 생성을 위한 사용

박진형 위경량[1] 조양진[1] 강상욱[1]

고려대학교 일반대학원 소재화학과 [1]고려대학교 소재화학과

니켈 나노입자(NiNPs)를 테트라글라임(Tetraglyme) 용매상에서 사용하여 효율적인 촉매반응으로 암모니아 보란에서 보라진으로 합성하였다. 최적의 조건은 3mol%의 니켈 나노입자를 테트라글라임에 암모니아 보란을 녹인 1.5 M 의 용액에 넣고 80 oC 온도에서 6 시간동안 반응한 후 30 Torr 로 유지한 진공을 유지하여 합성을 진행한 것이다. 보라진은 -45 oC, -78 oC, -196 oC 트랩을 이용하여 분리하였으며 -78 oC 트랩에 순수한 보라진이 53 % 수율로 얻어졌다. 생성된 보라진은 저압화학증착법(Low pressure chemical vapor deposition: LPCVD)을 이용한 고품질의 h-BN (white graphene) 과 대면적의 h-BN sheet 를 형성하는 분자전구체로 활용하였다. Ultra-thin h-BN(단막부터 다막층)은 니켈 호일(Ni foil)위에서 보라진과 암모니아의 최적의 비율로 합성하였고 암모니아의 다양한 부분압을 이용하여 막의 수를 조절하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An adsorption equilibrium and kinetic study of CO_2, N_2, CH_4, and CO on cucurbit[6]uril

노영경 문종호[1,*]

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Adsorption equilibrium and kinetics of 4 single gases (CO_2, N_2, CH_4, and CO) on two different types (powder and pellet) of an organic molecular porous material based on cucurbit[6]uril (CB[6]) was studied. The experiments were performed by a gravimetric method using a microbalance (MSB, magnetic suspension balance) in the temperature range of 10 to 40 ℃. The pressure of the adsorbate was increased in a stepwise manner from 0.0 (vacuum condition) to 2.0 atm and the uptake curves were measured at each pressure range. Langmuir and Langmuir-Freundlich models were employed to fit the equilibrium data of the pure single gases and a conventional micropore diffusion model was used to analyze the adsorption kinetic data. The enthalpy of adsorption and selectivity for CO_2 over other gases were estimated to understand the adsorption affinity of CB[6] toward various gases. Details of the work will be presented.

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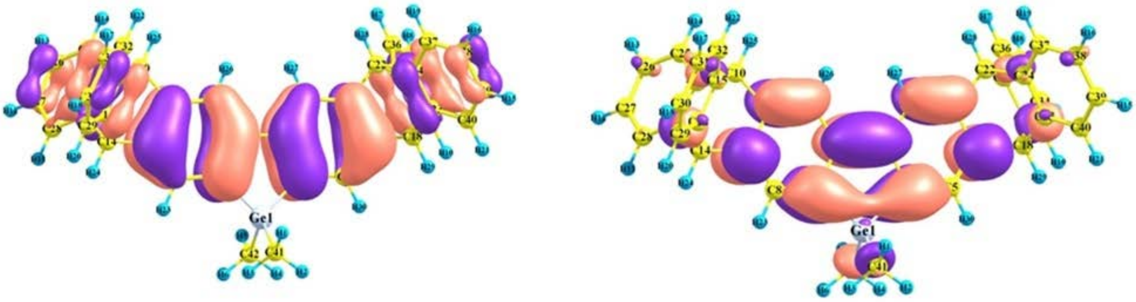
Synthesis and Optical Properties of Fluorene containing Germanium for OLED Applications

엄성용 손홍래[*]

조선대학교 화학과

Various functionalized germaflourene derivatives have been synthesized and their optical and electronic properties were investigated. The germafluorene compounds were synthesized by a stepwise reactions from 1,2,4,5-tetrabromobenzene to 2,2'-dibromobisfluorene with germanium tetrachloride in THF at row temperature. The germafluorene compounds were characterized by 1H-NMR, UV-Vis absorption, and photoluminescence spectroscopy. The optical absorption spectra showed an absorption edge at 285 nm, while a strong UV-vis photoluminescence at 350 nm is observed. These germafluorene compounds are served as light emissive layers. They possess relatively low LUMO energy levels while maintaining high HOMO-LUMO optical gaps. Differential scanning calorimetry measurements reveal that these germafluorene compounds exhibited very good thermal stability at extremely high temperature ca. above 350 oC. Organic light-emitting diodes have been fabricated using thermal evaporation technique which emit blue light with an excellent diode behavior under the forward bias. This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)



HOMO **LUMO**

B3LYP/6-31G(d)

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Aromatic Anhydride as a Ultra-Fast Curing Agent for the Synthesis of Epoxy-Based Polysiloxane Resins for High Refractive and Excellent Transparent Optical Properties

김성웅 손홍래*

조선대학교 화학과

The epoxy-based oligosiloxanes were synthesized from the reaction of 3-glycidoxypropyltrimethoxysilane, diphenylsilanediol (DPSD), and Ba(OH)2H2O via sol?gel condensation process. Previously known cross-linking agent such as a methyl hexa-hydrophthalic anhydride (MHHPA) for the synthesis of epoxy-based polysiloxane resins in the present of amine catalyst showed disadvantage in terms of curing time. To obtain suitable hardness for polysiloxane resins, the curing time to complete the reaction requires 12 hours. Here, we reported new aromatic anhydrides as a ultra-fast curing agent for the synthesis of epoxy-based polysiloxane resins. The curing process with non-aromatic anhydride requires usually more than 12 hours. However the curing process with aromatic anhydrides requires only about 30 min to obtain a suitable hardness. Structural analysis of epoxy-based oligosiloxane was determined by using 1H-NMR. By using new curing agent, the prepared epoxy-based polysiloxane resins exhibited an ultra-fast curing time, good refractive index, and high hardness and transmittance. Hardness, refractive index, and transmittance were measured by using Durometer(GS-702N), refractometer(NAR-1T SOLID), and UV-vis spectrometer(UV-2401 PC, Shimazu), respectively.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Camptothecin-Capped Silicon Quantum Dots As New Drug Delivery Materials

백상수 손홍래*

조선대학교 화학과

Camptothecin(CPT)-capped silicon quantum dots (Si QDs) were successfully synthesized from the reaction of ammonium chloride, magnesium silicide and camptothecinyltrichlorosilane. Optical characterizations of Si QDs were achieved by using ultraviolet-visible (UV-Vis) and photoluminescence (PL) spectroscopy. The morphologies of Si QDs were achieved by scanning electron microscope (SEM) and transmission electron microscope (TEM). CPT-capped Si QDs were characterized by nuclear magnetic resonance (NMR) and infra-red (IR) spectroscopy. Si QDs synthesized without camptothecinyltrichlorosilane were emitted the light at 450 nm with an excitation wavelength of 400 nm. CPT itself was emitted the light at 425 nm with an excitation wavelength of 370 nm. After the one-pot synthesis, CPT-capped Si QDs were emitted the light at 570 nm with an excitation wavelength of 480 nm. Optical characteristic of drug-capped silicon particles were investigated in PSB buffer solution. The release of CPT was measured by UV-vis spectrometer. The intensity of fluorescence of the Si QDs was measured with a drug release. The concentration of released drug exhibited non-linear relationship with a release time. Quantum yields for Si QDs, CPT, and CPT-capped Si QDs were measured. Detailed information about the photoluminescence will be discussed.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282).

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Synthesis and Characterization of Graphene Oxide/Silicon Nanowire Composite Materials

신동희 손홍래*

조선대학교 화학과

Graphene oxide (GO)/silicon nanowire (Si NW) composite materials were synthesized from the reaction of GO and Si NW via hydrosilylation in the presence of platinum catalyst. Single-crystalline SiNWs were fabricated by using an electroless metal assisted etching of bulk silicon wafers with silver nanoparticles that are deposited by wet electroless deposition. The etching of SiNWs is based on subsequent treatments in aqueous solutions of silver nitrate followed by hydrofluoric acid and hydrogen peroxide. Free-standing SiNWs were then obtained using ultrasono-method in chloroform. GO was prepared by the modified Hummer's method and used for the synthesis of GO/SiNW hybrimers. The morphology of GO/SiNW composite materials were characterized by EDS, TEM, and FE-SEM. Covalent bond between GO and SiNW was confirmed by using XPS and FTIR spectroscopy. BET measurement showed that GO/SiNW hybrimesr had a mesoporous. Detailed information about the characterization of GO/SiNW hybrimesr will be discussed.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Effect of Phenyl Substituents in Phenylvinyl Polysiloxane Resins for OLED Encapsulants

김성룡 손홍래*

조선대학교 화학과

Effect of phenyl derivatives on phenylvinyl polysiloxane (PVPS) resins was investigated for OLEDencapsulant application. Thermally stable transparent PVPS resins with high refractive index wassynthesized by the thermal curing reaction of phenylvinyl oligosiloxanes (PVOS). PVOS was obtainedby a sol?gel condensation process between vinyltrimethoxysilane (VTMS) and diphenylsilanediol(DPSD). We have investigated the effect of phenyl derivatives on PVOS resins. Instead of usingDPSD, dimestylsilanediol (DMSD) was used for the synthesis of mesitylvinyl oligosiloxane (MVOS).DMSD was synthesized from the reaction of 2 equivalents of mesityllithium and silicon tetrachloride,Mesityllithium was obtained from the reaction of bromomesitylene with n-buthyllithium. To obtainmesitylvinyl polysiloxane (MVPS) resins, MVOS was thermally cured at 150 oC for 3 hours. MVPSshowed a refracive index of 1.55 after 4 hours of reaction time. For the comparison of DPSD,tritylsilane triole (TST) synthesized from the reaction of trityllithium with silicon tetra chloride wasused for the synthesis of tritylvinyl oligosiloxanes(TVOS). The physical properties such as an opticaltransmittance, refractive index, and harness were measured according to the curing time and precursorcomposition.This research was financially supported by the Ministry of Education, Science Technology (MEST)and National Research Foundation of Korea (NRF) through the Human Resource Training Project forRegional Innovation. (2012H1B8A2026282)

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Synthesis of Phenyl-Vinyl-Based Polysiloxane Resins Using Linear Hydrosiloxane Oligomers as New Cross-Linking Agents

정성은 손홍래*

조선대학교 화학과

New cross-linking agents containing silicon-hydride such as linear hydrosiloxane oligomers were used for the synthesis of phenyl-vinyl-based polysiloxane resins via hydrosilylation reaction. Here, we discovered linear hydrosiloxane oligomers as a new cross-linking agent. Phenyl-vinyl-based oligosiloxanes were synthesized from the reaction of diphenylsilanediol and vinyltrimethoxysilane through a nonhydrolytic sol-gel condensation. Linear hydrosiloxane oligomers were obtained from the reaction of dichlorodimethylsilane and dichlorophenylsilane. Dimethylchlorosilane was used as a terminating group of linear hydrosiloxane oligomers. Structural analysis of phenyl-vinyl-based oligosiloxanes and linear hydrosiloxane oligomers were determined by using 1H-NMR. For the synthesis of polysiloxane resins, the reaction of phenyl-vinyl-based oligosiloxanes and linear hydrosiloxane oligomers in the present of Pt catalyst was carried out. Linear hydrosiloxane oligomers as a new curing agent provided the phenyl-vinyl-based polysiloxane resins showing a good refractive index, high hardness, and great transmittance. The comparison to previously known phenyltris(dimethylsiloxy)silane as a cross-linking agent has been reported. Hardness and refractive index, transmittance was measured using a coating with a thickness of 2mm. Durometer(GS-702N), refractometer(NAR-1T SOLID), and UV-vis spectrometer(UV-2401 PC, Shimazu) were used. This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Synthesis and Characterization of Mestylphenylvinyl Polysiloxane Resins for OLED Encapsulants

이성기 손홍래*

조선대학교 화학과

New thermally stable transparent polysiloxane resins with high refractive index, mesitylphenylvinyl polysiloxane (MPVPS) were synthesized from the thermal curing reaction of mesitylphenylvinyl oligosiloxane (MPVOS). MPVOS was obtained by a sol?gel condensation process between vinyltrimethoxysilane (VTMS) and mestylphenylsilanediol (MPSD). We have investigated the effect of phenyl derivatives on PVOS resins. Instead of using DPSD, MPSD was used for the synthesis of MPVOS. MPSD was synthesized from the reaction of 1 equivalent of mesityllithium and trichlorophenylsilane, Mesityllithium was obtained from the reaction of bromomesitylene with n-buthyllithium. To obtain MPVPS resins, MPVOS was thermally cured at 150 oC for 3 hours. MPVPS showed the refracive index of 1.56 after 3 hours of reaction time. For the comparison of DPSD, the physical properties such as an optical transmittance, refractive index, and harness were measured according to the curing time and precursor composition.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Synthesis and Characterization of Microwave-Exfoliated Graphene Oxide/Silicon Quantum Dot Composite Materials

안지훈 손홍래*

조선대학교 화학과

Microwave-exfoliated graphene oxide(MEGO)/silicon quantum dot (Si QD) composites have been successfully synthesized and characterized for the possible application of supercapacitor. Graphene oxide was synthesized by using modified Hummer's method and exfoliated by microwave to give MEGO. Hydride-terminated Si QDs were synthesized from the reaction of ammonium chloride and magnesium silicide. Activated MEGO was reacted with H-terminated Si QDs via hydrosilylation in the presence of platinum catalyst. MEGO/Si QDs composite materials were characterized by XRD, TEM and FE-SEM. A specific surface area was measured by the Brunauer-Emmett-Teller (BET) method. Detailed information for the composite materials will be discussed. This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Synthesis and Characterization of Phenyl-Vinyl-Based Polysiloxane /Silicon Quantum Dot Hybrimer

신기루 손홍래*

조선대학교 화학과

Phenyl-vinyl-based polysiloxane (PVPS)/silicon quantum dot (Si QD) hybrimer was synthesized from the reaction of PVPS and SI QDs via hydrosilylation in the presence of platinum catalyst. Silicon quantum dots (Si QDs) were used for the synthesis of organic-inorganic polysiloxane hybrimer. Si QDs were synthesized from the reaction of ammonium chloride and magnesium silicide to give hydride-terminated surface of Si QDs. Optical characterizations of silicon nanoparticles were achieved by using ultraviolet-visible (UV-Vis) and photoluminescence (PL). Si-H surface of the Si QDs was hydrosilylated with vinyl group of PVPS. The physical properties such as an optical transmittance, refractive index, and harness of PVPS/Si QDs hybrimer were investigated according to the curing time and precursor composition. Hardness, refractive index, and transmittance were measured by using Durometer(GS-702N), refractometer(NAR-1T SOLID), and UV-vis spectrometer(UV-2401 PC, Shimazu), respectively.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Photoluminescence Efficiency by FRET in Silicon Quantum Dots Capped with Silole Fluorophore

김강빈 손홍래*

조선대학교 화학과

Silicon Quantum Dots (Si QDs) capped with organic fluorophore such as siloles were successfully synthesized from the reaction of ammonium chloride, magnesium silicide, and dichlorotetraphenylsiloles in DMF. Optical characterizations of Si QDs were achieved by using ultraviolet-visible (UV-Vis) and photoluminescence (PL) spectroscopy. The morphologies of Si QDs were achieved by scanning electron micrograph (SEM) and transmission electron micrograph (TEM). Silole-capped Si QDs were characterized by nuclear magnetic resonance (NMR) and infra-red (IR) spectroscopy. Si QDs synthesized without silole were emitted the light at 450 nm with an excitation wavelength of 400 nm. The emission wavelength of tetraphenylsilole is 520 nm with an excitation wavelength of 360 nm. After the synthesis of Si QD/silole core/shell nanoparticles, core/shell nanoparticles were subjected to measure the PL. Si QD/silole core/shell nanoparticles exhibited an absence of PL for Si QDs and an enhancement of PL for silole by 40 times. This result can be interpreted by the efficient fluorescence resonance energy transfer (FRET) from Si QDs having large band gap to silole moiety having small band gap. Detailed information about the photoluminescence will be discussed.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282).

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New Synthesis of Methacrylate- and Epoxy-Based Polysiloxane Resins for the Application of LED Encapsulation

김종준 손홍래*

조선대학교 화학과

New methacrylate- and epoxy-based oligosiloxanes were synthesized from the reaction of 3-(methacryloyloxy)-propyltrimethoxy-silane (MPTS), 3-(glycidoxy)-propyltrimethoxysilane (GPTS), and diphenylsilanediol (DPSD) in the prescence of barium hydroxide monohydrate, $Ba(OH2)$ $H2O$ as a catalyst. The catalyst promotes the direct condensation reaction of the methoxy radical of MPTS and GPTS and the diol radical of DPSD to form siloxane bonds. This oligosiloxanes contained bi-functional groups such as methacrylate and epoxy group for the further condensation. New methacrylate- and epoxy-based polysiloxanes resins were obtained by using both photo-curing and thermal curing methods. To investigate the curing effect, the epoxy moiety of oligosiloxane was heat-treated and the methacrylate moiety of oligosiloxane was photo-treated. The physical properties such as an optical transmittance, refractive index, and harness were investigated according to the curing time and precursor composition. Hardness, refractive index, and transmittance were measured by using Durometer(GS-702N), refractometer(NAR-1T SOLID), and UV-vis spectrometer(UV-2401 PC, Shimazu), respectively.This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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Synthesis of High Quantum Yield Silicon Quantum Dots and Silicon Nanoparticles

조보민 손홍래*

조선대학교 화학과

Silicon quantum dots (Si QDs) and nanoparticles (Si NPS) was successfully synthesized from the reaction of ammonium chloride and magnesium silicide. Pholuminescnece (PL) and quantum yields of Si QDs have been measured. The change of quantum yield and optical characterization of Si QDs are measured depending on the reaction time. Highly luminescent Si QDs were obtained as the reaction time increased. TEM topograph of a typical nanoparticle reveals the tetrahedral geometry of the nanoparticle. The size of the nanocrystal is 250 nm. The SAED pattern is from several of the particles shown in the TEM image and thus single zone axis patterns are observed. The [111] zone axis pattern for diamond cubic is observed. Absorption measurement indicated that the Si QDs consisted of only silicon and hydrogen atom. Optical characterizations of Si QDs were measured by UV-Vis and PL spectroscopy. The size distribution and orientation of Si QDs were measured by TEM and XRD. TEM image displays the spherical Si QDs with the size of 2-4 nm. The monotonic shift of the PL as a function of excitation wavelength resulted in the excitation of different sizes of QDs that had different optical transition energies. This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation. (2012H1B8A2026282)

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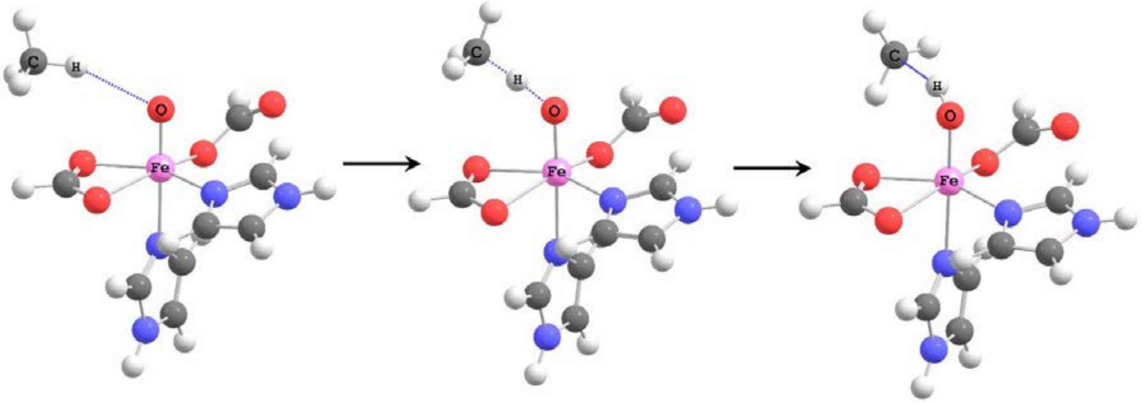
A Theoretical Study on the Methane Hydroxylation by Fe(IV)-Oxo Intermediate in Taurine/α-Ketoglutarate Dioxygenase: the Hydrogen Atom Transfer Mechanism and the Role of Tunneling Effect

Mai Khanh Binh 김용호*

경희대학교 응용화학과

Taurine/α-Ketoglurate dioxygenase (TauD) is one of the most important enzymes in α-Ketoglurate dioxygenase family, which involves in many important biochemical processes. The iron(IV)-oxo active species of TauD has the ability for activating C-H bond by taking oxygen at its non-heme iron center. Large kinetic isotope effect for the hydrogen transfer was found in the reaction of taurine with TauD. In this study, the variational transition state theory including multidimensional tunneling approximations was used to calculate rate constants and accurately predict the KIEs of the reaction of methane with TauD based on the quantum mechanically generated intrinsic reaction coordinates of the H-transfer. At 278 K, the calculated KIE is 38.3 and in good agreement with experimental data of 37.0 within the error limits of experiment. In the substrate binding process, the electron is moved from oxo ligand to iron atom and reduce Fe^{IV} to Fe^{III}. We suggest that the Fe^{IV}/Fe^{III} reduction is the driving force of the H-transfer reaction between CH_4 and Fe(IV)-oxo species of TauD. Tunneling is found to be very significant for the H-transfer and that the representative tunneling path (RTP) is very different from the MEP. At 278 K, the pre- and post-tunneling configurations appear at 5.0 kcal/mol below the top of the adiabatic energy barrier, where the hydrogen atom moves 0.33 Angstrom by tunneling from carbon to oxygen atom. Before the pre-tunneling configuration, mostly heavy atoms move closer to the reaction center and then the hydrogen atom suddenly hops.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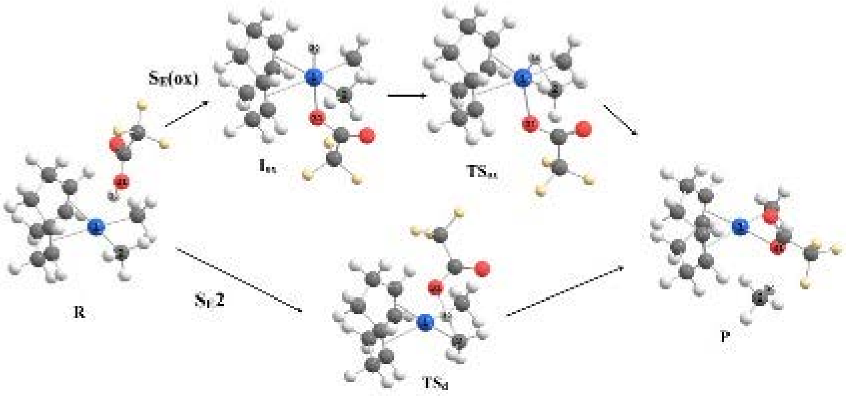
The Mechanism for the Protonolysis of Dimethylplatinum(II) Complex: Theoretical Studies Using Large Kinetics Isotope Effects as Mechanistic Indicator

Mai Khanh Binh 김용호*

경희대학교 응용화학과

Mechanistic pathway for the protonolysis of alkylmetal complex, which can be proceeded via concerted or stepwise routes, and the correlation between kinetic isotope effect (KIE) and mechanism are the interested issues. In this work, we demonstrated that variational transition state theory including multidimensional tunneling approximations allows accurate prediction of the KIEs and Arrhenius parameters for such systems. The calculated values of KIE, E_a^D-E_a^H and A_H/A_D ratio of the protonolysis of (COD)$PtMe_2$ and $ZnMe_2$ by TFA agree very well with experimental data. Both density functional theory (DFT) and dynamics calculations revealed that the protonolysis of (COD)$PtMe_2$, which exhibits abnormal large KIE, occurs via concerted pathway. In this route, we found that tunneling is very efficient for the proton transfer and the RTP is very different from the MEP. For the protonolysis of $ZnMe_2$, which always ocurs via concerted pathway, the adiabatic potential curve in the reactant side is very flat and small tunneling effect was obtained. Based on our calculations, we found that the abnormally large KIE (greater than 10 at room temperature - reveals the involvement of tunneling) can be used as an experimental indicator of the concerted pathway (S_E2 mechanism), but with other alkylmetal systems, which has normal KIE for the proton transfer in the protonolysis, these reactions can proceed via concerted or stepwise routes and the mechanisms of these systems must be considered carefully.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Reactions of organic halophsophines to Pd(0) complexes: synthesis and structures of new dinuclear phosphido -bridged palladium(Ⅱ) complexes

김용주* 최근영 이선계 김건우 **ZHENG ZHENNU**[1] 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Oxidative addition is one of fundermental step in the transition metal-catayzed organic reactions and sometimes gives unique transition metal intermediates. Although many studies on the oxidative addition of organic halides into the Pd(0) compounds were known, reactions of chlorophosphines toward Pd(0) compounds are still rare. In this work we have examined oxidative addition of various chlorophosphines into the Pd(0) compounds and obtained unique dinuclear phsphido-bridged Pd(II) complexes. Isolated complexes characterized by NMR and X-ray crystallgraphic analyses.

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Synthesis and structures of (π-allyl) Pd-NHC(N-heterocyclic carbene) complexes bearing pseudohalides (N3, NCS or SCN, NCO, CF3COO) and their catalytic application

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Various mononuclear (π-allyl) Pd-NHC complexes having pseudohalogen ligands were obtained from the reactions of bis(π-allyl) Pd chlorides with 2 equiv. of NHCs ligands. Then sequential substitution reactions with NaN3, KSCN, KOCN, AgOCOCF3 in aquous solvent produced coresponding [(π-allyl) PdX(NHC) complexes, respectively. The isolated complexes were characterized by spectroscopic analyses and some of X-ray diffraction study. Treatments with organic isothiocyanates (R-NCS) and Dimethyl acetylene dicarboxylate to the [(π-allyl)Pd(N3)(NHC)] caused dipolar cycloaddition for (π-allyl) Pd-NHC tetrazole-thiolato, [(π-allyl)Pd{SCN4(Ph)}(NHC)] and triazolato complexes, [(π-allyl)Pd{(N3C2)(COOMe)2}], in quantitative yield, respectively. Also, catalytic activies in Suzuki-Miyaura cross C-C coupling reactions using various (π-allyl) Pd-NHC pseudhalogen complexes were underwent.

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Mechanistic insights into the O-O bond cleavage in redox-inactive metal ion boundiron(III)-peroxo intermediates

방수희 권윤혜[1] 이용민[2,*] 남원우[3,*]

이화여자대학교 바이오융합과학과 [1]이화여자대학교 [2]이화여자대학교 기초과학연구소 [3]이화여자대학교 화학과

One primary goal in biomimetic research is to understand mechanisms of dioxygenactivation, structures of reactive intermediates, and reactivities of the intermediates involvedin catalytic oxidation reactions by metalloenzymes. The O-O bond cleavage is considered asan important step in dioxygen activation. Recently, the conversion from iron-peroxo speciesto iron-hydroperoxo, and then to iron-oxo species has been reported. However, mechanismof O-O bond cleavage regulated by Lewis acidity of metal ion has not been reported yet. Inthis presentation, we report that rate of O-O bond cleavage in redox-inactive metal ion-boundiron(III)-peroxo species was markedly enhanced by one-electron reductants (i.e., ferrocenederivatives) and Lewis acidity of metal ion such as Sc^{3+}, Y^{3+} and Lu^{3+}. These results indicate that electron transfer is involved in the rate determining step and the O-O bond strength in the strong Lewis acid-bound iron(III)-peroxo species might be weakened because of the strong binding of metal ion to peroxo moiety. The conversion from redox-inactive metal ion-bound iron(III)-peroxo to iron(IV)-oxo was also investigated by spectroelectrochemical method.

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o-Carborane-Triarylborane Dyad as a Dual Sensor for Fluoride

송기철 박지현[1] 도영규[*] 이민형[1,*]

한국과학기술원(KAIST) 화학과 [1]울산대학교 화학과

o-Carborane (1,2-*closo*-$C_2B_{10}H_{12}$) substituted triarylborane (*closo*-1) was synthesized and converted into a corresponding *nido*-carborane (*nido*-1). The identity of *closo*-1 and *nido*-1 has been characterized by multinuclear NMR spectroscopy, elemental analysis, and mass spectrometry. The crystal structure of *nido*-1 was determined by X-ray diffraction method. Photophysical measurements upon fluoride addition indicated that while *closo*-1 shows high fluoride ion affinity through the trigonal-planar boron center, degradation to *nido*-carborane (*nido*-1) leads to turn-on fluorescence response toward fluoride. Details of the dual fluoride sensing properties of *closo*-1 before and after degradation to *nido*-1 will be discussed with theoretical calculations.

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Selective Sensing of Cyanide Ions in Buffered Water at pH 7 by Multi-phosphonium Triarylboranes

송기철 **NGUYEN VAN NGHIA**[1] 도영규[*] 이민형[1,*]

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A series of mono-, di-, tri-phosphonium substituted triarylboranes, $[Mes_2BAr^P]I$ ([2]I), $[MesBAr^P_2]I_2$ ($[3]I_2$), and $[BAr^P_3]I_3$ ($[4]I_3$) (Ar^P = 4-$(MePh_2P)$-2,6-Me_2-C_6H_2) were prepared. The crystal structure of $[4]I_3$ determined by X-ray diffraction study reveals peripheral decoration of aryl groups with phosphonium moieties. The triarylboranes, [2]I-$[4]I_3$ bind both fluoride and cyanide ions in DMSO/H_2O (7:3 v/v) mixture with high binding constants (K). Comparison of the K values of triarylboranes for fluoride reveals that fluorophilicity increases with the increasing number of phosphonium moieties: $[2]^+ < [3]^{2+} < [4]^{3+}$. A similar trend is also observed in the cyanide binding with K values that are greater by 2-4 orders of magnitude than those in the fluoride binding. The tri-phosphonium borane $[4]Cl_3$, a water-soluble form of $[4]I_3$, was further utilized in evaluating the anion affinity in water. While $[4]^{3+}$ is shown to hardly bind fluoride in buffered water at pH 7, it binds cyanide with a high binding constant (1.7×10^7 M^{-1}).

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Triarylborane-Phenanthroimidazole Conjugates as a Ratiometric Fluorescent Sensor for Fluoride

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한국과학기술원(KAIST) 화학과 [1]울산대학교 화학과

Triarylborane-phenanthroimidazole conjugates 1 and 2 linked by a biphenylene and phenylene group, respectively, were prepared and characterized. Both compounds are highly fluorescent (Φ = 0.49 - 0.74 for 1 and Φ = 0.71 - 0.92 for 2) and show a positive solvatochromism. Upon fluoride binding to the boron center, they exhibit a ratiometric fluorescence response (?λ_{em} = 84 nm for 1 and 63 nm for 2 in acetone) accompanying a vivid emission color change. Photophysical data and TD-DFT studies suggest that intramolecular charge transfer (ICT) transition from a phenanthroimidazole donor to a borane acceptor in the neutral 1 is switched to π-π^* transition of phenanthroimidazole moiety after fluoride binding. Due to the greater elevation of LUMO level by fluoride complexation, the resulting fluoride adduct $[1F]^-$ fluoresces at the apparently blue-shifted region. Details of synthesis, characterization, and fluoride binding properties of 1 and 2 will be discussed.

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Redox-Inactive Metal Ion Effect on the Reactivity of Mononuclear Non-Heme Manganese(IV)-Oxo Complex

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이화여자대학교 화학나노과학과 [1]이화여자대학교 기초과학연구소 [2]이화여자대학교 바이오융합과학과 [3]이화여자대학교 화학과

Redox-inactive metal ions play pivotal roles in regulating reactivities of high-valent metal-oxo species in a variety of enzymatic and chemical reactions. A mononuclear nonheme $Mn^{IV}(O)$ complex bearing a pentadentate N5 ligand and its Sc^{3+}-bound complex have been synthesized and characterized with various spectroscopic methods. The reactivities of the $Mn^{IV}(O)$ complex are markedly influenced by binding Sc^{3+} ions in oxidation reactions, such as ~2200-fold increase in sulfoxidation (i.e., oxygen atom transfer) but ~180-fold decrease in the C-H bond activation (i.e., hydrogen atom transfer). The present results provide the first example of a nonheme $Mn^{IV}(O)$ complex binding redox-inactive metal ions that shows a contrasting effect of redox-inactive metal ions on the reactivities of metal-oxo species in the oxygen atom transfer and hydrogen atom transfer reactions.

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Characterization and Reactivity of Redox-Inactive Metal Ion-Bound Iron(III)-Peroxo

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Iron-oxygen species in the metalloenzymes are key intermediates in catalytic cycle of dioxygen activation. Recently, iron(III)-peroxo, iron(III)-hydroperoxo and iron(IV)-oxo have been characterized spectroscopically. Brønsted acid (H^+) binds to iron(III)-peroxo species to generate iron(III)-hydroperoxo species, and then convert to iron(IV)-oxo intermediate. Relative reactivity studies reveal that the iron(III)-hydroperoxo species are viable oxidants in both nucleophilic and electrophilic reactions. Herein, we tried to generate redox-inactive metal ion-bound iron(III)-peroxo species instead of Brønsted acid-bound iron(III)-peroxo species in order to understand the effect of redox-inactive metal ions, which have the different Lewis acidity. Redox-inactive metal ion-bound iron(III)-peroxo species, $[(TMC)Fe(III)(O_2)]^+$-Mn^+ ($Mn^+ = Sc^{3+}$ and Y^{3+}; TMC = tetramethylcyclam), were synthesized by adding redox-inactive metal ions (Sc^{3+} and Y^{3+}) into the solution of isolated iron(III)-peroxo species, $[(TMC)Fe(III)(O_2)]^+$, and characterized by various physicochemical methods, including UV-vis, ESI-MS, resonance Raman and EPR. The reactivities of these intermediates were investigated with 1,4-cyclohexadiene for electrophilic reactivity and cyclohexanecarboxaldehyde for nucleophilic reactivity.

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Anionic 3-D Microporous Metal-organic Framework with Two Different Kinds of 3-Connected Ligands

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울산과학기술대학교(UNIST) 친환경에너지공학부

The solvothermal reaction of zinc(II) nitrate hexahydrate and two kinds of triscarboxylic acid ligands, 1,3,5-benzenetricarboxylic acid (H_3BTC) and 1,3,5-benzenetribenzoic acid (H_3BTB), in anhydrous *N,N'*-dimethylacetamide (DMA) led to an anionic 3-dimensional (3-D) microporous metal?organic framework (MOF), $(NH_2(CH_3)_2)_3[Zn_6(BTC)_4(BTB)]$. The $Zn_2(COO)_5$ metal cluster as a 5-connected trigonal bipyramidal secondary building unit (SBU) in the framework is composed of three carboxylates as three bladed bidentate bridging ligands at the equatorial positions of the dinuclear zinc(II) center and two monodentate carboxylates at the axial sites of the SBU. The 5-connected SBU is interconnected via two different kinds of the ligands as 3-connected nodes to form 3-D network of an unprecedented 3,3,3,5-connected net topology The charge balance of the framework structure and the 1H NMR spectrum of the dissociated framework by an acid suggest that the framework is of an anionic framework and the dimethylammonium cation derived from the hydrolysis of the solvent DMA serves as a counter cation for the charge balance of the framework. The gas sorption behaviors of this anionic MOF will also be discussed.

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Dye-Sensitized Solar Cells for Greenhouse application

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The light manipulation is very important in greenhouse as well as other environmental factors to cultivate and improve the quality. We have developed dye-sensitized solar cells using novel sensitizer with enhanced transmittance of red (625-675 nm) and blue (425-475 nm) waveband to control the illumination condition in the greenhouse. Novel ruthenium bipyridyl sensitizers with general formula $(Me_3PhN)_4[Ru(dcbpy)_2\text{-}(NCS)_2]$ (JJ-7) and $(Me_3BnN)_4$ $[Ru(dcbpy)_2\text{-}(NCS)_2]$ (JJ-9) have been synthesized and demonstrated as efficient sensitizers in dye-sensitized solar cells for greenhouse application. Under standard AM 1.5 sunlight, the solar cell of JJ-7 using a liquid-based electrolyte exhibits a short-circuit photocurrent density of 8.49 mA/cm^2, an open-circuit voltage of 0.83 V, and a fill factor of 0.71, corresponding to an overall conversion efficiency of 4.96% on 5 μm TiO_2 film. The transmittances of JJ-7 and JJ-9 exhibits 62.0% and 61.0% at red (660 nm) and 18.0% and 15.0% at blue (440 nm) wavelength for cultivation on 5 μm TiO_2 film, respectively.

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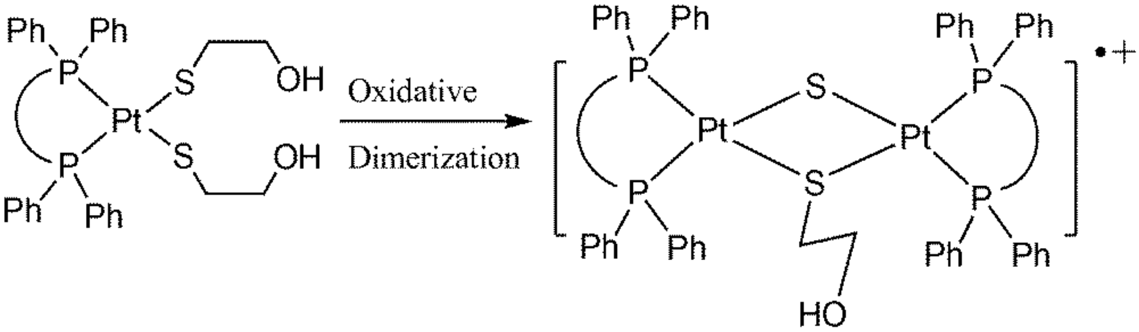
Oxidative Dimerization of (diphosphine)Pt(SEtOH)$_2$

전효경 노동윤*

서울여자대학교 화학과

Two heteroleptic Pt(II) complexes, (P2)Pt(SEtOH)$_2$ where P2 is 1,2-bis(diphenylphosphino)ethane (dppe) and 1,1’-bis(diphenylphosphino)ferrocene (dppf), were synthesized and characterized by NMR and X-ray structure analyses. The analysis of (dppf)Pt(SEtOH)$_2$ by MALDI-TOF mass spectroscopy shows the fragment with a loss of two -SEtOH ligand, $[M\text{-}2SEtOH]^{2+}$, as the prominent peak. Also, the most prominent peak in MALDI-TOF mass spectra was a product of oxidative dimerization process, $[(P2)Pt(\mu\text{-}S)(\mu\text{-}SEtOH)Pt(P2)]^{+}$. The detailed dimerization process, as well as their electrochemical and structural properties, will be presented. (NRF2010-0011478)



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Photochemical Properties and Shape Evolution of CdSe QDs in Non-injection Reaction

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Highly monodispersed CdSe quantum dots (QDs) were prepared without injection procedure. The influence of various cadmium alkyl fatty acids such as Cd-myristate(C14), Cd-palmitate(C16), Cd-steatate(C18) was studied for the optical properties of CdSe NCs in non-injection method. A series of Cd salt of long chain fatty acids, including Cd(myristate), Cd(palmitate) and Cd(stearate) has been prepared, and all metallic precursors and surfactants were mixed together followed by increasing temperature with controlled manner. This reaction resulted in highly monodispersed and bright zinc blend QDs. The bright point was found to be dependent on the Cd precursor used. The bright point was found at higher energy region with increasing carbon number of the fatty acid. The Full width at half maximum (FWHM) of all QDs obtained by this method was fallen in the range of 22-27 nm. In addition, the effects of specific ligands which have been known to lead anisotropic growth of the nanocrystals in injection method were investigated. The use of alkylphosphonic acid and alkyl amine was found to produce extremely monodisperse and high quantum yield of CdSe QDs. This procedure was proven to be able to yield large quantity zinc blend CdSe QDs (2g) by one pot reaction. The use of controlled amount of TDPA and ODA resulted in tetrapod and match shapes of QDs, which was first reported in non-injection method. These results clearly demonstrated the appropriate combination of precursors can provide a high quality of CdSe nanocrystals in terms of quantum yield, monodispersity and shape controls in non-injection method.

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Synthesis, crystal structures and magnetic properties of two Mn(III) azide complexes incorporating tetradentate schiff bases.

송정화 임광수 홍창섭*

고려대학교 화학과

We prepared two manganese complexes. $[Mn_2(L1)_2(N_3)_2]$ [1; L1=2,2’-[(1,2-ethanediyl)bis(nitrilopropylidyne)bisphenol], bridged by phenoxide and a one-dimensional chain $[Mn(L2)(N_3)]$ [2; L2 =2,2’-{(1,2-ethanediyl)bis[nitrilo(phenyl)-methylidyne]}bisphenol], linked by azide. For 1, each Mn central environment in the dimeric moiety bridged by the phenoxides of the L1 ligands can be described as a distorted octahedron made up of three oxygens from L1 ligand and three nitrogens from L1 ligand and azide. Remarkably, the replacement of L1 with L2 allows the distinct structural variation from the dimeric motif to a one-dimensional linear chain. The Mn center in compound 2 adopts a distorted octahedral geometry comprising two oxygens from L2 ligand and four nitrogens from L2 ligand and azides. Compounds 1 and 2 were characterized by elemental analysis, IR, and single crystal X-ray diffraction. Detailed structural and magnetic studies will be given in the presentation.

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Synthesis, structure and properties of a three-fold interpenetrated metal organic framework

김영아 임광수 홍창섭*

고려대학교 화학과

Multitopic ligands have been of interest due to their potential to generate MOFs that have application in gas storage, sensing, lunminescence and catalyst. In this regard, we prepared H_2L (=3,3'-dimethoxy-4,4'-biphenyldicarboxylic acid) with methoxy groups. The reaction of H_2L and Zn(II) allows for the formation of a new 3D MOF with 3-fold interpenetration.Secondary building unit consists of one-oxygen and four-zinc centers, which are linked by three ligands. One of four zinc centers is coordinated with two DMF molecules.We will present the detailed structure and sorption properties.

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Synthesis, structures and magnetic properties of dysprosium(III) complexes with D_{4d} local symmetry

임광수 홍창섭*

고려대학교 화학과

We prepared two Dy(III) compounds, $[Dy(L_{OMe})_2(H_2O)_2]PF_6$ (1) and $Dy(L_{OMe})_2(NO_3)$ (2), where L_{OMe} = (dimethyl phosphito-P)cobaltate. Compounds 1 and 2 were characterized by elemental analysis, IR, PXRD and single crystal X-ray diffraction. Compound 1 crystallizes in the orthorhombic system with the space group $P2_12_12$ and consists of a PF_6^- anionic part and a $[Dy(L_{OMe})_2(H_2O)_2]^+$ cationic one. The central Dy^{3+} is coordinated by eight oxygen atoms, six of which come from two L_{OMe}^- ligands and two from coordinated water molecules. Compound 2 crystallizes in the monoclinic system with the space group $P2_1/c$. The Dy^{3+} center is coordinated by eight oxygen atoms from two L_{OMe}^- ligands and a nitrate anion. Each Dy ion adopts a square anti-prism geometry and the local symmetry is nearly D_{4d}. Detailed structural and magnetic studies will be given in the presentation.

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Synthesis and Characterisation of Bio-inspire Iron Complexes as Catalysts for Hydrocarbon Oxidation

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이화여자대학교 바이오융합과학과 [1]이화여자대학교 화학과

Bio-inspired catalytic hydrocarbon oxidations with iron complexes are challenging topics in biochemistry of indispensable enzymes. As part of our continuous efforts to develop models of heme-containing enzymes, we have reported a high-valent iron (IV) oxo porphyrin π-cation radical complex for catalytic oxygenations of hydrocarbons. The iron (IV)?oxo porphyrin π-cation radicals with different axial ligands have been prepared and studied in various oxidation reactions, in an effort to understand the electronic effects of porphyrin and axial ligands on the chemical properties of the intermediates. Based on the above results, we synthesized and characterised of our final goal of the new molecular catalysts compound H, [Fe(III)PFC-Im], where the imidazole group act as a axial ligand equivalent to histidine (His) in cytochrome c oxidase (CcO). Now, we are trying to study the generation of iron (V)?oxo species by reacting of [Fe(III)PFC-Im] with PhIO as artificial oxidant in CH_2Cl_2 : MeOH (v/v = 1:1) at -40 ˚C. Further study of the intermediate in C-H bond activation and oxygen atom transfer reaction etc., will be discussed in this presentation.

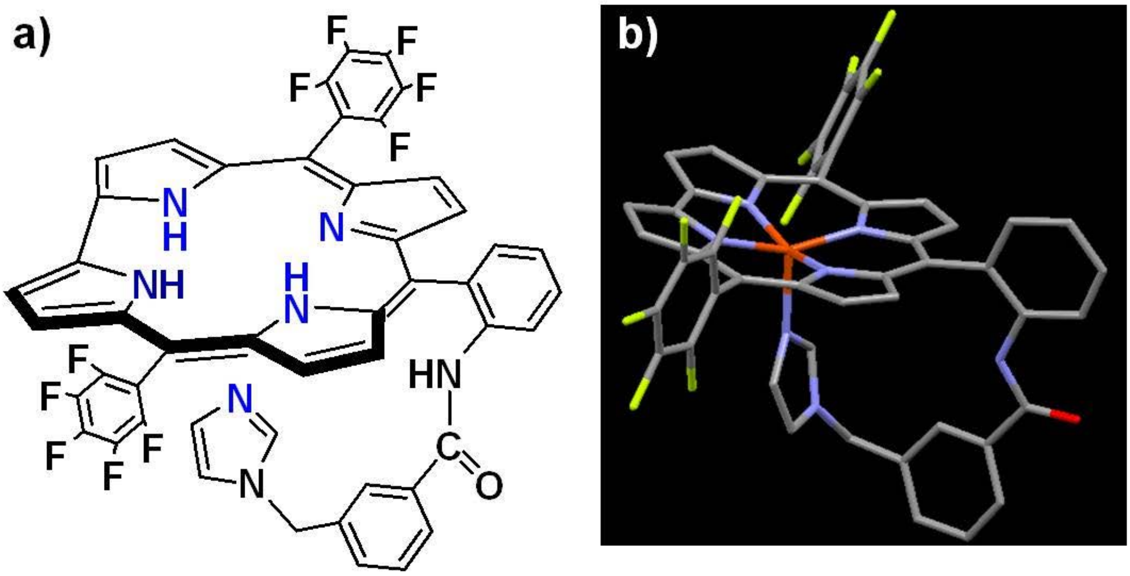

Figure 1. a) Schematic structure of PFC-Im ligand, and b) X-ray crystal structures of compound H, [Fe(PFC-Im)]

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Crystal structure and magnetic property of circular dinuclear Cu(II) complex

원미선 김양[1] 조정환

고신대학교 화학신소재학과 [1]고신대학교 화학 신소재학과

The syntheses, crystal structures, and magnetic properties of low-dimensional transition metal complexes continue to receive a great deal of attention, in part motivated by the desire to uncover new functional materials. Circular dinuclear Cu(II) complex [Cu2L2] incorporating 2,2'-((1E,1'E)-((1,3-phenylenebis(methylene))bis(azanylylidene))bis(methanylylidene))diphenolate (L) was synthesized and its X-ray crystal structure and variable temperature magnetic property determined. Its X-ray crystal structure shows that each Cu(II) centre is bound to one nitrogen and oxygen atoms from each ligand, L.

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Preparation and characterization of chlorobridged tetranuclear Cu(II) bispidine complex

한소영 원미선 김양[1] 조정환

고신대학교 화학신소재학과 [1]고신대학교 화학 신소재학과

The bispidine platform has proven to be extremely useful for the generation of multidentate ligands, in particular ditopic species suited to the formation of binuclear complexes. In the case of Cu, the separation of the metal ions in these binuclear species can be such as to provide useful models of copper oxidase enzymes, especially of intermediate species involving oxygen coordination. We report herein the characterisation of the complex of a binucleating bispidine derivative with copper(II) chloride in which chloride bridging in the solid state leads to the presence of centrosymmetric tetranuclear units in which there are inequivalent inner and outer magnetic centres.

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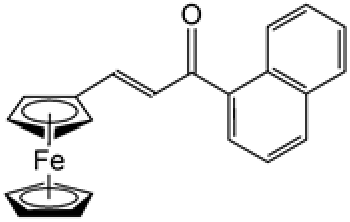
Ferrocenyl Chalcones with Naphthalenyl Group: Electrochemical and Fluorescence Properties

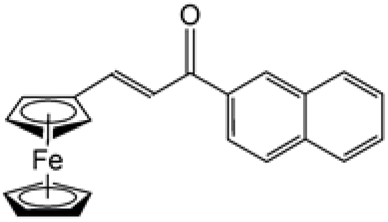
이지원 송성예 전효경 노동윤*

서울여자대학교 화학과

Ferrocenyl chalcones, 1Naph-C(O)CH=CH-Fc (1Naph-Fc) and 2Naph-C(O)CH=CH-Fc (2Naph-Fc), were prepared by a base-catalyzed aldol condensation and spectroscopically characterized. They exhibit one reversible redox cycle for the ferrocenyl moiety and one irreversible oxidation peak for the naphthalenyl moiety. The details of electrochemical properties and fluorescence properties will be presented in comparison with their isomers, Fc-1Naph and Fc-2Naph.



1Naph-Fc



2Naph-Fc

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Synthesis of a New Face-to-Face dinuclear Bis(macrocylic) Nickel(Ⅱ) Complex

김주영 강신결 곽지훈[1]

대구대학교 화학과 [1]순천대학교 화학교육과

Ethylene glycol reacts selectively with one of the two cyanomethyl group in $[NiL^1(OAc)]^+$(L^1=1,8-bis(cyanomethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane) in the presence of $HClO_4$ to yield $[NiL^2]^{2+}$ bearing one N-$CH_2C(=NH)OCH_2CH_2OH$ pendant arm. The complex $[NiL^3]^{2+}$ bearing two N-$CH_2C(=NH)OCH_2CH_2OH$ pendant arms can also be prepared by the reaction of $[NiL^2]^{2+}$ with ethylene glycol. In the presence of triethylamine, $[NiL^2]^{2+}$ undergoes intermolecular nucleophilic addition to yield the face-to-face dinuclear complex $[NiL^4]^{4+}$, where two macrocyclic units are linked together by two N-$CH_2C(=NH)OCH_2CH_2OC(=NH)CH_2$-$N$ linkages. Each mononuclear unit of the dinuclear complex has *cis*-octahedral coordination geometry.

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Reactions of Azide ion with *N*-Cyanoethyl pendant Arms of Tetraaza Macrocyclic Nickel(Ⅱ) and Copper(Ⅱ) Complexes

이지영 강신결

대구대학교 화학과

Sodium azide reacts with two *N*-CH_2CH_2CN groups of $[NiL^1]^{2+}$ (L^1 = 2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}0^{7.12}$]docosane) to yield $[Ni(H_2L^2)]^{2+}$ bearing two tetrazole pendant arms that are not involved in coordination in the solid state. On the other hand, the anion reacts with only one of the two *N*-CH_2CH_2CN groups in $[CuL^1]^{2+}$ to produce $[Cu(HL^3)]^{2+}$ bearing one tetrazole pendant arm that is coordinated to the central metal ion. Two deprotonated forms, $[Ni(HL^2)]^+$ and $[NiL^2]$, as well as the deprotonated form $[CuL^3]^+$ can be isolated selectively from aqueous solutions of the complexes. Synthesis and coordination behaviors of the nickel(Ⅱ) and copper(Ⅱ) complexes are presented.

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Metal-Template Synthesis and Characterization of Unsaturated Tetraaza Acyclic and Pentaaza Macrocyclic Nickel(II) Complexes

장보우 강신걸

대구대학교 화학과

The reaction of 7-amino-4,4-dimethyl-5-azaheptan-2-one with ethylenediamine in the presence of the metal ion produces the unsaturated tetraaza acyclic nickel(II) complex $[NiL^1]^{2+}$ (L^1 = 4,6,6-trimethyl-3,7-diaza-non-3-en-1,9-diamine) with a 5-6-5 chelate ring sequence. Various 14-membered pentaaza macrocyclic nickel(II) complexes, $[NiL^2]^{2+}$ (L^2 = 1-alkyl derivatives of 1,3,6,10,13-pentaazacyclotertradeca-6-one), can be prepared by the reaction of $[NiL^1]^{2+}$ with alkyl amines ($R\text{-}NH_2$) and formaldehyde. The dinuclear complex $[Ni_2L^3]^{4+}$, in which two 14-membered tetraaza macrocyclic units are linked together by a $N\text{-}CH_2CH_2\text{-}N$ linkage has also been prepared. All the nickel(II) complexes have square-planar coordination geometry. Synthesis and characterization of the unsaturated macrocyclic complexes are presented.

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Synthesis of new MOF through heterovalent-mixed-metal approach and its gas sorption behavior.

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한양대학교 응용화학과

Some metal-organic frameworks (MOFs) based on high valent metal ions, such as Ti or Zr, and carboxylate ligands are known to exhibit hydrothermal stability which is required for practical applications. Those MOFs, however, are limited in diversity, and in general it is very difficult to discover a new phase as single-crystalline materials. Therefore, we attempthed to synthesize new MOFs that contain both divalent and tetravalent metal ions within the same framework. In one of these attempts, we successfully obtained a new porous MOF in which two types of heterovalent metal ions are included with well-defined stoichiometry. The crystal structure, gas sorption properties and stability in water are reported.

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Calix[4]arene-based supramolecular Gels Triggered by K^+ or Rb^+

황두미 이은지 이심성 박기민*

경상대학교 화학과

Calixarene derivatives with multiple binding sites and flexible conformation frequently promote an effective cross-linking to form a polymeric network that is critical for gelation. To investigate the calix[4]arene derivative-based gelator, $(Et_3NH)_2{\cdot}H_2CTA$ was prepared from the reaction of calix[4]arene tetraacetic acid (H_4CTA) and triethylamine in methanol. Upon addition of the aqueous solution of K^+ and Rb^+ to the methanolic solution of $(Et_3NH)_2{\cdot}H_2CTA$, the respective metallogels $[K_2@H_2CTA]_n$ (1) and $[Rb\{Rb_{1.5}@H_{1.5}CTA]_n$ (2) with network structures possessing solvents were generated immediately (*see below*). In the experiment for the sol-gel phase transition stimulated by the temperature change, 2 exhibits the reversible process many times without significant degradation. While upon heating gel 1 was converted to the sol state but did not recover the gel state again after cooling, indicating the sol-gel process is not reversible under this condition. The observed gel-stability and the different sol-gel reversibility could be arise from the structural characteristics of gels formed. In order to investigate the structure-property relationship for gels 1 and 2, the related single crystals of each species was obtained. According to the crystal structures, 1 and 2 exhibit a self-assembled network topologies of a typical polymer gel formed by H-bonds and a coordination polymer gel linked by coordination bonds, respectively. In this presentation, we report the formation and the properties of the metal-triggered supramolecular gels based on calix[4]arene derivative as well as their crystal structures.


LiCl
NaCl
KCl
RbCl
CsCl

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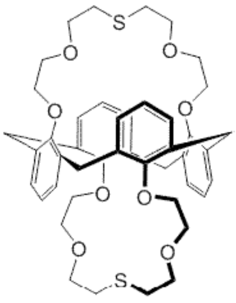
Beyond the Dipotassium(I) Complex of Calix[4]-*bis*-thiacrown: X-ray and NMR Studies on Discrete Homonuclear Species and Heteronuclear Network

김자연 이심성[*] 이재영[1]

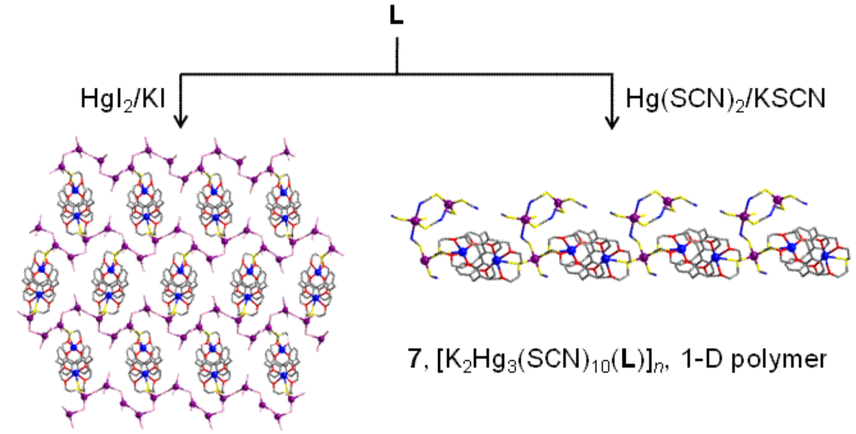
경상대학교 화학과 [1]건양대학교 나노바이오화학과

In the extension of our previous work on the exocyclic coordination polymers of calix[4]-*bis*-monothiacrown (L) exhibiting a photoluminescence switching behavior,[1] its new networking patterns via homo- and heteronuclear system are reported. In the reactions of L with $Hg(SCN)_2$ and HgI_2 gave commonly 1D coordination polymers 1, $[Hg_2(SCN)_4(L)]n$ and 2, $\{[Hg_2I_4(L)]\cdot CH_2Cl_2\}_n$ with a similar network pattern, in which Ls are linked by -X-Hg-X_2-Hg-X- (X=SCN for 1, X=I for 2). CdI_2 also gave a 1D coordination polymer 3, $[Cd_2I_4(L)]n$ showing a similar pattern. Interestingly, the reaction of CdI_2 in the presence of HgI_2 afforded a 1D coordination polymer 4, $[Cd_3Hg(L_2)I_8]_n$ linked with -I-Cd-I_2-Cd-I- and -Hg(I_2-Cd-I_2)-, alternatively. Treatment of L with KI in the presence of CdI_2 afforded a discrete endocyclic dipotassium(I) complex 5, $[K_2(L)][Cd_2I_6]\cdot CH_2Cl_2$, in which the square-type dicadmium(II) hexaiodide cluster $[Cd_2I_6]^{2-}$ exists in a separated form. The reaction of L with KI in the presence of HgI_2 afforded a 2D brick-wall type coordination polymer 6, $[K_2Hg_4I_{10}(L)]n$ with the endocyclic dipotassium(I) complex linked by exocyclic mercury(II) iodide cluster backbone. In addition, the reaction of L with KSCN in the presence of $Hg(SCN)_2$ afforded an endo/exocyclic heteronuclear complex 7, $[K_2Hg_3(SCN)_8(L)]n$ with a 1D polymeric structure. To obtain the further inforamtion on the behavior of the dipotassium(I) complexation of L and also the reactivity of the O_4S crown rings towards the hard and soft metal ion species, the competition complexation studies of L in the presence of potassium(I) and silver(I) (as hexafluorophosphate) in solution were performed by ^1H NMR. The result from NMR confirms that potassium(I) forms more stable dinuclear-type complexes with L than silver(I) in solution.

Reference 1. Lee, J. Y.; Kim, H. J.; Jung, J. H.; Sim, W.; Lee, S. S. *J. Am. Chem. Soc.* 2008, *130*, 13838.



L



7, $[K_2Hg_3(SCN)_{10}(\mathbf{L})]_n$, 1-D polymer

6, $[K_2Hg_4I_{10}(\mathbf{L})]_n$, 2-D polymer

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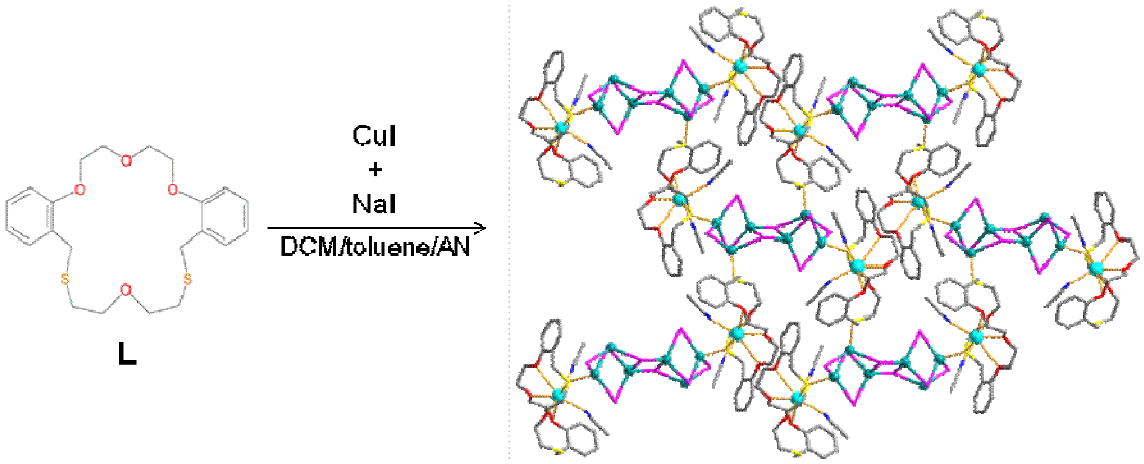
Assembly of Soft and Hard Metal Complexes of an O_4S_2-Macrocycle Displaying Endocyclic Monomer, Exocyclic Dimer, and Endo/Exocyclic Heteronuclear Polymer Structures

류현수 이심성*

경상대학교 화학과

An O_4S_2-macrocycle L incorporating dibenzo subunits was synthesized and structurally characterized by X-ray analysis. The X-ray crystal structures of six complexes (1-6) have been determined, and a range of structural types and coordination modes, including discrete to continuous forms, mono- to multinuclear, and endo- to exocyclic structures involving M-S and M’-O bonds are presented. First, reactions of L with heavy metal salts such as HgI_2, CdI_2, and $Pb(ClO_4)_2$, afforded the exocyclic mononuclear isostructural complexes $[M(L)I_2]$ (1: M = Hg, 2: M = Cd) as well as a typical endocyclic mononuclear complex $[Pb(L)(ClO_4)_2]$ (3). Reaction of, L with silver(I) nitrate afforded the exocyclic dimer, $[Ag_2(L)_2(NO_3)_2]$ (4), linked with the square-type Ag-$(NO_3)_2$-Ag unit. Furthermore, the straightforward one-pot reaction of L with CuI in the absence and presence of NaI resulted in the isolation of the exocyclic dimer $[Cu_2(L)_2I_2]$ (5) linked with the square-type Cu-I_2-Cu unit and the (Na^+/Cu^+) heteronuclear endo/exocyclic complex $[Na_2(L)_2(CH_3CN)_4(\mu_2\text{-}Cu_6I_8)]_n$ (6) with an infinite structure, respectively. In 6, the endocyclic macrocyclic Na^+ complex units are linked by the twisted ribbon-type cluster $[Cu_6I_8]^{2+}$ resulting in the unique 2D network.



L

6, $[Na_2(L)_2(CH_3CN)_4(\mu_2\text{-}Cu_6I_8)]_n$

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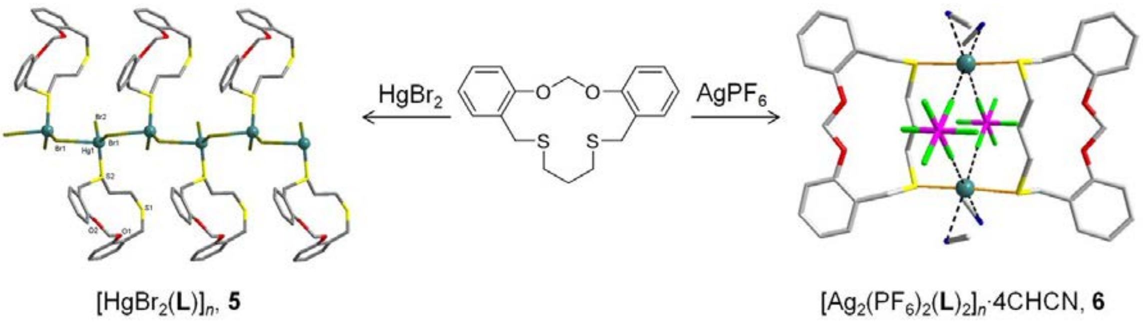
Comparative Structural Study of the Complexation Behavior of Copper(I), Silver(I), Palladium(II), and Mercury(II) with a 14-Membered O_2S_2-Macrocycle

김슬기 이은지 이심성*

경상대학교 화학과

Coordination behavior of the 14-membered dibenzo-O_2S_2-macrocycle, L, with the soft metal ions such as Cu(I), Ag(I), Pd(II), and Hg(II) is reported. The X-ray crystal structures of the complexes have been determined, and a range of less common structural types, including mono-, di-, and multinuclear species with discrete and infinite forms were obtained. L reacts with copper(I) Iodide to yield an infinite complex $[Cu_4I_4(L)]_n$ (1), in which the macrocycles are linked by cubane-type Cu_4I_4 cluster. While, the parallel reactions of copper(I) bromide and chloride afforded an isostructural $[Cu_2X_2(L)]_n$ (2: X = Br, 3: X = Cl) with one-dimensional polymeric structure linked by square-type Cu_2X_2 cluster. Reactions of L with HgX_2 (X = I and Br) yielded the one-dimensional species $[Hg_2I_4(L)]_n$ (4) and $[HgBr_2(L)]_n$ (5), respectively. Reaction of L with $AgPF_6$ afforded a bicyclic dimer complex $[Ag_2(L)_2](PF_6)_2{\cdot}4CH_3CN$ (6), in which two PF_6^- ions weakly bridge two Ag atoms in a bidentate manner to form a three-dimensional bicycle. In the reaction of L with $Pd(NO_3)_2$, a bis(O_2S_2 macrocycle) complex $[Pd(L)_2](NO_3)_2$ (7) was isolated.



$[HgBr_2(\mathbf{L})]_n$, **5**

$[Ag_2(PF_6)_2(\mathbf{L})_2]_n{\cdot}4CHCN$, **6**

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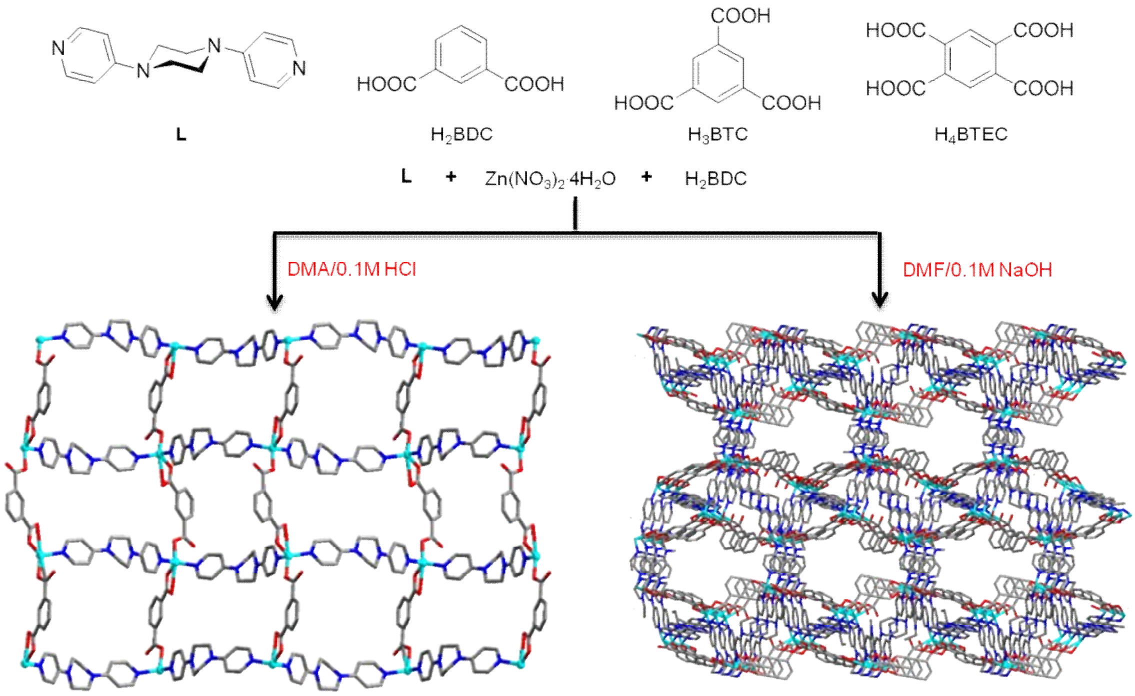
Multi-dimensional MOFs Based on 1,4-Bis(4-pyridiyl)piperazine and Aromatic Carboxylic Acid

주희영 박기민* 이심성*

경상대학교 화학과

Solvothermal reactions of 1,4-bis(4-pyridiyl)piperazine (L) with zinc(II) nitrate in the presence of aromatic carboxylic acids (H_2BDC, H_3BTC, and H_4BTEC) enabled the isolation of metal-organic frameworks (MOFs) (1-4). The reaction of L, $Zn(NO_3)_2{\cdot}4H_2O$, and H_2BDC in DMA yielded a 2D coordination polymer $\{[Zn(L)(BDC)]{\cdot}2DMA{\cdot}2H_2O\}_n$ (1). When DMF was used in the same reaction instead of DMA, interestingly, a supramolecular isomer $\{[Zn_2(L)_2(BDC)_2]{\cdot}xDMF\}_n$ (2) was isolated. In addition, the reaction of L with $Zn(NO_3)_2{\cdot}4H_2O$ in the presence of H_3BTC and H_4BTEC gave a 3D polymeric species $\{[Zn_3(BTC)_2]{\cdot}(L){\cdot}(H_2O)_4\}_n$ (3) and a grid-type 2D network $\{[Zn_2(BTEC)]{\cdot}(L)\}_n$ (4), respectively. In the gas sorption isotherms at 77 K, 1 shows the N_2 adsorption up to 120 mL/g (P/P_0 0 ~ 1).



2D Zn(II) Coordination Polymer **1**, $\{[Zn(\mathbf{L})(BDC)]\cdot 2DMA\cdot 2H_2O\}_n$

3D Zn(II) Coordination Polymer **2**, $\{[Zn_2(\mathbf{L})_2(BDC)_2]\cdot xDMF\}_n$

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3D Pillared-Layered Co(II) MOFs with Long Spacer Ligand and Linear Dicarboxylic Acids

박인혁 **Anjana Chanthapally**[1] 김자연 이심성* **Jagadese J. Vittal**[1,*]

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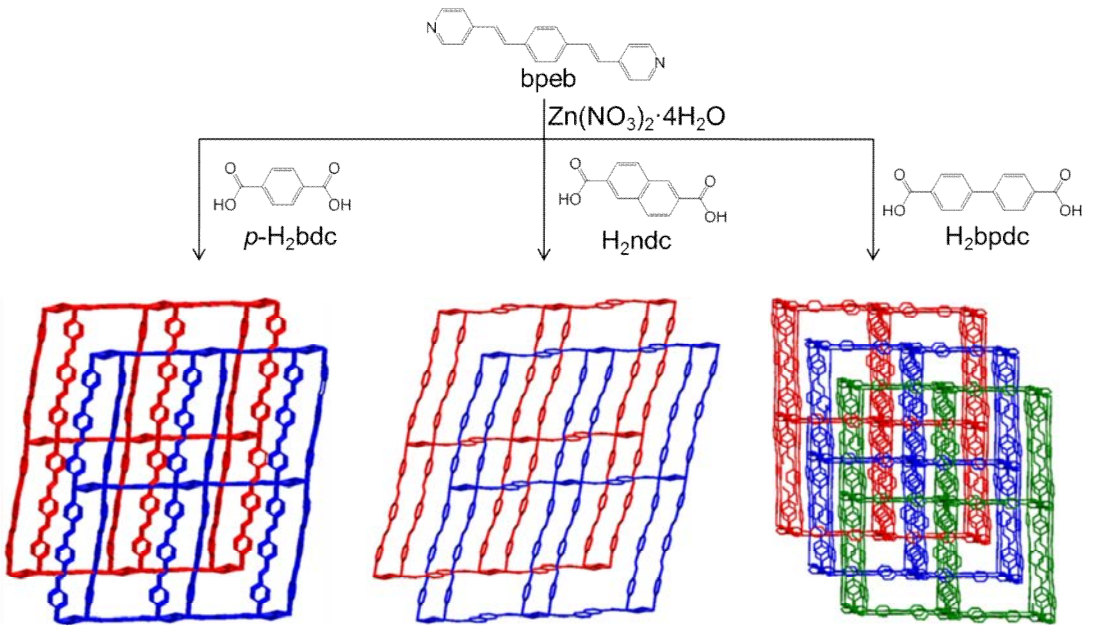
Three Co(II) MOFs (1-3) of a long olefinic dipyridyl spacer ligand (bpeb) and linear dicarboxylic acids (p-H_2bdc, H_2ndc, or H_2bpdc) showing different conformations are reported. The assembly reaction of bpeb with Co(II) in the presence of p-H_2bdc allowed us to isolate a 2-fold interpenetrated 3D pillared-layer MOF, $\{[Co_2(p\text{-bdc})_2(\text{bpeb})_2]\cdot DMF\cdot 4.5H_2O\}_n$ (1) with a *trans-trans-trans* and a *trans-cis-trans* conformations of bpeb as a pillar ligand. When the linear dicarboxylic acid was changed with H_2ndc in same reaction, again we obtained a 2-fold interpenetrated 3D pillared-layer MOF, $\{[Co_2(\text{ndc})_2(\text{bpeb})_2\cdot 1.5DMF\cdot 3H_2O\}_n$ (2) with a larger pore size than that of 1 adopting the trans-cis-trans conformation of bpeb. When the H_2bpdc was employed, a similar 3D MOF, $\{[Co(\text{bpdc})(\text{bpeb})]\cdot DMF\cdot 0.5DMSO\cdot H_2O\}_n$ (3) in which the bpeb shows *trans-cis-trans* conformation and its smaller pore is smaller due to the 3-fold interpenetration. Although the three 3D MOFs prepared satisfy the conditions for the photodimerization but, to our surprise, they were found to be photo-inactive. The conformational changes of bpeb and the pore sizes in each MOF depending on the linear dicarboxylic acids were discussed.



1, $\{[Co_2(p\text{-}bdc)_2(bpeb)_2]\cdot DMF\cdot 4.5H_2O\}_n$ **2**, $\{[Co_2(ndc)_2(bpeb)_2]\cdot 1.5DMF\cdot 3H_2O\}_n$ **3**, $\{[Co(bpdc)(bpeb)]\cdot DMF\cdot 0.5DMSO\cdot H_2O\}_n$

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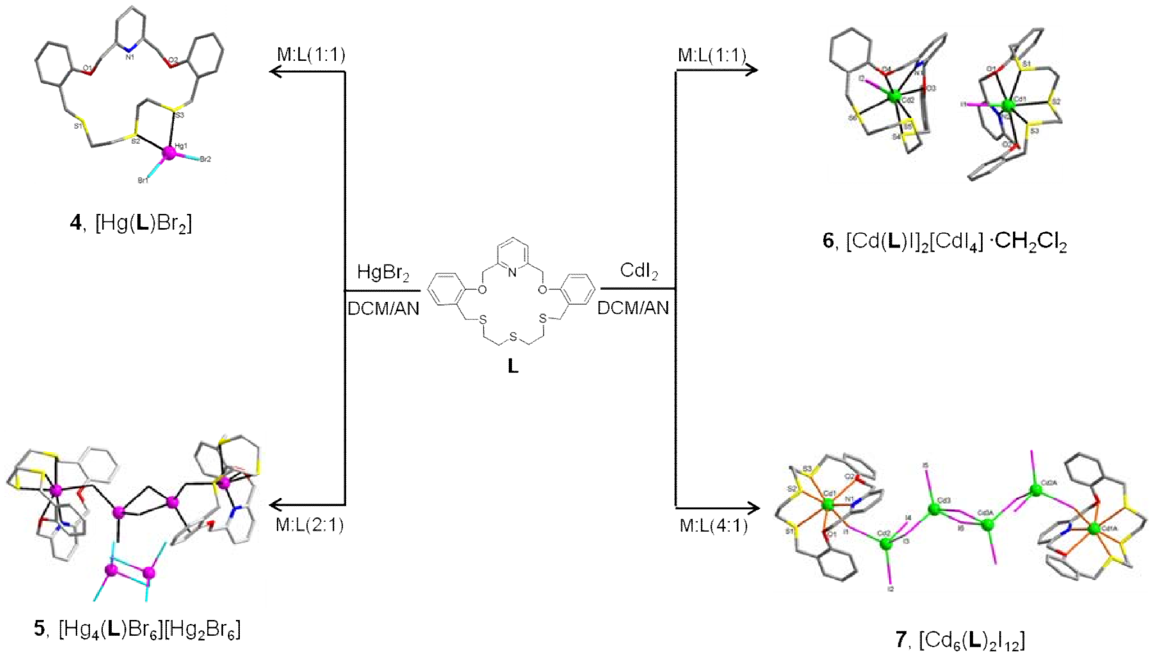
Mole-Ratio Dependent Metallosupramolecules of Thiaoxaaza-Macrocycle

이형환 이심성*

경상대학교 화학과

The pyridine-containing thiaoxaaza-macrocycle L was synthesized by dithiol-dichloride coupling reaction using Cs_2CO_3 in DMF under high dilution condition. Comparative investigation of the coordination behavior of L with Ag(I), Cu(I), Hg(II), and Cd(II) is reported. The X-ray structures of seven complexes (1-7) were determined, and a range of structural types and coordination modes including mono- to multinuclear and discrete to continuous ones, is shown to occur. In the reaction with $AgNO_3$, L forms a rare example of a 1D coordination polymer $\{[Ag_2(L)(NO_3)_2]\cdot CH_3CN\}_n$ (1) incorporating endo/exocyclic metal ion coordination. The reaction of L with mercury(II) perchlorate gave an endocyclic complex $[Hg(L)](ClO_4)_2$ (2). In the reaction with CuI, L forms an exocyclic 1D coordination polymer $[Cu_2(L)I_2]_n$ (3) linked by Cu_2I_2-rhomboid giving a zigzag chain. The reaction of L with $HgBr_2$ afforded the mole-ratio dependent products $[Hg(L)Br_2]$ (4: 1 equiv of $HgBr_2$) and $[Hg_4(L)Br_6][Hg_2Br_6]$ (5: 2 equiv of $HgBr_2$) (*see below*). In the reaction of L with CdI_2, again, $[Cd(L)I]_2[CdI_4]\cdot CH_2Cl_2$ (6: 1 equiv of CdI_2) and $[Cd_6(L)_2I_{12}]$ (7: 4 equiv of CdI_2) were isolated depending on the mole-ratio of CdI_2 (*see below*).


M:L(1:1)
HgBr$_2$
DCM/AN
M:L(2:1)
CdI$_2$
DCM/AN
M:L(1:1)
M:L(4:1)
L
4, [Hg(L)Br$_2$]
5, [Hg$_4$(L)Br$_6$][Hg$_2$Br$_6$]
6, [Cd(L)I]$_2$[CdI$_4$] ·CH$_2$Cl$_2$
7, [Cd$_6$(L)$_2$I$_{12}$]
O1
N1
O2
S1
S2
S3
Hg1
Br1
Br2
Cd1
Cd2
Cd3
Cd2A
Cd3A
Cd1A
I1
I2
I3
I4
I5
I6

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Ag(I) Coordination Networks of Bis(cyanobenzyl)sulfide Ligands: Ligand Isomer Effect and Mole-Ratio Dependent Metallosupramolecular Isomerism

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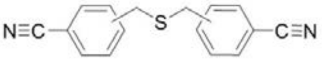
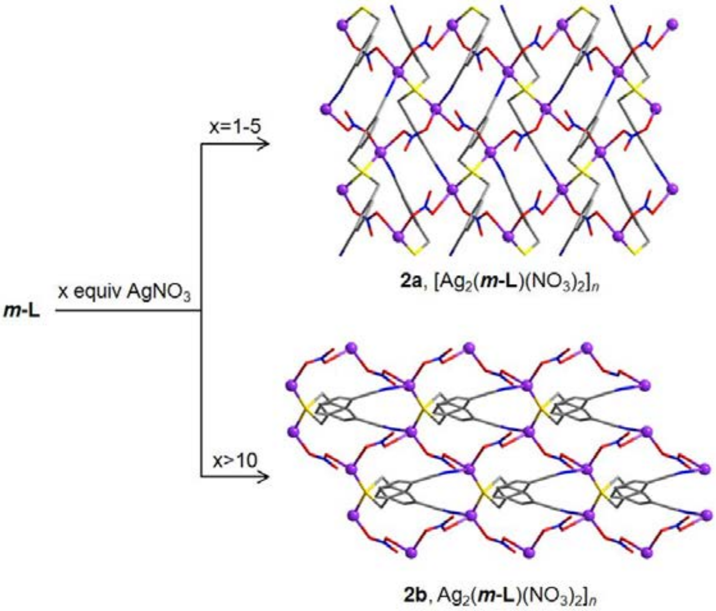
경상대학교 화학과

Regioisomers of bis(cyanobenzyl)sulfide incorporating a xylyl group in the *ortho* (*o*-L), *meta* (*m*-L), and *para* (*p*-L) positions were employed to examine the effect of ligand isomers on the networking assembly with silver(I) nitrate. *o*-L yielded a 1-D loop-type coordination polymer 1, $[Ag(o\text{-}L)NO_3]_n$, while *m*-L under the same condition gave supramolecular isomers 2a and 2b of the type $[Ag_2(m\text{-}L)(NO_3)_2]_n$ with different 2-D network structures depending on the mole-ratios of reactants (*see below*). Both of the supramolecular isomers 2a and 2b are consist of the 2-D layers constructed by the combination of a zigzag $-(AgNO_3)_n-$ inorganic chains with *m*-L acting as a bridging ligand. Notably, the overall structural motifs of the supramolecular isomers 2a and 2b are mainly due to the conformational variation of the ligand: *anti*-conformation in 2a and *syn*-conformation in 2b. *p*-L afforded a 3-D network $[Ag_2(p\text{-}L)(NO_3)_2]_n$ (3) made up of the double-stranded $(Ag\text{-}L)_n$ backbones further bridged by anion.



o-L
***m*-L**
***p*-L**



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Synthesis and characterization of new MOF having the fluorite topology

박우정 전형필*

한양대학교 응용화학과

It is very difficult to observe the fluorite topology in metal-organic frameworks (MOFs) because the 4,8-connectivity requires two types of building blocks which are tetrahedral and cubic, respectively. Therefore, a rational approach would use ligands with a rigid tetrahedral backbone and attempt to form the secondary building unit having the connectivity of cubic nodes. In this work we demonstrate that such an elaboration is not necessary and only a judicious choice of organic ligands as simple as the derivatives of terephthalic acid is sufficient to realize the noble topology in MOF. We report the synthetic approach, crystal structure and various properties of a new MOF having the 4,8-connected fluorite topology.

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BODIPY 유도체를 기반으로 한 분자 로직 게이트의 제조

최희경 이지하 정종화*

경상대학교 화학과

본 연구에서는 분자 로직 게이트를 제조하기 위해서 화합물 1 을 7 단계에 걸쳐 합성하였다. 이렇게 합성된 화합물 1 을 자성체 나노 입자 Fe_3O_4에 고정화 시켰다.

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발표분야: 무기화학

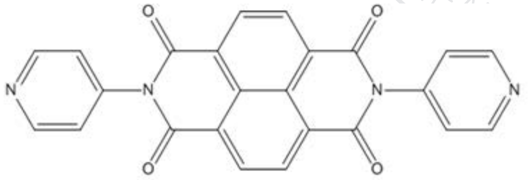
발표종류: 포스터, 발표일시: 수 16:00~19:00

이성분계 하이드로 젤의 형광특성 연구

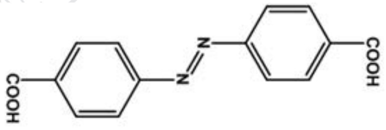
이지하 정종화*

경상대학교 화학과

이성분계 하이드로 젤의 제조는 화합물 1 과 2 를 일정 비율로 섞어서 물에서 준비하였다. 하이드로 젤은 화합물 1 용액에 약 0.8 당량의 화합물 2 가 첨가 될 때까지 형성되었으나, 그 이상에서는 형성하지 않았다. 이렇게 준비된 하이드로 젤의 특성은 전자현미경, 형광분광기, XRD 및 시분해능 형광 분광기를 이용하였다. 하이드로 젤 형광 스펙트럼은 화합물 2 의 양이 증가할수록 장파장 쪽으로 이동하였으며, life time 이 증가하였다. 이는 하이드로 젤에서 화합물 1 과 2 사이에 전하 이동이 일어나기 때문이다



1



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발표코드: **INOR.P-141**

발표분야: 무기화학

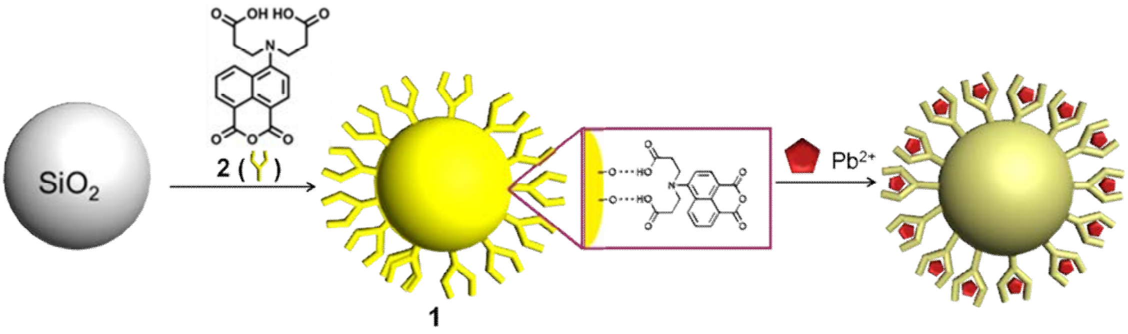
발표종류: 포스터, 발표일시: 수 16:00~19:00

나프탈렌 유도체가 고정화된 SiO_2 나노입자를 이용한 Pb^{2+} 검출에 대한 연구

이진혁 정종화*

경상대학교 화학과

본 연구는 Pb^{2+} 이온을 검출하기 위해서 유기-무기 하이브리드 소재를 제조하였다. 납 검출용 TLC 는 나프탈렌 유도체가 고정화된 SiO_2 를 이용하였다. 리간드 2 가 SiO_2 나노입자에 결합이 되었고 나프탈렌 유도체의 고정화에 대한 구체적인 분석은 FT-IR, TGA 등을 이용하였다. 그 결과 리간드 2 가 SiO_2 나노입자에 34.95% 가 흡착이 된 것을 확인하였다. 나노입자 1 의 형광변화는 pH 7.4 수용액에서 형광 분광기를 이용하여 관찰하였다. 그 결과 나노입자 1 은 550 nm 에 강한 형광스펙트럼을 나타내었으나, Pb^{2+} (10 당량) 을 첨가한 결과 550 nm 의 스펙트럼은 급격하게 감소 하였다. 반면에 수용액 나노입자 1 은 다른 금속이온 (Cu^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Hg^{2+}, Fe^{2+}, Na^{2+}, Ni^{2+}, Zn^{2+}, Mg^{2+}) 의 경우는 어떤 형광 선택적 변화도 유도하지 않았다. 이는 수용액나노입자 1 은 Pb^{2+} 이온과 선택적으로 결합하기 때문이다.



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G-Quadruplex DNA를 검출할 수 있는 파이렌-이미다조리움 유도체를 도입한 그래핀 형광센서의 제조

박소현 정종화*

경상대학교 화학과

본 연구에서는 파이렌-이미다조리움 유도체(JY-1)와 그래핀을 이용하여 G-quadruplexes DNA 를 검출하고자 하였다. 그래핀의 표면의 기능화는 파이렌-이미다조리움 유도체를 π-π stacking 에 의해서 고정하였고, 다양한 DNA 와 선택적인 상호작용에 대한 연구는 형광분광기를 이용하여 수행하였다. 먼저 파이렌-이미다조리움 유도체가 고정화된 그래핀을 수용액에 첨가한 후에, DNA 를 넣어서 형광 스펙트럼 변화를 관찰하였다. 그 결과, 구아닌 3 개 이상을 가지고 있는 다양한 DNA 와 선택적인 결합으로 인해 강한 형광 스펙트럼을 나타냈다. 이는 그래핀 표면에 고정화 된 파이렌-이미다조리움 유도체가 떨어져 DNA 와 상호작용을 하기 때문이다. 그리고 그래핀-파이렌 이미다조리움 유도체는 약 pM 농도의 DNA 를 검출할 수 있었다.

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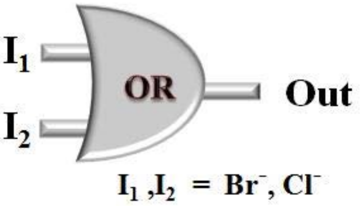
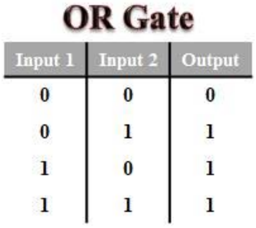
Coordination Polymer Gel with Co^{2+} ion and Its Application to Logic Gate

정성호 정종화*

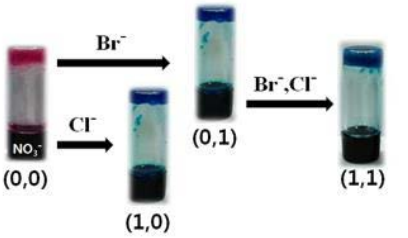
경상대학교 화학과

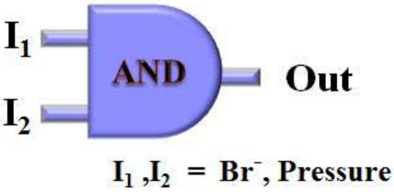
금속 배위 고분자 젤의 배위 메커니즘을 연구 하기 위해 이미다졸기를 가지고 있는 리간드 1 을 이용하여 배위환경에 따라 색이 변화는 코발트 배위 고분자 젤에 대해서 연구 하였다. 유기용매 조건에서 코발트의 음이온이 NO_3^-인 경우 리간드 1 이 배위되어 붉은색 배위 고분자 젤을 형성 하였으며, 코발트의 배위 환경이 6 배위 착물을 형성 할 경우 붉은색 배위 고분자를 형성한다는 것을 결정을 통해 확인 하였다. 그리고 음이온이 Cl^-, Br^- 이온인 경우 푸른색 배위 고분자 젤을 형성 하였으며, 이것은 코발트에 리간드 1 이 배위되어 4 배위 착물을 형성하여 푸른색을 나타낸다는 예상 할 수 있었다. 또한 색변화를 통해 로직게이트인 AND 와 OR 게이트에 응용 할 수 있었다.

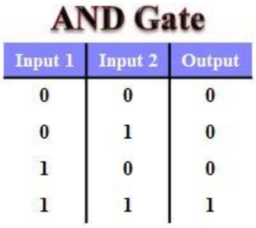



OR Gate

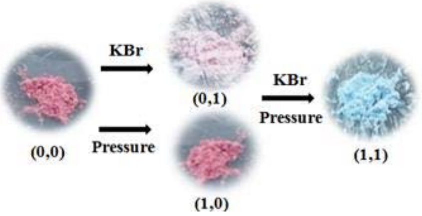
Input 1	Input 2	Output
0	0	0
0	1	1
1	0	1
1	1	1






AND Gate

Input 1	Input 2	Output
0	0	0
0	1	0
1	0	0
1	1	1



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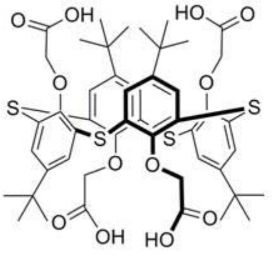
Thiacalix[4]arene을 기반으로 한 화학적 센서 Gel

김가영 정종화[*]

경상대학교 화학과

자가조립은 분자에 대한 규명과 기능적인 소재로서 개발할 수 있는 기반을 보여준다. 이러한 자가 조립을 바탕으로 형성되는 배위 고분자 젤은 조직 공학, DDS(drug delivery system) 그리고 화학센서로서 광범위한 범위에서 응용되고 있다. 본 연구에서는 MOF (metal-organic framework) 화학에서 널리 바탕으로 사용되는 Calix[4]arene 을 기반으로 화합물 p-tert-butyl-thiacalix[4]arene tetraacetic acid(H_4TCTA, 1)를 제조하여 Co^{2+} 과 함께 화학적 센서로서의 배위 고분자 젤의 기능을 연구 하였다. 1 에 Co^{2+}를 첨가하여 DMF/H_2O 조건에서 젤을 제조하여 붉은색을 나타내었으나, 온도 증가 및 Cl^- 농도 증가에 의해서 푸른색으로 변화하였다. 이는 Co^{2+} 착물이 6 배위 화합물에서 4 배위 화합물로 변화하기 때문이다. 이러한 결과를 이용하여 Cl^-에 선택적으로 감응하는 센서 개발을 시도하였다. 그 결과 Co^{2+} 착물 젤은 Cl^-를 포함하는 화합물에 대해서 붉은색에서 푸른색으로 변화하였다. 따라서 Co^{2+} 착물 젤은 Cl^-를 검출할 수 있는 센서로 활용가능 할 것으로 판단된다.



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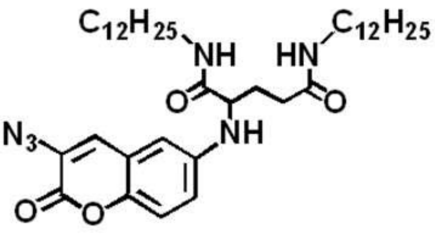
Organogel based on azidocoumarin derivative

박혜경 이지하 정종화*

경상대학교 화학과

화합물 1 은 형광체로서 쿠마린기, 그리고 소수성 특성을 부여하기 위해서 긴 알킬 사슬을 도입하였다. 특히 화합물 1 이 자기조립에 의해서 초분자 젤을 형성할 수 있도록, 수소결합을 형성할 수 있는 glutamic acid 를 도입하였다. 합성된 화합물 1 은 NMR, IR, MS 그리고 원소분석을 통하여 구조를 확인하였다. 화합물 1 의 초분자 젤 형성은 다양한 유기용매(DMF, DMSO, Acetonitile, Acetone, EA, Ethanol, THF, Toluene, Benzene, Hexane, $CHCl_3$, H_2O)에서 테스트한 결과 DMSO, Acetone, Ethanol 에서 나타났다. 그리고 DMSO 에서 형성한 초분자 젤의 특성은 UV-Vis, PL, SEM 등으로 연구하였다. DMSO 에서 형성된 젤의 형광을 측정한 결과, 438 nm 에서 강한 세기를 나타내었다. 또한 SEM 을 통하여 fiber 형태의 젤이 형성된 것을 확인할 수 있었다.



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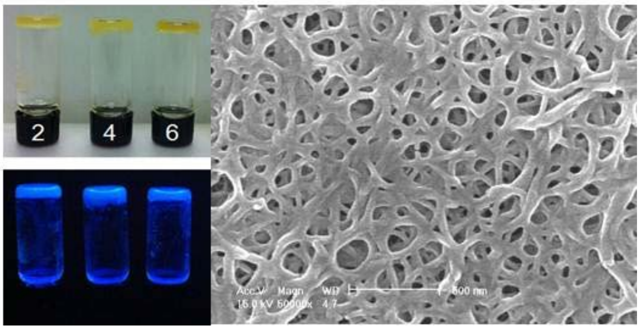

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자기조립 발광성 리간드를 이용한 중금속 센서 개발

이효희 정성호 정종화*

경상대학교 화학과

Terpyridine 을 기반으로 한 tripodal 리간드를 합성하였으며, 이의 광학적 성질과 특정 금속에 대한 화학적 센서로서의 성질을 연구하였다. 형광스펙트럼 측정 결과, 리간드에 대하여 Zn^{2+}, Cd^{2+}이 형광이 유발되며 선택적인 red shift 를 하는 것을 확인할 수 있었다. 이는 Aggregation-induced emission (AIE) 효과이며, metal-to-ligand-charge-transfer process 을 원인으로 추측하고 있다. 또한 리간드에 대하여 Fe^{2+}이 선택적으로 결합하여 자홍색으로 발색되는 것을 확인할 수 있었다.

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칼릭스 아렌과 크라운에테르가 도입된 금 나노입자를 이용한 도파민의 센싱 연구

안진호 박재현 정성호 이지하 정종화*

경상대학교 화학과

본 연구진은 기존에 보고된 칼릭스 크라운이 도파민의 인식에 효과적이라는 사실에 착안하여 보다 간단한 센싱 체계의 확립을 위해 칼릭스 아렌과 크라운에테르를 금 입자 표면에 도입하였다. 호스트로서 칼릭스 아렌과 크라운 에테르를 도입한 금 나노입자와 게스트로서의 도파민 분자가 파이-파이 스택킹과 수소결합을 통해 금 나노입자의 엉김현상을 유발한다. 그로 인해 기존에 붉은색을 유지하던 금 나노입자의 색이 변하게 되는데, 이 현상을 동적광산란, 자외선-가시광선 분광광도계, 수소-핵자기공명분광기, 투과전자현미경을 통해 분석 하였다. 벤젠 유도체를 포함하는 생체 내의 다른 신경 전달물질을 대조군으로 삼아 자외선-가시광선 분광광도계를 측정하여 센서로서의 활용 가능성을 확인 하였다. 이번 연구를 통해 본 연구진은 호스트-게스트 화학에 금 나노입자를 도입하여 보다 간단하고, 쉽게 도파민을 센싱하는 체계를 구축할 수 있었다..

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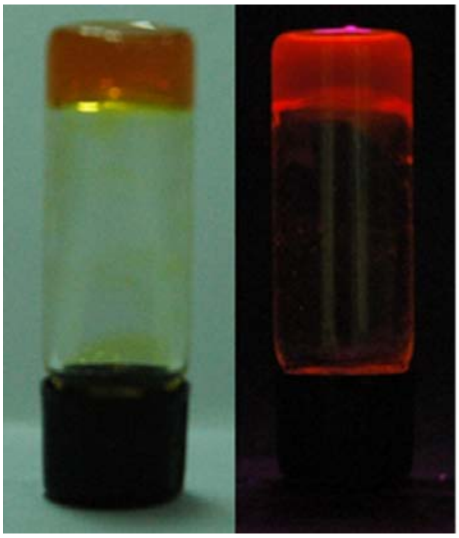
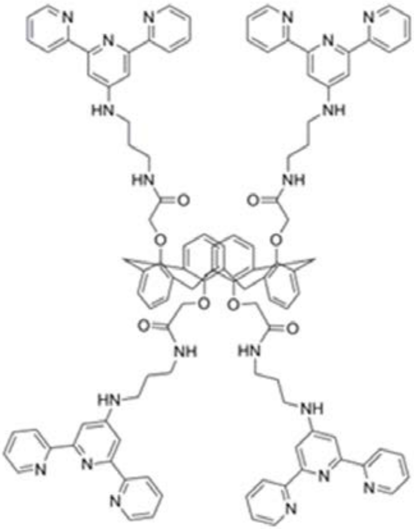
Platinum(II) Terpyridine과 Calix[4]arene이 도입된 Metallogel의 연구

박재현 정성호 이지하 정종화*

경상대학교 화학과

d^8 의 전자배치를 가지는 Pt^{2+}는 Terpyridine 과 안정한 사각평면착물을 형성한다. 이러한 Pt^{2+}착물은 아주 특별한 형광특성을 나타내며 이것은 용매와 금속이온의 검출, 광촉매적인 특성, 그리고 생화학적활성에 대한 많은 연구가 이루어지고 있다. Ligand 와 4 당량의 $PtCl_2$는 DMSO 용액에서 4 배위 착물을 형성한다는 것을 Job's plot 법과 ESI-MS 로 확인하였다. 그리고 Calix[4]arene 을 도입함으로써 분자의 3 차원 구조와 대칭성을 부여하였고 H_2O 와 수소결합을 형성할 수 있게 아마이드기를 도입했다. 이를 바탕으로 DMSO 와 H_2O 에서는 주황색의 MetalloGel 이 만들어졌으며 분광학적, 물리적특징을 연구하였다. Metallogel 은 435nm 부근에 강한 UV 흡수가 나타났다. 이는 dπ(Pt)에서 π*(terpy)전하가 이동하는 Metal-to-lignad charge transfer(MLCT)이며, DMSO 용액 상태에서는 형광특성이 나타나지 않았지만 MetalloGel 에서는 660nm 의 강한 형광을 나타내었다. Aggregation-Induced Emission(AIE) 효과이며, 이는 Pt….Pt 와 π-π interactions 의한 Metal-Metal-to-lignad charge transfer(MMLCT)으로 볼 수 있다





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Application of Diverse Technique for Supramolecular Crystallography at 2D Beamline in Pohang Light Source

문도현

포항가속기연구소 빔라인부

The 2D beamline at Pohang Light Source in Korea has been designed to operate in the photon-energy range of 6~20 keV (2.0 ~ 0.61?) based on a bending magnet in PLS II. It is dedicated to single crystal crystallography with inorganic/organic, supramolecule and MOF crystals. The experiment station is equipped with high speed and high sensitivity of an ADSC Quantum Q210 area detector containing a 210mm^2(4096 x 4096 pixel) detection area, high accuracy one-axis goniometer, a cryojet for cooling sample using a liquid nitrogen its controlled 90~400K range, a helijet for extremely low temperature achievement using a liquid helium its 9K temperature, and a scintillation fluorescence detector for simple XANES. Recently, we install the high power laser(250~2100 nm) and Xenon lamp (300W) for catalytic and photoreactivity research. I will provide new technique and challenge work for your extreme research. The status of beamline, equipments and several fabrication techniques will be presented on this poster, also I will find a good collaborator.

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Fluorescent Chemosensor Based on Bispicolylamine for Selective Detection of Magnesium Ions

강희경 이정하 김 철[1,*] 김진홍[*]

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An assay to quantify the presence of magnesium ions with a chemosensor of bispicolylamine covalently attached to coumarin as a fluorephore was developed using a ratiometric fluorescence enhancement approach. Upon treatment with magnesium ions, the fluorescence wavelength of the chemosensor at 367 nm was shifted to 413 nm and the intensity was also enhanced. The formation of a 1:2 complex between the chemosensor and magnesium ions was confirmed based on the spectral changes of UV-vis, fluorescence, and NMR as well as Job's plot. As the concentration of Mg^{2+} was increased, the fluorescence at 413 nm gradually increased along with decreasing that of the chemosensor at 367 nm. The maximum wavelength and intensity of the emission of the complex with Mg^{2+} were discriminated from those of other metal ions, such as Ca^{2+}, Zn^{2+}, etc.

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Fluorescent Chemosensor Containing Phenol-Pyridyl for Selective Detection of Aluminum Ions

김수진 이정하 이가예 김 철[1,*] 김진홍[*]

이화여자대학교 화학·나노과학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

The frequent use of aluminum foil, vessels, and trays for convenience might moderately increase the Al^{3+} concentration in food. After absorption, aluminum will become distributed to all tissues in humans and animals, and accumulates in the bone. The iron binding protein is the main carrier of Al^{3+} in plasma and Al^{3+} can enter the brain and reach the placenta and fetus. Al^{3+} may persist for a very long time in various organs and tissues before it is excreted in the urine. Al^{3+} has been implicated as a causative factor in Alzheimer's Disease and has been associated with damage to the central nervous system in humans. In this study, A phenol-pyridylimine probe was utilized as an optical sensor to quantify the presence of aluminum ions using a turn-on fluorescence enhancement approach. The high sensitivity was the result of FRET amplification of the receptor subunit fluorescence emission. The complex stability constant (Ks) for the stoichiometric 1:1 complex of the sensor with aluminum ions was obtained by fluorimetric titration. Remarkably, fluorescence output was not significantly affected by other trivalent cations, particularly Ga^{3+} and In^{3+}.

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Electrochemical Regeneration of NADH Using $[Cp^*Rh(bpy)(H_2O)]^{2+}$ on Modified ITO Electrodes

김수진 이가예 김진홍*

이화여자대학교 화학·나노과학과

Functionalized ITO electrodes are used to regenerate NADH using $[Cp^*Rh(bpy)(H2O)]^{2+}$ (Cp* = pentamethylcyclopentadienyl, bpy = 2,2’-bipyridine) electrochemically in a buffer solution. Amino- and mercapto-functionalized electrodes featured higher activity and stability for electrocatalytic generation of NADH than a bare ITO electrode. Effect of metal nanoparticles was also studied on modified ITO electrodes and the addition of platinum nanoparticles even resulted in improved activity. The electrochemical regeneration was somewhat affected in the presence of dioxygen, but not significantly. In addition, a conversion of carbon dioxide was carried out utilizing the electrochemically generated NADH and formate dehydrogenase to produce formic acid.

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Temperature effect on synthesis of gibbsite and boehmite from typical imogolite synthesis method

이호익 손대원* 고재형[1]

한양대학교 화학과 [1]한양대학교 고분자 물리화학 연구실

The natural minerals have been investigated in their unique properties such as chemical reactivity, optical properties, high elastic modulus, thermal stability, and a high specific surface area over the past two decades. Gibbsite (α -aluminum trihydroxide, α-Al(OH)3] and boehmiate (α-aluminum oxyhydroxide, α -AlOOH) are the most common aluminum hydroxide. We synthesized successfully aluminum hydroxide minerals from imogolite synthesis method and investigated the temperature effect on determining gibbsite and boehmite structure. Inorganic minerals gibbsite plate, boehmite, and imogolite are synthesized by controlling temperature via one synthesis method. Gibbsite and boehmite are controlled by adjusting temperature. At low temperature, gibbsite nucleate crystallize along the (002) with (200), (110) and (011) face and formed lozenge-shaped morphology. At high temperature, boehmite nucleates on the internal and external surfaces of the decomposed gibbsite particles as clusters of fine crystallites. The boehmite crystallites further coalesce and grow into fibrous particles within the decomposed matrix of gibbsite. These inorganic minerals are conformed by TEM and XRD.

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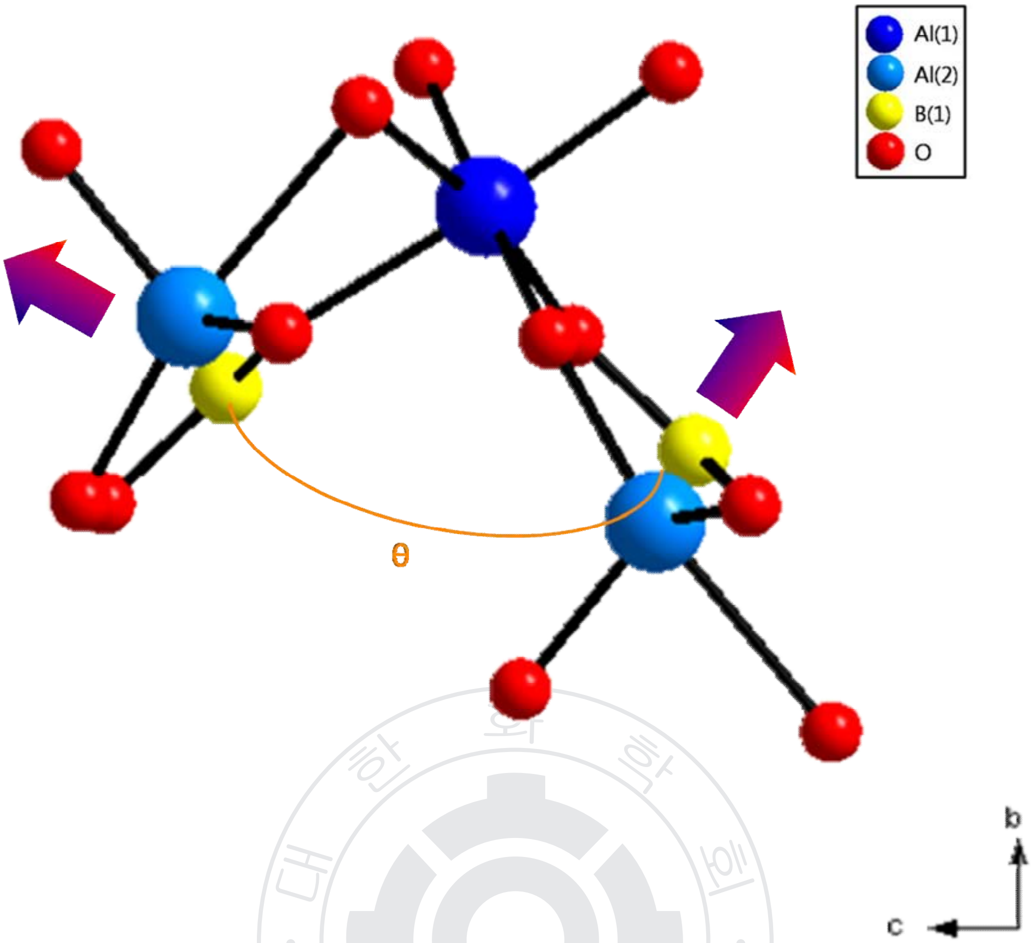
Structure-NLO property relationships in polar noncentrosymmetric aluminoborate solid solutions, $Al_{5-x}Ga_xBO_9$ (x = 0.0-0.5)

신이슬 옥강민*

중앙대학교 화학과

Solid solutions of polar noncentrosymmetric aluminoborate, $Al_{5-x}Ga_xBO_9$ (x = 0, 0.1, 0.2, 0.3, 0.4, and 0.5), have been synthesized through standard solid-state reactions. The phase purities, crystal structures, and solid solution behavior of the reported materials have been investigated by powder X-ray diffraction. Solid solutions of $Al_{5-x}Ga_xBO_9$ crystallize in the polar noncentrosymmetric space group, $Cmc2_1$, with a three-dimensional structure consisting of distorted MO_4, MO_5, MO_6, and BO_3 polyhedra (M = Al or Ga). Powder second-harmonic generating (SHG) measurements on the Al_5BO_9 using 1064 nm radiation, indicate the material has a SHG efficiency of approximately 2 times that of α-SiO_2 and is not phase-matchable (type 1). Further nonlinear optical (NLO) measurements on the $Al_{5-x}Ga_xBO_9$ solid solutions indicate a sharp increase in SHG efficiency up to 10 times that of α-SiO_2 for $x \geq 0.4$. As the B(1)-Al(1)-B(1) angle increases, an optimal orientation of BO_3 groups can be achieved, which results in the increase of net moments. Close structural examination suggests that the alignment of the asymmetric π-delocalization of BO_3 groups is responsible for the increase of SHG efficiency.


Al(1)
Al(2)
B(1)
O
θ
b
c

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Study of the Effects on the O_2 Reactivity Chemistry of Copper(I) Complexes with an Aminoacid-Based Chelate Liand.

이수연 정현진 이동헌

전북대학교 화학과

Copper(I)-dioxygen adducts or derived spesies pertinent to copper protein O_2-binding and activation are currently of considerable interest in bioinorganic chemistry.The topic of thioether sulfur ligation in copper(I)-dioxygen adducts have attracted more recent attention. A sulfur atom as a ligand at the active sites of various metalloenzymes has been well documented. DβM (dopamine β-monooxygenase) and PHM (peptidyl glycine α-hydroxylating monooxygenase) each contain a methionine residue as one of the lignads at the catalytic site. These proteins serve important roles in neurotransmitter or regulatory hormone biosynthesis. Furthermore, The nonheme iron enzyme CDO(cysteine dioxygenase) catalyzes the oxygenation of cystein by O_2 to give cystein sulfinic acid, which is essential for the biosynthesis of pyruvate and taurine. This enzyme is also vital for the maintenance of healthy levels of cysteine in the body.We have synthesis a sulfur containing ligands derived from L-methionine ethyl ester (L = 2-Ethylthio-N,N-bis(pyridine-2-yl)methylethanamine) Liand and it's copper(I) complex. The Cu(I) complex reacted with O_2 to produce sulfoxide derivative of thioether-amine ligand. We plan to study other new sulfur containing ligands derived from L-methionine and cysteine. And this research rendered service to an understanding of the discovery and influence of sulfur containing ligands with metal complexes reactivity.

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Colorimetric Anion Sensing of Cu(II) Complex withN,N'-dimethyl-N,N'-bis(pyridin-2-yl)methanediamine

정현진 박경세[1] 이동헌

전북대학교 화학과 [1]군산대학교 화학과

Anions have been recognized as a significant analyte in diverse fields including environmental, industrial, biological, and medical ones. In particular, a colorimetric anion sensor has been recently appreciated because of its capability that allows a simple and quick analysis. The interaction of N,N'-dimethyl-N,N'-bis(pyridin-2-yl)methanediamine (DMPA, 1) ligand with $Cu(ClO_4)_2$ salts yields compound of stoichiometry $[(DMPA)_2Cu](ClO_4)_2$, 2. Complex 2 was tested as potential anion sensors toward ions such as SCN^-, Cl^-, Br^- and I^- in organic solvents by utilizing a colorimetric method and was found to be feasible candidates for colorimetric detection of anions. Slow decomposition of 2 in methanol unexpectedly led to the formation of an alkoxo-bridged tetranuclear copper(II) cubane, 3. 3 is product of an oxidative N-dealkylation reaction, which took place on DMPA and methanol used as a solvent under the used conditions. The compound was characterized by a single crystal X-ray crystallography. Two copper ions of the tetranuclear copper(II) cluster each are five-coordinated in a square-planar geometry while the other two copper ions are six-coordinated in a octahedral geometry.

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Silver(I) and Pd(II) and Ni(II) N-Heterocyclic Carbene Complexes; Synthesis, characterization and Catalytic Application

배호연 정현진 이동헌

전북대학교 화학과

Recently, N-heterocyclic carbenes(NHCs) have become a very important class of ligands in organometallic chemistry and catalysis. Furthermore, metal complexes of N-heterocyclic carbene(NHCs) have become extremely important in catalytic processes such as cross-coupling, metathesis, and C-H bond activation. Especially the readily available Ag^{I}-NHC complex is the most commonly used NHC transfer reagent. A great number of metal complexes have been obtained via transmetalation from Ag^{I}-NHCs.Here we have described a convenient method for the synthesis of metal-complexes using Ag^{I}-NHC complexes as the carbene sources. Ag^{I}-NHC complexes are very useful precursors for other metal-NHCs complexes. Metal-NHCs complexes were obtained from the silver complexes by the transmetallation reactions with metal chloride.We are planning to synthesize a variety of transition metal and we are going to survey the potential applications of these new NHC complexes as materials or homogeneous catalysts.

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카바졸과 안트라센 계열의 청색 유기 EL 물질의연구

안상원 이승희

홍익대학교 화학시스템공학과

현재 OLEDs(Organic Light Emitting Diodes)의 물질과 소자에 대한 연구가 활발히 진행되고 있다 이 OLED 의 장점은 빠른 반응속도와 우수한 선명도, 그 외에 자체발광 하고 온도에 강하고 낮은전력에서도 구동가능하다는 장점이 있다. 하지만 RGB 물질 중 청색 물질은 큰 밴드갭 때문에,녹색과 적색에 비해 효율과 수명 그리고 선명도에 대한 문제점을 보이고 있다이러한 문제점을 해결하기 위해 본 실험에서는 새로운 청색 발광 물질을 합성을 하였다. 기존의 실험에서 사용한 anthracene 과 carvazole 에 치환기를 붙여 Tg 를 측정하고 입체장애에 의한 OLED 소자의 성질을 살펴 보았다

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In-situ Plasmonic Reaction Monitoring of a Single Au@Ag Nanocube with Sulfide Ions

이찬형 송현준*

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Precise surface plasmon tuning of metal-based nanostructures is essential in the view of fundamental aspects as well as photonic applications. Sulfide ions (S^{2-}) readily react with silver atoms (Ag^0) at room temperature. Using this reaction, the addition of sulfide ions into the Au@Ag core-shell nanocubes yields stable Au@Ag/Ag_2S core-shell nanocubes, which lead to the continuous shifts of the plasmon extinction maximum to the longer wavelength from 500 to 750 nm, and covers the entire visible range.Since the localized surface plasmon resonance (LSPR) spectra of Au@Ag nanocubes are highly sensitive to local refractive index change induced by compositional variation from Ag (n_{Ag} ~ 0.05) to Ag2S (n_{Ag2S} ~ 2.9), it is possible to observe the change of LSPR spectra of Au@Ag nanocubes occurred by the generation of Ag_2S layer on the surfaces of nanocubes.We use dark field microscopy (DFM) to study the change of LSPR spectra of individual Au@Ag nanocube at a single particle level. When sulfide ions are added into Au@Ag nanocubes, the ions are reacted with specific rates. It is possible to quantitatively measure the rate of compositional variation from Ag to Ag_2S on surfaces of particles by calculating plasmon extinction maximum shift of the LSPR peak in times progress.

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Photoluminescent Cu(I) Coordination Polymers Based on N/S Donor Ligands.

조성화 이상진 전영은 김태호 김진은*

경상대학교 화학과

Four copper(I) coordination polymers with ligands (L^1 and L^2), $[Cu_2I_2L^1{}_2]_n$ (**1**), $\{[Cu_2I_2L^1]\ CH_3CN\}_n$ (**2**), $\{[Cu_2I_2L^2{}_2]\ CH_2Cl_2\}_n$ (**3**), and $[Cu_2I_2L^2]_n$ (**4**), have been successfully synthesized and structurally characterized by single-crystal X-ray diffraction. Structural transformations between the polymers were controlled by the appropriate solvent composition, mole ratio, or temperature.

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Solvent-Controlled Supramolecular Isomerism in Three Cu(I) Coordination Polymers Based on (2-Pyrazinylcarbonyl)thiomorpholine

전영은 조성화 이상진 김태호 김진은*

경상대학교 화학과

A one-dimensional(1-D) and two-dimensional(2-D) coordination polymers $\{[\mathrm{CuI}\mathbf{L}]\mathrm{CH_3CN}\}_n$(**1**), $\{[\mathrm{CuI}\mathbf{L}]\mathrm{CH_2Cl_2}\}_n$ (**2**), and $\{[\mathrm{CuI}\mathbf{L}]\mathrm{CHCl_3}\}_n$ (**3**) with a (2-Pyrazinylcarbonyl)thiomorpholine (**L**), has been prepared by self-assembly. Three coordination polymers are supramolecular iosmerism by solvent molecules.Polymers **1**, **2**, and **3** interconnected by rhomboid Cu-I_2-Cu units were a 1-D looped chain(1 and 3), 2-D network(2) structures, respectively. Very interestingly, Photolumenescent properties and crystal structures of coordination polymers are very different according to solvent molecules.

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Self-Assembled Nanocomposites fo Graphene-Layered Double Hydroxide with Highly Efficient Visible Light Photocatalytic Activity

Gunjakar Jayavant Laxman 김인영 황성주*

이화여자대학교 화학·나노과학과

Highly efficient photocatalysts for visible light-induced O_2 generation are synthesized via an electrostatically-derived self-assembly of Zn-Cr-LDH 2D nanoplates and the graphene 2D nanosheets. In the self-assemble nanohybrids, the positively-charged Zn-Cr-LDH nanosheets are immobilized on the surface of negatively-charged graphene nanosheets with the formation of mesoporous house-of-card stacking structure. A strong electronic coupling between the Zn-Cr-LDH nanoplates and reduced graphene oxide (RGO)/graphene oxide (GO) nanosheet gives rise a prominent increase of visible light absorption with remarkable depression of photoluminescence signal. The self-assembled Zn-Cr-LDH?RGO nanohybrids display an high photocatalytic activity for visible light-induced O_2 generation with a rate of ~1.20 mmol h^{-1} g^{-1}, which is much superior to those of the pristine Zn-Cr-LDH material (~0.67 mmol h^{-1} g^{-1}). The Zn-Cr-LDH-RGO nanohybrid shows a higher activity than the Zn-Cr-LDH-GO nanohybrid, providing strong evidence for the superior role of the RGO nanosheet as an electron reservoir. The present findings clearly demonstrate that the RGO nanosheets can be used as an effective platform for improving the photocatalytic activity of 2D nanostructured inorganic solids through the depression of charge recombination.

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Crystal Structures and Photophysical Properties of Cu(I) Coordination Polymers

이상진 조성화 전영은 김태호 김진은*

경상대학교 화학과

Six copper(I) coordination polymers with ligands (L^1, L^2, and L^3), $[Cu_2I_2L^1{}_2]_n$ (1), $\{[Cu_2I_2L^1]\ CH_3CN\}_n$ (2), $\{[Cu_2I_2L^2{}_2]\ CH_2Cl_2\}_n$ (3), and $[Cu_2I_2L^2]_n$ (4), $[Cu_2I_2L^3{}_2]_n$ (5), $\{[Cu_2I_2L^3]\}_n$ (6), have been successfully synthesized and structurally characterized by single-crystal X-ray diffraction. Structural transformations between the polymers were controlled by appropriate solvent composition, mole ratio, or temperature.

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Catecholase Activity of a Non-coupled Dinuclear Copper Carboxamide Complex

<u>shuranjan sarkar</u> 이홍인

경북대학교 화학과

Tyrosinase, a dinuclear copper enzyme, actuates dioxygen to form a side-on peroxodicopper(II) or end-on trans-peroxodicopper(II) complex, which is able to oxidize phenols to corresponding catechols. Numerous synthetic side-on peroxodicopper(II) or end-on trans-peroxodicopper(II) complexes with simple amine ligands have been discussed in that the complexes authentically reproduced the spectrum of oxygenated tyrosinase, Cu(III)-bis-oxide species, upon phenolate addition at low temperatures. These species decay with hydroxylation of the aromatic ring via an electrophilic aromatic substitution mechanism, as seen in the enzyme. Herein, we describe a new non-coupled dinuclear copper complex with chelating pyridyl-based dicarboxamido ligand that shows unusual catalytic activity for the oxidation of various phenols. The complex was characterized by various spectroscopic techniques and the catalytic activities were monitored by the GC-Mass, UV-kinetics and EPR spectroscopy.

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Photophysical and Electroluminescent Properties of Iridium Complexes with *o*-Carborane Substituted $C^{\wedge}N$-Chelating Ligand

배혜진 도영규[*] 이민형[1,*]

한국과학기술원(KAIST) 화학과 [1]울산대학교 화학과

Heteroleptic $(C^{\wedge}N)_2$Ir(acac) ($C^{\wedge}N$ = 5-*CBbtp* (1); 4-*CBbtp* (2); 5-*CBbtp* = 2-(2-benzothienyl)-5-(2-methyl-*ortho*-carboran-1-yl)-pyridinato-C^2,N, 4-*CBbtp* = 2-(2-benzothienyl)-4-(2-*n*-butyl-*ortho*-carboran-1-yl)-pyridinato-C^2,N, acac = acetylacetonate) complexes bearing *o*-carborane substituted $C^{\wedge}N$-chelating ligand were prepared and characterized. While 1 exhibits a deep-red phosphorescence band centered at 644 nm (Φ_{em} = 0.05), which is red-shifted compared to that of unsubstituted $(btp)_2$Ir(acac) (3) (λ_{em} = 615 nm), 2 is non-emissive in solution at room temperature. In contrast, both complexes are emissive at 77 K and in solid state. An electroluminescent device incorporating 1 as an emitter displayed overall good performance in terms of external quantum efficiency with deep-red phosphorescence. Details of synthesis, characterization, photophysical and electroluminescent properties of 1 and 2 will be presented along with theoretical calculation.

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CO_2/EO copolymerization and ligand variation for a salen-cobalt(III) complex tethering 4 quaternary ammonium salts

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아주대학교 분자과학기술학과

A cobalt(III) complex of a salcy-type ligand tethering 4 quaternary ammonium salts, which is constructed with trans-1,2-diaminocyclohexane is as highly active (TOF, 25900 h^{-1}; TON, 518000; 2.72 kg polymer per g cat) in CO_2/ethylene oxide (EO) copolymerization as it is in CO_2/propylene oxide (PO) copolymerization. High-molecular-weight polymers (M_n, 200000-300000) with strictly alternating repeating units were generated. The related cobalt(III) complexes were prepared through variations of the ligand framework by replacing the trans-1,2-diaminocyclohexane unit with 2,2-dimethyl-1,3-propanediamine, trans-1,2-diaminocyclopentane, or 1,1'-binaphthyl-2,2'-diamine or by replacing the aldimine bond with ketimine. These ligand frameworks are thought to favour the formation of the cis-β configuration in complexation, and the formation of the cis-β configuration was confirmed through NMR studies or X-ray crystallographic studies of model complexes not bering the quaternary ammonium salts. Complexes which adopt the cis-β configuration even in DMSO did not show any activity for CO_2/PO copolymerization, whereas complex constructed with trans-1,2-diaminocyclopentane and fluctuated in DMSO between the coordination and de-coordination of the acetate, showed fairly high activity. This fluxional behaviour may play a role in polymerization.

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Reactivity Comparison for Metal-Oxygen Species Bearing Common *N*-methylated Macrocyclic Ligands

강현아 조재흥[1,*] 남원우[2,*]

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Metal-active oxygen adducts are key intermediates detected in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. Here, we report the differences in the structure and reactivity of the active oxygen complexes (i.e., $[Mn^{III}(12\text{-}TMC)(O_2)]^+$ vs $[Mn^{III}(12\text{-}TMC)(O)]_2^{2+}$; 12-TMC = 1,4,7,10-tetramethyl-1,4,7,10-tetraazacyclododecane) on the basis of the detailed comparison of these systems with the same ligand. In addition, the reactivity of end-on Cr(III)-superoxo and Cr(IV)-oxo species (i.e., $[Cr^{III}(14\text{-}TMC)(O_2)(Cl)]^+$ vs $[Cr^{IV}(14\text{-}TMC)(O)(Cl)]^+$; 14-TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane), has been investigated in C-H bond activation.

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Design of acid-free proton conducting materials

이길령 **Yakiyama Yumi Masaki Kawano***

포항공과대학교 첨단재료과학부

Now preparation of efficient proton-conducting system is one of the most active fields in the material chemistry especially for the proton exchange membrane (PEM) for automobile. To date, introduction of acidic moiety is commonly accepted as one of the effective strategy to achieve high proton conductivity. On the other hand, the efforts to prepare highly conductive materials without any acidic backbones are not well made. With the consideration of the safety problem and further development of this field, it is quite meaningful to investigate non-acidic system with focusing the multi-interactivity of the components. Recently, we have newly designed and synthesized highly symmetrical ligand named TPHAP. The biggest feature of this molecule is to form weak intermolecular interactions very actively. Because of this multi-interactivity of TPHAP, its potassium salt shows remarkable proton conductivity under high humidity condition even without any acidic groups. Here, we discuss the conduction mechanism from the structural information of K^+TPHAP^- system based on the view of its multi-interactive nature.

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Design of Redox-Active Multi-Interactive Ligand and Its Coordination Network

구진영 Yakiyama Yumi Masaki Kawano*

포항공과대학교 첨단재료과학부

Redox activity and weak intermolecular interactions play crucial roles in various reactions in sophisticated biologic systems to maintain our life. Especially, how to control these functions are the key issues for new material design in this century. Coordination network is one of the ideal systems to achieve designable materials which can be constructed by self-assembly of metal connectors and ligands. Here, we will show our recent work on the redox-active diazaphenalene-based coordination networks with focusing ligand design and physical properties. The ligand 2,5,8-tripyridyl-1,3-diazaphenalene (TPDAP) is nitrogen modified analogue of our representative multi-interactive ligand, TPHAP. The central diazaphenalenyl skeleton is known for its fascinating redox active nature. Because of multi-interactivity and high symmetric structure, TPDAP is expected to give various porous coordination networks. Furthermore, the central DAP-based redox activity will provide the unique magnetic/electronic properties. The precise control of these natures will give unprecedented molecular materials such as highly efficient heterogeneous catalytic system.

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Effect of the ring size of macrocyclic ligands on the electrophilic reactivity of Fe^{IV}(O)complexes

소희 홍승우[1] CHO KYUNG BIN MICHAEL 이용민[2] 남원우[3,*]

이화여자대학교 바이오융합과학과 [1]이화여자대학교 화학나노과학부 [2]이화여자대학교 기초과학연구소 [3]이화여자대학교 화학과

Nonheme iron-oxygen complexes are capable of carrying out chemically challenging and important oxidative transformations which are essential for life. In biomimetic studies, the influence of the ring size of macrocyclic ligands on the reactivity of Fe^{IV}(O) have yet to be reported. In this work, $[Fe^{IV}(O)(13\text{-}TMC)]^{2+}$ (13-TMC = 13-membered tetramethylcyclam) complex was synthesized and characterized with various spectroscopic methods such as UV-vis, electrospray ionization mass (ESI-MS), EPR and resonance Raman spectroscopies. Then, the electrophilic reactivities of $[Fe^{IV}(O)(13\text{-}TMC)]^{2+}$ (1) and $[Fe^{IV}(O)(14\text{-}TMC)]^{2+}$ (2) (14-TMC = 14-membered tetramethylcyclam) were investigated in the C-H bond activation and oxygen atom transfer reactions. In both C-H bond activation and oxygen atom transfer reactions, reactivities of 1 was 3~5 order greater than those of 2. To understand the differences of electrophilic reactivity of 1 and 2, the redox titration of two complexes by ferrocene derivatives were carried out, resulting that Ered value of 1 (0.61 V *vs.* SCE) was 0.22 V more positive than 2 (0.39 V *vs.* SCE). The reactivity enhancement might be explained by the difference of electronic configurations caused by their geometric structures.

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Remarkable Solvent, Porphyrin Ligand, and Substrate Effects on Participation of Multiple Active Oxidants in Manganese(III) Porphyrin-Catalyzed Oxidation Reactions

배정미 황인홍 노진영 김 철[1]

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The participation of multiple active oxidants generated from the reactions of two Mn(III) porphyrin complexes containing electron-withdrawing and -donating substituents with peroxyphenylacetic acid (PPAA) as a mechanistic probe was studied by carrying out catalytic oxidations of cyclohexene, 1-octene, and ethylbenzene in various solvent systems, namely, toluene, CH_2Cl_2, CH_3CN, and H_2O/CH_3CN (1/4). With an increase in the concentration of the easy substrate cyclohexene in the presence of (TMP)MnCl 1a with electron-donating substituents, the ratio of heterolysis to homolysis increased gradually in all solvent systems, suggesting that (TMP)Mn-OOC(O)R species 2a is the major active species. When the substrate was changed from the easy one (cyclohexene) to difficult ones (1-octene, ethylbenzene), the ratio of heterolysis to homolysis increased a little or did not change. (F_{20}TPP)Mn-OOC(O)R species 2b generated from the reaction of (F_{20}TPP)MnCl 1b with electron-withdrawing substituents and PPAA also gradually becomes involved in olefin epoxidation (although to a much lesser degree than with (TMP)Mn-OOR 2a) depending on the concentration of the easy substrate cyclohexene in all aprotic solvent systems except for CH_3CN, whereas Mn^V=O species is the major active oxidant in the protic solvent system. With difficult substrates, the ratio of heterolysis to homolysis did not vary except for 1-octene in toluene, indicating that a Mn(V)=O intermediate generated from the heterolytic cleavage of 2b becomes a major reactive species. We also studied the competitive epoxidations of *cis*-2-octene and *trans*-2-octene with two manganese(III) porphyrin complexes by MCPBA in various solvents under catalytic reaction conditions. The ratios of *cis*- to *trans*-2-octene oxide formed in the reactions of MCPBA varied depending on the substrate concentration, further supporting the contention that the reactions of manganese porphyrin complexes with peracids generate multiple reactive oxidizing intermediates.

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Characterization and Reactivity of High-Valent Ruthenium-Oxo Species

김진화 서미숙 남원우[1]

이화여자대학교 바이오융합과학과 [1]이화여자대학교 화학과

The water oxidation to evolving dioxygen is catalyzed at the oxygen-evolving center (OEC) in photosystem II (PSII) in photosynthesis. Despite recent development on the structural information of OEC, the mechanism of water oxidation at molecular level still remains unclear. In recent study, many ruthenium-oxo species act as an efficient water oxidation catalyst in model complex for chemical transformation of wide range of organic substrate. Here we are reporting the generation and characterization of high-valent mononuclear nonheme ruthenium-oxo complex, $[Ru^{IV}(tpy)(bpm)(O)]$ (tpy=2,2':6',2''-terpyridine, bpm=2,2'-Bipyrimidine) by reaction of $[Ru^{II}(tpy)(bpm)(OH_2)](ClO_4)_2$ with PhIO in presence of TFA (TFA=Trifluoromethanesulfonic acid) (5%) in CH_3CN with many spectroscopic methods. Also their reactivity aspects towards externally added various substrates such as 1,4-cyclohexadien for C-H activation reaction and $PhSCH_3$ for oxygen atom transfer reaction.

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Zn^{II} coordination polymers constructed by malonate and bipyridyl ligands: Photoluminescence and heterogeneous catalytic reactivity

황인홍 이명미 김현 노진영 김 철[1] 김영미[2] 김성진[3]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터 [2]이화여자대학교 화학-나노과학과 [3]이화여자대학교 화학과

Four three-dimensional Zn^{II} frameworks containing malonates and various bipyridyl pillars (4,4'-bpy (1), bpa (2), bpe (3), and bpp (4)) have been prepared, and their structures were determined by X-ray crystallography. In all four frameworks, malonate ligands bridge three Zn ions to form two-dimensional layers, and these layers are connected by bipyridyl pillars to form three-dimensional frameworks with general formula $[\{Zn(H_2O)(\mu\text{-malonate})\}_2(\mu\text{-bipyridyl})]$ containing water or acetonitrile solvates. Reactivity study of the compounds 1 - 4 showed that they catalyzed the heterogeneous transesterification reactions of phenyl acetate and could be reused without a significant loss of activity through five runs with ester. Emission spectra of 2 and 3 were observed at 347-365 nm (λ_{ex} = 313 nm) for 2 and 363 nm (λ_{ex} = 328 nm) for 3, while compounds 1 and 4 showed no luminescence properties. The thermal stabilities of these complexes were also examined.

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Tandem catalysis with site-isolated Lewis acid-Brønsted base metal-organic frameworks

홍순상 윤민영[1] 김용휘 김기문*

포항공과대학교 화학과 [1]Department of Chemistry, University of California Berkeley

In light of growing demand for efficient heterogeneous catalysts for chemical processes, the synthesis of metal-organic frameworks (MOFs) have become immensely important because of their potential applications in heterogeneous catalysis. We prepared a MOF accommodating both acid and base catalytic moieties in the same framework, NH_2-MIL-101(Al), by site isolation of the catalytic moieties, which is difficult to achieve in a homogeneous catalyst system. This MOF, without any post-synthetic modification, functions as a bifunctional site-isolated Lewis acid-Brønsted base heterogeneous catalyst for tandem Meinwald rearrangement-Knoevenagel condensation reactions. The Lewis acidic Al(III) sites catalyze Meinwald rearrangement of epoxides with remarkable selectivity for substrates, which generate aldehydes via benzylic 3° carbocation, and the Brønsted basic amino groups in organic linkers catalyze Knoevenagel condensation of resulting aldehyde with malononitrile in tandem.

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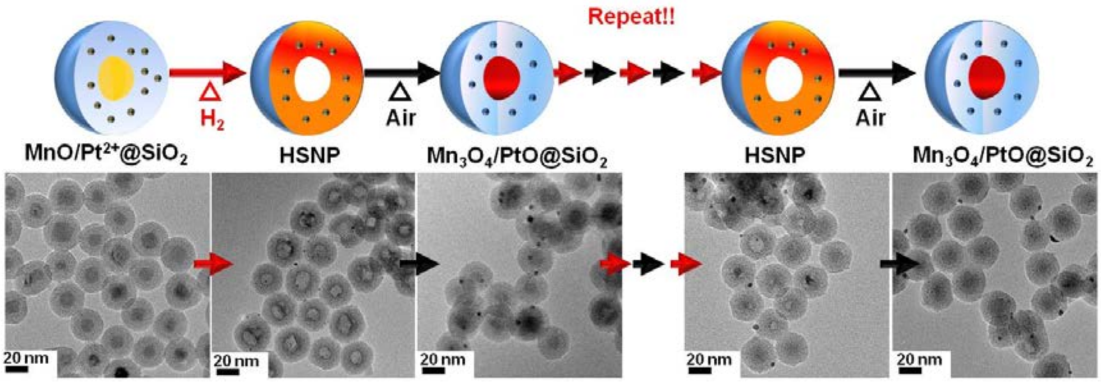
Reversible and Cyclical Transformations between Solid and Hollow Nanostructures in Confined Reactions of Manganese Oxide and Silica within Nano-sized Spheres.

김진구 김수민 이인수*

포항공과대학교 화학과

Annealing of $MnO@SiO_2$ nanospheres in a reducing gas environment resulted in the transformation of the core-shell structure into a hollow structure as a result of outward diffusion of MnO species into the thermodynamically more stable silicate phase. When the hollow silicate nanospheres were oxidized, the interior cavities were refilled with a Mn_3O_4 phase segregated from the silicate phase, and the hollow structure reverted to the initial core-shell structure. More interestingly, when catalytically active Pt nanocrystals were introduced into the manganese oxide/silica system, the Mn_3O_4 was readily reduced to the chemically reactive MnO, even at low temperature, which enabled reconversion of the solid nanospheres with a Mn_3O_4 core to hollow nanostructures during reductive annealing. Therefore, when $MnO@SiO_2/Pt(II)$ nanospheres were subjected to an oxidation/reduction cycle by repeatedly switching the flowing gas between air and hydrogen, the nanospheres underwent a reversible change between solid and hollow structures, depending on the gas environment. The solid-to-hollow-to-solid transformation was successfully cycled many times simply by repeatedly switching the flowing gas during annealing.


Repeat!!
MnO/Pt^{2+}@SiO$_2$
△
H$_2$
HSNP
△
Air
Mn$_3$O$_4$/PtO@SiO$_2$
HSNP
△
Air
Mn$_3$O$_4$/PtO@SiO$_2$
20 nm
20 nm
20 nm
20 nm
20 nm

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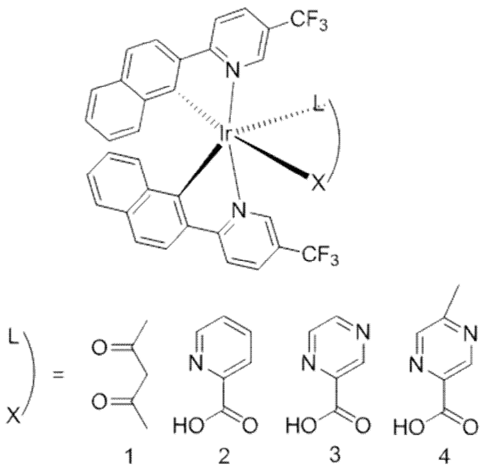
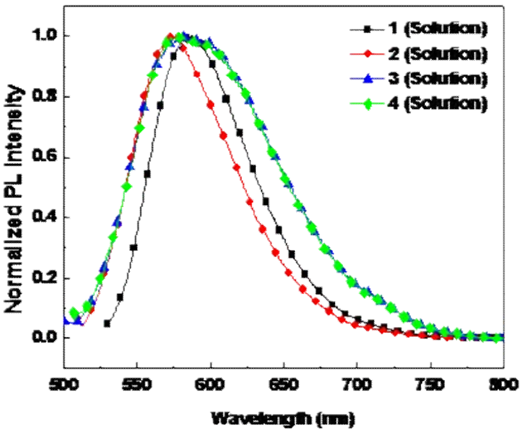
Heteroleptic Iridium(III) Complexes Containing 2-(Naphthalen-2-yl)-5-(trifluoromethyl)pyridine for Orange-Red Phosphorescent Organic Ligth-Emitting Diodes (OLEDs)

윤성재 신재민[1] 김민지[2] 강성권[3] 김영인[1,*]

부산대학교 첨단정보및디스플레이소재협동 [1]부산대학교 화학교육과 [2]부산대학교 첨단소재화학협동과정 [3]충남대학교 화학과

Normally, the emission wavelength of an Ir(III)-ppy complex is red-shifted when an electron donating group is introduced to the phenyl moiety of ppy, the π-conjugation length of the ligand is extended or an electron-withdrawing group is added to the pyridyl moiety of ppy.In this study, the electron-withdrawing trifluoromethyl group in the pyridyl moiety and aromatic group in the phenyl moiety of phenylpyridine were introduced to tune the energy band gap of the complexes. Heteroleptic iridium(III) complexes for organic light-emitting diodes (OLEDs); $(N^\wedge C)_2Ir(L^\wedge X)$, where N^C= 2-(naphthalene-2-yl)-5-(trifluoromethyl) pyridine (npCF3py) and L^X= acetylacetone (acac), picolinic acid (pic), pyrazine-2-carboxylic acid (prz) and 5-methylpyrazine-2-carboxylic acid (mprz); $(npCF3py)_2Ir(acac)$ (1), $(npCF3py)_2Ir(pic)$ (2), $(npCF3py)_2Ir(prz)$ (3) and $(npCF3py)_2Ir(mprz)$ (4) were synthesized. The complexes exhibited the photoluminescence at 572 ~ 587 nm in solution and 565 ~ 583 nm in film. The iridium(III) center of complex 1 adopts a distorted octahedral coordination geometry with cis metalated carbon and trans nitrogen atoms.


CF3
N
Ir
L
X
N
CF3
L
X
=
O
O
N
HO
O
N
N
HO
O
N
N
HO
O
1
2
3
4


1 (Solution)
2 (Solution)
3 (Solution)
4 (Solution)
Normalized PL Intensity
0.0
0.2
0.4
0.6
0.8
1.0
500
550
600
650
700
750
800
Wavelength (nm)

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Zinc Sensors with lower binding affinities

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Zinc sensors based on 2,3-dipicolylamine (DPA) and quinoline have been synthesized. They fluoresced in the presence of Zn^{2+} and remained fluorescence when other metal ions were present. The fluorescence enhancement of the sensors was selective for Zn^{2+} over other metal ions, like Cd^{2+}. In vitro studies with fibroblasts showed cell fluorescence when sensor and Zn^{2+} were combined. As seen by single crystal X-ray analysis, four nitrogens from the 2,3-QA sensor bind Zn^{2+}. This tetradentate coordination leads to these sensors having lower binding constants than the pentadentate sensors based on 2,2-DPA.

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Synthesis and Characterizaition of New Pd(II) Complexes with Ligand pyridin-2-ylmethylbenzenamine Derivatives

김성훈 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have prepared new palladium complexes $PdLnCl_2$ with ligands Ln (L_1~L_4), where (L_1=2,6-dimethyl-N-((pyridin-2-yl)methyl)benzenamine), L_2 = (3,5-dimethyl-N-((pyridin-2-yl)methyl)benzenamine), L_3= (2,4,6-trimethyl-N-((pyridin-2-yl)methyl)benzenamine), L_4 = (2,6-diisopropyl-N-((pyridin-2-yl)methyl)benzenamine). All new Pd(II) complexes are characterized by spectroscopic methods and X-ray single crystal diffraction. The catalytic activity of new Pd(II) complexes for MMA polymerization in the presence of MMAO were investigated along with the effect of temperature control.

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Phosphorescent Heteroleptic Cyclometalated Iridium(III) Complexes with 2-(2,3,4-Trifluorophenyl)pyridine

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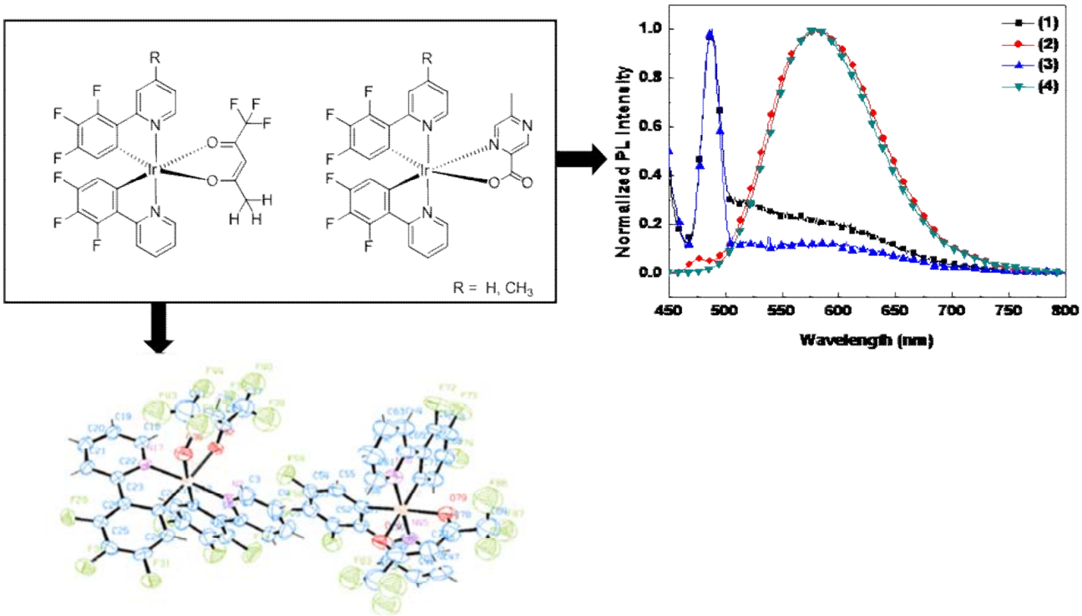
부산대학교 화학교육학과 [1]부산대학교 첨단정보 및 디스플레이소재협동과정 [2]충남대학교 화학과 [3]부산대학교 화학교육과

We synthesized heteroleptic cyclometalated Ir(III) complexes for an application of OLEDs; (C^N)$_2$Ir(L^X), where C^N= 2-(2,3,4-trifluorophenyl)pyridine(tfppy), 4-methyl-2-(2,3,4-trifluorophenyl)pyridine(tfpmpy) and L^X = 1,1,1-trifluoro-2,4-pentanedione(tfacac), 5-methylpyrazine-2-carboxylic acid (mprz); (tfppy)$_2$Ir(tfacac) (1), (tfppy)$_2$Ir(mprz) (2), (tfpmpy)$_2$Ir(tfacac) (3) and (tfpmpy)$_2$Ir(mprz) (4). The crystal structure of complex (2) has a distorted octahedral coordination geometry as N(17)-Ir(1)-N(2) (175.7(2)), C(13)-Ir(1)-O(36) (176.8(3))and C(13)-Ir(1)-N(17) (96.7(3). The PL spectra of the complexes show the emission are at 488 and 596 nm, with quantum yields of 2 and 30% in solution. The complexes (3) and (4) showed a blue-shift emissions compared to complexes (1) and (2), respectively. This properties indicate that the conjugation effect of 4-substituted metyl group increased the electron density of the pyridine ring resulting in an increase of the LUMO energy level.


R = H, CH3
Ir
(1)
(2)
(3)
(4)
Normalized PL Intensity
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
450
500
550
600
650
700
750
800

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Two Different Geometries of Co(II)/Co(I) Complexes with N,N,N’,N’-tetra-[(3,5-dimethyl-1-pyrazolyl)methyl]-p-phenylenediamine ligand

임종완 류상훈[1,*]

심인고등학교 화학 [1]안동대학교 공동실험실습관

Variety of pyrazole-based ligands were used for the study of metal-chelating property in coordination chemistry. N,N,N’,N’-tetra-[(3,5-dimethyl-1-pyrazolyl)methyl]-p-phenylenediamine having two pyrazole groups which were bridged by phenylenediamine so afford large chelating spatial for the formation of polynuclear complex. Dinuclear Co(II) complex was formed in the reaction of $CoCl_2{\cdot}6H_2O$ with N,N,N’,N’-tetra-[(3,5-dimethyl-1-pyrazolyl)methyl]-p-phenylenediamine. The crystallographic analysis of the complex revealed that the two N of pyrazole and two Cl atoms are bound to Co with tetrahedral geometry. Chlorine atoms are bound to Co metal in the *cis* position and the Co-Cl distance was 2.231 Å. In constrast to $CoCl_2{\cdot}6H_2O$ the reaction of $Co(OAc)_2{\cdot}6H_2O$ with pyrazole ligand formed Co_4N_4 Cubane Cluster. The complex Co_4N_4 $(O_2CMe)_4(py)_4$ consists of four each of Co^+ and N atoms occupy at alternate corners of cube to form a $[Co_4N_4]^{4+}$ core with Acetate ligand bridging the Co^+ ions along four face diagonals of the cube. The four Co atoms form an approximate tetrahedron with Co…Co separation of ~2.75 Å. The average Co-N distance is of the order of 2.114 Å. In addition of crystallographic study, IR property and Raman Effect also will be discussed.

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Coordination polymers composed of metallomacrocycles and 1,4-cyclohexanedicarboxylate ligand

김소연 김주창*

부경대학교 화학과

Metallomacrocycles such as [Ni(cyclam)](ClO4)2 and [Zn(L)](NO3)2 (L = 3,14-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.07.12]docosane) were subjected to react with cis-1,4-cyclohexanedicarboxylic acid (cis-CHDC), trans-1,4-cyclohexanedicarboxylic acid (trans-CHDC) or cis,trans-1,4-cyclohexanedicarboxylic acid mixtures under basic reaction conditions, respectively. The coordination tendencies of CHDC to the corresponding metallomacrocycles were different depending on the nature of the macrocycles as well as the types of hydrogen bonds, resulting in the formation of monomeric or polymeric reaction products. The solid state structures, thermal and spectroscopic properties of Ni(II) and Zn(II) metallomacrocycles bearing CHDC ligands are described in this presentation.

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Supramolecules assembled by hexaaza macrocyclic copper(II) complexes

김영환 김주창*

부경대학교 화학과

Hexaaza macrocyclic copper(II) complexes of [{Cu(L+2H)}2(?-tp)](ClO4)6?2H2O (1), [Cu(L+2H)(H2O)2](ClO4)2?(ndc)?2H2O (2), [Cu(L)(CH3CN)2](ClO4)2 (3), [Cu(L1+2H)](ClO4)4 (4), [Cu(L1)](ClO4)2?2H2O (5) (L = 3,10-bis(3-(1H-imidazol-1-yl)propyl)-1,3,5,8,10,12-hexaazacyclotetradecane, L1 = 3,10-bis(3-(2-methyl-1H-imidazol-1-yl)propyl)-1,3,5,8,10,12-hexaazacyclotetradecane, tp = terephthalate, ndc = 2,6-naphthalene dicarboxylate) have been synthesized and structurally characterized by X-ray diffraction method. Complexes 1-5 were self-assembled by intermolecular interactions such as hydrogen bonds, C-H???? and ?-? interactions, resulting in the formation of a corresponding supramolecule, respectively. In this presentation, we describe the structures and properties of 1-5 in detail.

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Synthesis of Dichloro Zn(II) Complexes with Ligands*N*,*N*-bis(1-pyrazolyl)methyl Aniline Derivatives and Their Application to rac-Lactide Polymerization.

김성훈 최성혜 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

Polylactide is one of the most important biodegradable polymers due to their biomedical and pharmaceutical applications. Ring-Opening-Polymerization (ROP) of lactide using non- hazardous zinc complexes has attracted great attention than highly toxic tin and lead complexes.The Zn(II) dichloro complexes based on ligands such as *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-dimethylbenzenamine, *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-3,5-dimethylbenzenamine, *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-diethylbenzenamine, *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-diisopropylbenzenamine, have been synthesized in high yield and purity. The crystal structure of complexes was determined by X-ray crystallography. Methylated Zn(II) complexes were employed and evaluated as an initiator for ROP of rac-Lactide. The heterotactic PLA with Pr up to 87 % can be obtained by using the Zn complex containing ligand *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-diisopropylbenzenamine in CH_2Cl_2at -50℃.

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Selective Isotropic or Anisotropic Nanoscale Growth of Coordination Polymers

박신애 이희정 오문현*

연세대학교 화학과

Porous coordination polymers (CPs) have been the subject of intense research owing to their fascinating properties and applications, such as gas storage, gas separation, catalysts, optics, and recognition. Currently, various ongoing researches have been devoted to the fabrication of nano- and micro-scaled coordination polymer particles (CPPs) and CP thin films to extend their applicability. As several hybrid nano-materials with more than two components have been suggested as candidates for multi-functional materials, CPPs with well-controlled hetero-compositions will offer a great chance to extend the applicability of CPPs and CPs. Here, we report on the precise and controlled synthesis of hetero-compositional CPPs through the selective isotropic and/or anisotropic nanoscale growth of CPs.

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Physical Properties of Polymer, Graphene and Metal Composites

오영희* 현일환 정아름 이은경 김윤미

동의대학교 화학과

Graphene/transition metal nanostructured composites have been prepared from the graphene, and metal salts in alcoholic solution. Polymers containing the graphene/metal composites were prepared in the different ratios of composites/polymer and examined. The structures and the properties of the composites including thermal property have been investigated.

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Crystal structures and properties of hexaaza macrocyclic nickel(II) complexes

유슬기 김주창[*]

부경대학교 화학과

A hexaaza macrocyclic nickel(II) complex, [Ni(L)](ClO4)2?2H2O (L = 3,10-bis(3-(2-methyl-1H-imidazol-1-yl)propyl)-1,3,5,8,10,12-hexaazacyclotetradecane), and its derivatives have been synthesized and structurally characterized by X-ray diffraction method. Due to the presence of imidazole pendants on the macrocycle L, the obtained nickel(II) complexes show various types of intermolecular interactions. The detailed structures of the complexes as well as the formation of supramolecules by the self-assembly processes will be described in this presentation.

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X-ray Structure and Magnetic Properties of Tris(2-minoethyl)amine Complexes of Nickel(II) Combined with Ferrocyanide.

서민지 곽지훈[1,*]

순천대학교 화학과 [1]순천대학교 화학교육과

The coordination chemistry derived from tren, tris(2-minoethyl) amine, ligand is interesting because it implies wide variety of biochemical and catalytic activities. Also, this multidentate ligand has the great flexibility in coordination pattern and it can be applied in crystal engineering, such as preparation of multimetallic complexes, two or three dimensional structures, etc. we obtained dimeric complex of [(tren)Ni(?-Cl2)Ni(tren)](ClO4)2 (1) and one-dimensional polymeric ring chain of {[Fe(CN)6][Ni(tren)]2[Ni(tren)(H2O)]2}Cl2(ClO4)2?4H2O (2), by the reaction of potassium ferricyanide, nickel chloride and tren. In this presentation, single crystal X-ray structures and magnetic properties of 1 and 2 are discussed

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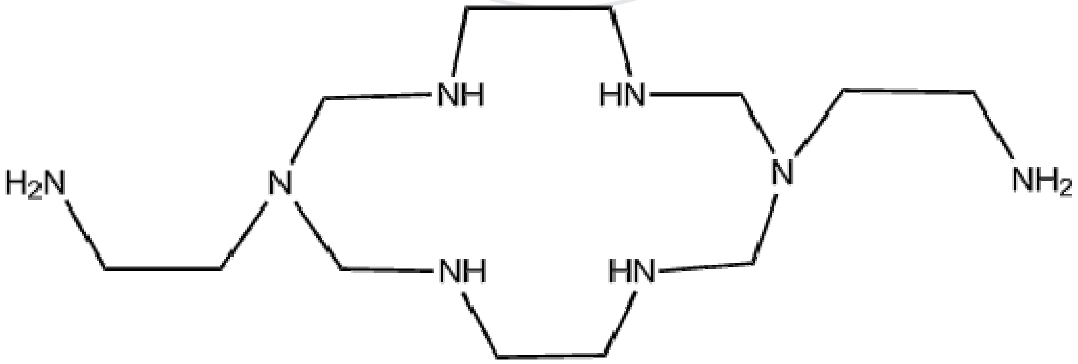
Guest Controlled Selective Binding of Nickel(II) and Copper(II) Macrocyclic Complex Having Pendant Arms

이재명 곽지훈[1,*]

순천대학교 화학과 [1]순천대학교 화학교육과

Molecular recognition is important not only to prepare supramolecules but also host-guest chemistry. Especially host-guest chemistry is applied to the molecular devices and biological sensor. Usually, this system has been developed by the modification of active site and/or binding site in host molecule. Here we developed a new conceptual host-gust system, in which guest molecule has a redox active site and a potentially coordinating site as well. We get the complexes of nickel(II) and copper(II) of A combined crown ether. Here, we present the X-ray structrure of the complexes and the guest controlled binding properties of them as well.



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Synthesis of QD layer-encapsulated colloidal silica nanospheres and LED application.

유혜인 장호성[1] 이광렬[2] 우경자[3,*]

한국과학기술연구원(KIST) 분자인식연구센터 [1]한국과학기술연구원(KIST) 미래융합기술연구본부 [2]고려대학교 화학과 [3]한국과학기술연구원(KIST) 나노재료연구센터

Quantum Dots (QDs) encapsulated by silica have great physicochemical stability, biocompatibility, durability and feasibility for surface functionalization and manipulation. Therefore, they have attracted great attention in various applications such as bio-imaging, sensors, displays and LEDs.We encapsulated a homogeneous QD layer near the surface of colloidal silica nanosphere by using electrostatic interaction between QDs and surface-engineered silica nanosphere. These QD layer-encapsulated nanospheres (SQS) with an appropriate silica shell thickness display high improvement in their optical emission, compared to their corresponding QDs.Based on these great advantages of SQS, we fabricated white LED by incorporating red-emitting SQS and Ce-doped YAG phosphors together on a blue LED chip. The performance of the resultant white LED was evaluated using various combinations focusing on color rendering index and emission efficiency, which showed nice improvement.

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Postsynthetic Lignad Exchange of 3-D Metal-Organic Framework

정석 신선영 나명수*

울산과학기술대학교(UNIST) 친환경에너지공학부

The preparations of the two isoreticular MOFs, Ni(HBTC)(dabco)] (2) and [$Ni_2(HBTC)_2(bipy)_{0.6}(dabco)_{1.4}$] (3) (where, H_3BTC = 1,3,5-benzenetricarboxylic acid; dabco = 1,4-diazabicyclo[2.2.2]octane; and bipy = 4,4'-bipyridine), were demonstrated via the postsynthetic ligand exchange of [Ni(HBTC)(bipy)] (1). By soaking 1 in a high concentration of dabco DMF solution, all of the aromatic bipy pillaring linkers in 1 were completely exchanged by the shorter aliphatic dabco pillaring linkers to form the isoreticular MOF, 2, with reduced pore dimension and volume. In contrast, the soaking of 1 in a low concentration of dabco DMF solution led to the MOF, 3, with the partially and selectively exchanged additional component, dabco linker. Controlling the concentration of dabco, not only 2 with completely exchanged dabco but also 3 with selectively exchanged dabco in the alternating layers could be obtained. The structural characteristics, PXRD patterns and sorption behaviors of the three MOFs will be discussed in the presentation.

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Synthesis of Au-coated TiO_2 Nanorod Array and Its Application as a Raman Substrate

지인애 방진호*

한양대학교 응용화학과

Rapid, accurate detection of pollutants has become more important in the development of environmental technologies. Surface-enhanced Raman spectroscopy (SERS) stands out because of its high sensitivity, spectroscopic precision, and no interference from water. The recent development of Raman substrates, on which Raman scattering is significantly enhanced *via* strong local electromagnetic fields arising from metal nanostructures. One-dimensional (1D) nanostructures coupled with Ag or Au have been explored as efficient substrates as they can offer great Raman enhancement, reproducibility, and structural uniformity. 1D nanostructures of ZnO, TiO_2, and Si decorated with the noble metals are representative examples of this effort, and among them TiO_2 has received more attention because of its superior chemical stability and excellent photochemical properties. TiO_2 nanotubes or nanorods have been utilized as a 1D scaffold. Inspired by this report, we prepared a new Raman substrate, where Au nanoparticles (NPs) were deposited on hydrophobic TiO_2 nanorod array (Au/TiO_2). The Au/TiO_2 array found its utilization as a Raman substrate to amplify Raman signals, and we also observed that its photocatalytic properties rendered this substrate reusable.

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Mesoporous Co_3O_4 Nanoflower Integrated on a Three-Dimensional Carbon Network for Pseudocapacitor Electrode

곽지혜 방진호[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

As an electrical energy storage device, supercapacitors have found attractive applications in consumer electronic products and alternative power source due to their high energy density, fast discharge/charge time, low level of heating, safety, and long-term operation stability. Among various transition metal oxides, cobalt oxide has received a great attention because of a high specific capacitance and high stability. In this study, cobalt oxide nanoflowers were directly grown onto carbon fiber paper via a simple chemical synthesis route in order to maximize the utilization of cobalt oxide surface for high capacitance. The synthesized cobalt oxide nanoflowers featured large specific surface area, mesoporosity, and a nanostructure with open channels for efficient electrolyte diffusion, which were responsible for excellent charge storage performance. Also, the cobalt oxide nanoflowers deposited on carbon fiber paper were found to be stable during long-term operation.

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Mesoporous $Ni(OH)_2$ Nanotubes on Carbon Fiber Paper for Pseudocapacitor Electrode

이은주 방진호*

한양대학교 응용화학과

Supercapacitors offer high power density, fast charge-discharge characteristics, and long lifetime, but their energy density is unfortunately incomparable to that of LIBs. Thus, their utilization has been more limited in comparison to LIBs. In this respect, a great deal of effort has been devoted to enhancing the energy density of supercapacitors. A variety of transition metal oxides and hydroxides have been explored as electrode materials of pseudocapacitors. Among them, $Ni(OH)_2$ has received significant attention due to its high theoretical specific capacitance, high chemical stability, well-defined redox behavior, and low cost. $Ni(OH)_2$, however, suffers from low conductivity and poor long-term durability.To overcome these obstacles, $Ni(OH)_2$ has typically been either incorporated with activated carbon during electrode fabrication or directly grown on various carbon structures (e.g., carbon nanotubes or graphene). Despite the benefits of these strategies, the physical mixing and synthesis of nanocomposite powders still suffers from aggregation of $Ni(OH)_2$, phase separation, poor connectivity between carbon additives, and a need for the use of a binder that prohibits full utilization of active electrode material. In this study, we present a new strategy to alleviate these problems in which mesoporous $Ni(OH)_2$ nanotubes were directly integrated onto carbon fiber paper (CFP). One-dimensional $Ni(OH)_2$ nanostructures, assembled onto CFP without a binder, provide a large surface area and porous structure that facilitate the access of ions and relieve strain induced during charge/discharge cycling. Due to these synergic benefits, the $Ni(OH)_2$/CFP electrode exhibited a superior performance and good long-term cyclability.

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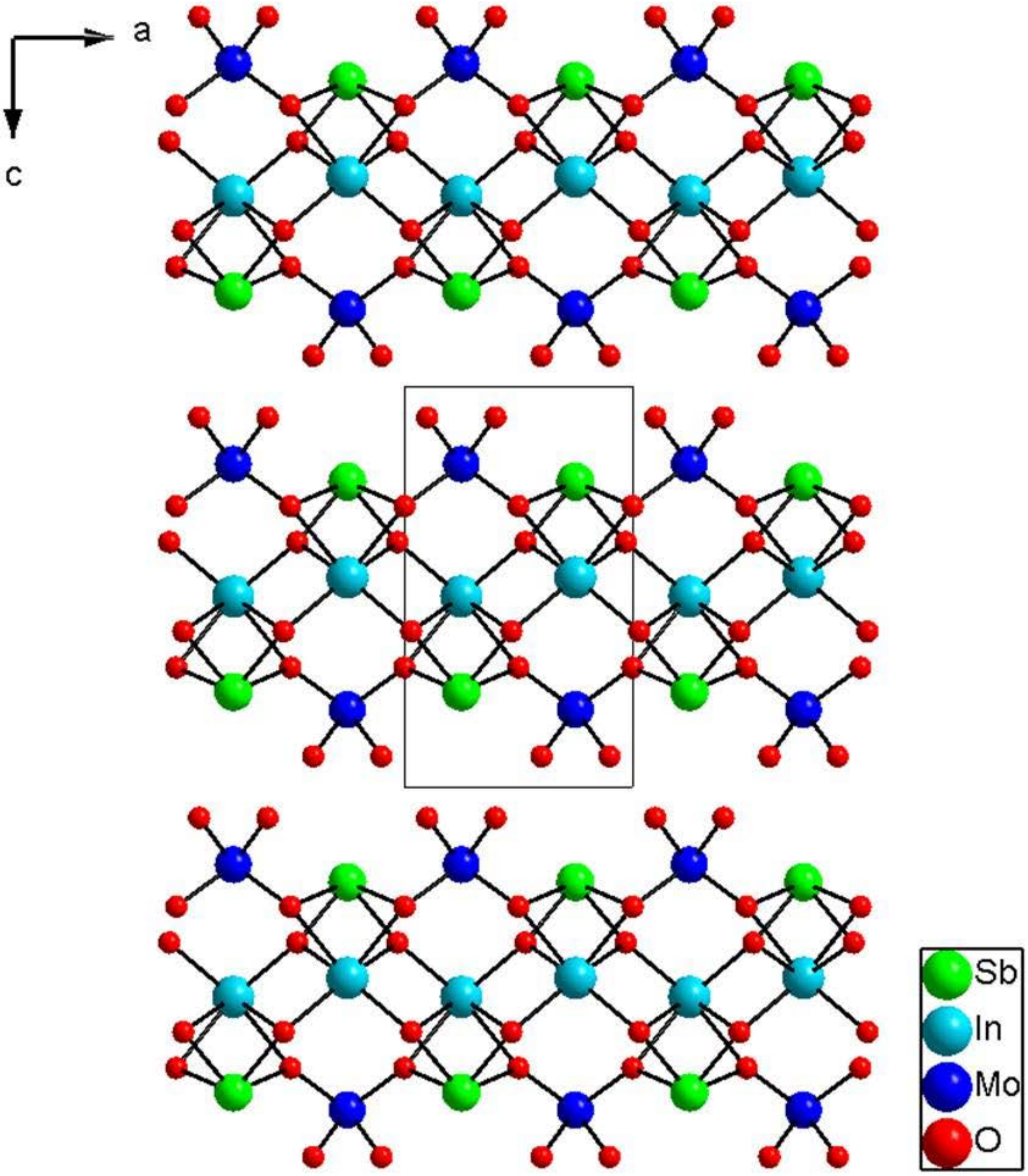
Solid-State Synthesis, Structure, and Characterization of a New Mixed Metal Oxide, $InSbMoO_6$.

이남희 옥강민[*]

중앙대학교 화학과

Centrosymmetric (CS) $InSbMoO_6$ has been synthesized by a standard solid-state reaction using In_2O_3, Sb_2O_3, MoO_3 as reagents. Single crystal X-ray diffraction was used to determine the crystal structure of the reported material. The $InSbMoO_6$ exhibits a layered crystal structure consisting of InO_8 polyhedra, MoO_4 tetrahedra, and asymmetric SbO_4 polyhedra. Powder X-ray diffraction, Scanning Electron Microscope/Energy-Dispersive Analysis by X-ray (SEM/EDAX), Infrared spectroscopy, and thermogravimetric analyses for the reported material are also presented. Crystal data for $InSbMoO_6$: orthorhombic *P*mmn (No. 59), Unit cell dimensions, a = 5.1367(10) Å, b = 5.3522(10) Å, c = 9.0131(2) Å.


a
c
Sb
In
Mo
O

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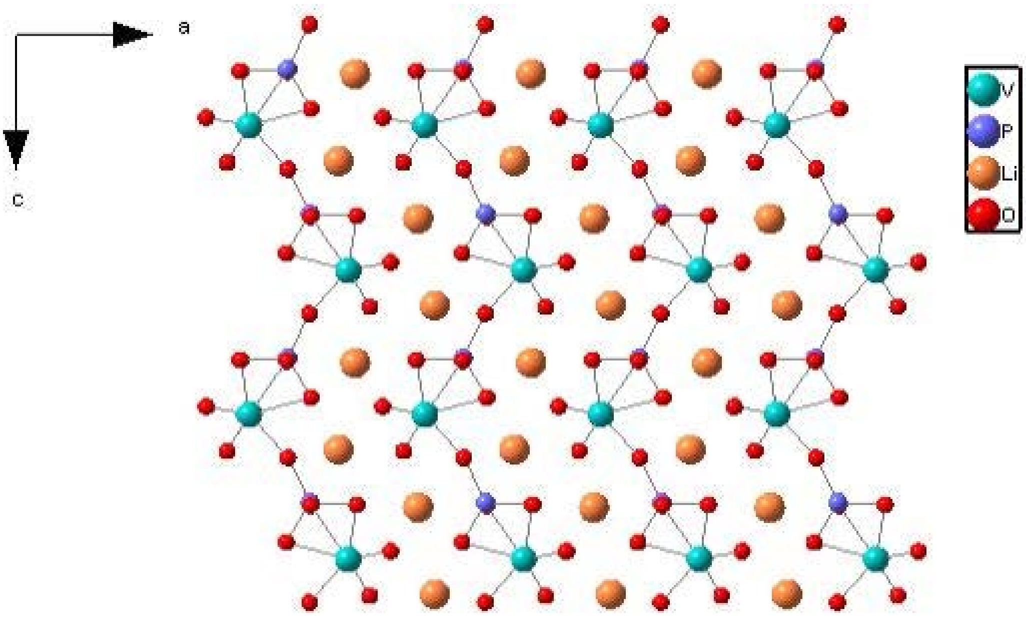
Synthesis, Structure, Second-Harmonic Generation (SHG), and Piezoelectric Properties of a Noncentrosymmetric vanadium phosphate, Li_2VPO_6

이은표 옥강민*

중앙대학교 화학과

The large scale synthesis, structural analysis, second-harmonic generation, and piezoelectric properties of a vanadium phosphate, Li_2VPO_6 are presented. The reported material has been prepared by a standard solid-state reaction using Li_2CO_3, V_2O_5, and $NH_4H_2PO_4$ as reagents. The phase purity and crystal structure of the reported material have been confirmed by powder X-ray and neutron diffractions. The noncentrosymmetric (NCS) 2D layered structure is composed of distorted VO_6 octahedra and PO_4 tetrahedra. The V^{5+} cations distort either along the [101] or [-101] directions due to the alignment of distorted VO_6 octahedra, which results in a polar crystal structure. Powder second-harmonic generating (SHG) measurements on Li_2VPO_6 using 1064 nm radiation, indicate the material has a SHG efficiency of approximately 10 times that of α-SiO_2 and is not phase-matchable (type 1). Converse piezoelectric measurements for the material exhibit a piezoelectric coefficient, d_{33}, of 12 pm V^{-1}.


a
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Design of a Redox-Active Ligand Having Acidic and Basic Coordination Sites.

하주연 구진영 **Yakiyama Yumi Masaki Kawano**[*]

포항공과대학교 첨단재료과학부

Organic N-containing heterocycles and carboxylate parts have been recognized as useful coordination units for the construction of coordination network. In this study, we have newly designed and synthesized redox-active as well as multi-interactive 4-[4’,7’-di(4”-pyridyl)-diazaphenalenyl]benzoic acid which contains carboxylic and pyridyl groups as coordination sites in the molecular structure. To our best knowledge, there is no ligand which possesses both acid-base sites and redox ability in one molecule in porous coordination chemistry. This unique structure will realize various network formations by controlling their coordination nature. Furthermore, the redox ability originated from the central diazaphenalenyl skeleton will provide unique magnetic properties in assembled structure. Here, we will report the preparation and the properties of our new ligand.

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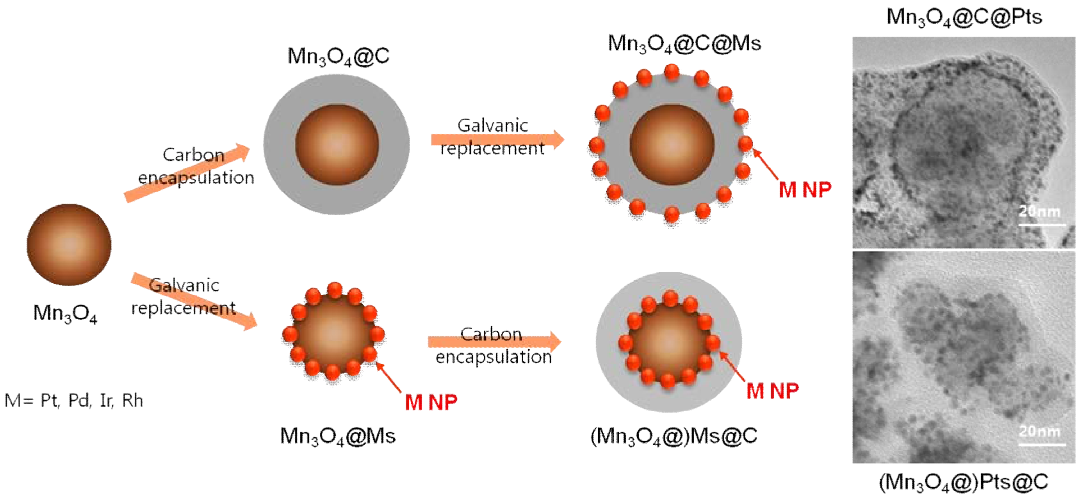
Differential Functionalization of Interior and Exterior Surfaces of Hollow Carbon Nanosphere through the Location-controlled Metal Depostion Process with Mn_3O_4@Carbon Nanospheres

이동규 김수민 이인수*

포항공과대학교 화학과

Due to their good electrical conductivity, high chemical inertness, large surface area, and controllable surface properties, hollow carbon spheres are attractive candidates as catalyst support materials. Here, we report the novel method of decorating surfaces of the hollow carbon nanospheres with catalytically active metal nanocrystals through employing the recently discovered galvanic replacement reactions involving manganese oxide surface. In the developed process, the immersion of the Mn_3O_4@C nanospheres, which are composed of Mn_3O_4 core and carbon shell, in aqueous solutions of noble metal ions produced catalytic nanocomposite, in which a high density of ultrafine nanocrystals of catalytic noble metals, such as Pt, Pd, Rh, and Ir, are stably immobilized in a homogeneously dispersive state on the outer surface of the hollow carbon nanosphere. Furthermore, the process was also applicable to control the location of the deposited metal nanocrystals in the carbon shell and, thus, enabled the differential functionalization of inner and exterior surfaces of the hollow carbon nanosphere.


Mn$_3$O$_4$@C
Mn$_3$O$_4$@C@Ms
Mn$_3$O$_4$@C@Pts
Carbon encapsulation
Galvanic replacement
M NP
20nm
Mn$_3$O$_4$
Galvanic replacement
Carbon encapsulation
M NP
M NP
20nm
M= Pt, Pd, Ir, Rh
Mn$_3$O$_4$@Ms
(Mn$_3$O$_4$@)Ms@C
(Mn$_3$O$_4$@)Pts@C

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2-Dimensional Ferrite/Carbon Nanocomposites as Li-ion Secondary Battery Anodes

장병철 박원철[1,*]

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We prepared monodisperse ferrite nanoparticles embedded in carbon materials via a simple salt-template heating process. Metal-oleate complex was used as the precursor for ferrite and carbon. The ferrite/carbon nanocomposites had a 2-dimensional (2-D) layered structure through the salt-template process. The electrochemical performances of the nanocomposites were strongly affected by the size of the ferrite nanoparticles and the morphology of the nanostructures. The smaller-sized nanoparticles and the 2-D nanostructures were more efficient for fast Li ion diffusion process during the electrochemical discharge/charge reaction. Consequently, the 2-D nanocomposites showed enhanced cycling stability and rate performance compared to the 3-D agglomerated composite materials.

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One-dimensional Cu(II) coordination polymers containing C_{2h}-symmetric terphenyl-3,3'-dicarboxylate linker

김현철 허성*

한국외국어대학교 화학과

Metal-organic frameworks (MOFs) are multifunctional nanoporous materials for various applications. They can be utilized for gas sorption, catalytic system, and drug delivery. We recently prepared a new C_{2h}-symmetric terphenyl dicarboxylate linker, terphenyl-3,3'-dicarboxylate (3,3'-TPDC), and a corresponding Zn-MOF containing 3,3'-TPDC and 1,4-diazabicyclo[2,2,2]octane (DABCO). The Zn-MOF is consisted of three-dimensional-like (3D-like) framework resulted from very efficient non-covalent stacking of the 2D layers compared with other grid structural MOFs which usually contain both the C_{2h}-symmetric dicarboxylate bridging ligand and a N-donor strut linker, DABCO or 4,4'-bipyridyl. We attempted to prepare MOFs derived from other transition metals and the 3,3'-TPDC ligand. For example, the dinuclear Cu(II) paddlewheel secondary building unit (SBU) consisted of 3,3'-TPDC might produce an interesting new Cu-MOF with unique topology which is structurally distinct from the well-known HKUST-1. Here we report two different Cu(II) 1D coordination polymers with the bridging ligand 3,3'-TPDC. Two 1D coordination polymers with distinct structural features were obtained through the reaction between Cu(II) ion and 3,3'-TPDC. Keeping the reaction mixture in a vial for several days at room temperature afforded two different crystalline products. The first form is a violet-colored rice-shaped crystal (1) and the second form is a blue-colored needle (2). The blue crystal is a major product. In contrast, a very small amount of violet crystals was recovered. Both compounds were structurally characterized by single crystal X-ray diffraction and their magnetic properties will be discussed.

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Facile Synthesis of Novel Rattle Structured Nanomaterials for Drug Delivery and Nanoscaled Reaction

최은진 박원철*

서울대학교 융합과학기술대학원 나노융합학과

Rattle structured nanomaterials, which contain a movable core in nanocapsules, have recently attracted much attention since the optical, electric, and magnetic properties of the core can be added to the nanomaterials. In this study, we synthesized rattle structured nanomaterials composed of gold nanorods in a mesoporous silica nanocapsule (AuNR@mSiO_2) using a novel solution-based consecutive process. The rattle structured AuNR@mSiO_2 nanomaterials were highly uniform and well dispersed in aqueous solution. Both the hollow space and the thickness of the mesoporous silica shell were easily changed by adjusting the amount of each chemical agent. We also studied the drug-loading properties and the controllably regrowth the core nanoparticles of the nanomaterial. The rattle structured nanomaterials are expected to be used as nanoreactors and in biomedical applications.

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Crystal Growth of $(CH_3)_2NH_2CuCl_3$ Single Crystals

박가람 오인환[1] 박승일

한국원자력연구원 중성자과학연구부 [1]한국원자력연구소 중성자과학연구부

It is well known that a low dimensional system can show various interesting, sometimes complex and/or useful, magnetic properties. To investigate the relation between the dimensionality and the magnetic behavior, it is crucial to have an adequate crystal structure.

Organometallic (dimethylammonium-bis(μ_2-chloro)-chlorocuprate) $(CH_3)_2NH_2CuCl_3$ (Cu-DMA) is known as a S = 1/2 Heisenberg alternating chain (HAC) magnet. Recent inelastic neutron scattering experiment showed inconsistent behavior to the previous results based on the susceptibility and the crystal structural investigation by X-rays[1]. To investigate further, it is imperative to have a good quality single crystal of a large size appropriate for neutron scattering experiments since the interaction of the neutrons with matter is relatively weak.

Recently, it has been reported that good quality single crystals were obtained using an evaporation method using alcohol as the solvent at 35℃ [2]. Following this example, we synthesized single crystals with different solvents at various temperatures to make suitable samples for the investigation of the crystal structure and the magnetic behavior by neutron scattering method. In this presentation, we will discuss the results of the crystal growth and X-ray powder diffraction.

[1] M.B. Stone et al., Phys. Rev. Lett. 99 (2007) 087204

[2] L.M. Chen et al., Journal of Crystal Growth 312 (2010) 3243

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콜로이달 합성을 통한 2차원 층상구조 형태를 가진 4족, 5족 전이 금속 칼코젠화합물 합성

김민경 천진우

연세대학교 화학과

2 차원 층상구조 물질의 물질적 특성에 대해 물질적 특성에 대한 연구가 진행되고 있으나 나노 입자의 정형화된 형태를 유지하는 합성 방법의 연구는 미흡하다. 이 연구에서는 2 차원 층상구조 물질을 이루는 transition-metal chalcogenide (TMC) 나노입자 합성에 전반적으로 적용될 수 있는 합성 protocol 을 제시하고자 한다. 다른 나노 입자와는 다르게 2 차원 층상구조 TMC 물질은 매우 불안정한데 그 이유로는 나노 입자 형성 과정 시 reactive 한 elemental chalcogene radical 의 존재때문인 것을 알아냈다. 이 연구에서는 먼저 정형화된 형태를 유지하는 titanium sulfide 와 selenide 합성 방법 소개 및 size control 이 가능함을 보이며 더 나아가 4 족, 5 족 transition-metal sulfide (TiS_2 , ZrS_2 ,HfS_2 ,VS_2 ,NbS_2 , TaS_2) 와 selenide ($TiSe_2$,$ZrSe_2$,$HfSe_2$, VSe_2 , $NbSe_2$, $TaSe_2$) 나노 입자를 합성했다. chalcogen source 로는 sulfur source 로는 CS_2 가 적합한반면에 selenide source 로는 element Se 가 매우 적합한 물질임을 발견했으며 2 차원 층상구조 TMC 나노 입자 형성에 S 와 Se element 의 radical 이 미치는 영향에 대해서도 간략하게 소개한다.

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Selective Trapping of Labile S_3 in a Porous Coordination Network and the Direct X-ray Observation

Hiroyoshi Ohtsu 최완욱 **Masaki Kawano***

포항공과대학교 첨단재료과학부

Trisulfur, S_3, is one of basic allotropes but still mysterious labile species over the long sulfur history. We succeeded in selective trapping of S_3 in a pore of a thermally stable coordination network and determination of the crystal structure by *ab initio* X-ray powder diffraction analysis. The S_3 in a pore has a C_{2v} bent structure like ozone as expected from microwave spectra. The S_3 trapped network is remarkably stable in an ambient condition and inert to photo-irradiation. Furthermore, we succeeded in unique transformation of S_3 to S_6 in the network by mechanical grinding or heating in the presence of NH_4X (X =Cl and Br) and the reverse-transformation of S_6 to S_3 by photo-irradiation. We also determined the S_6 encapsulated network structure by *ab initio* X-ray powder diffraction analysis.

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발표분야: 무기화학

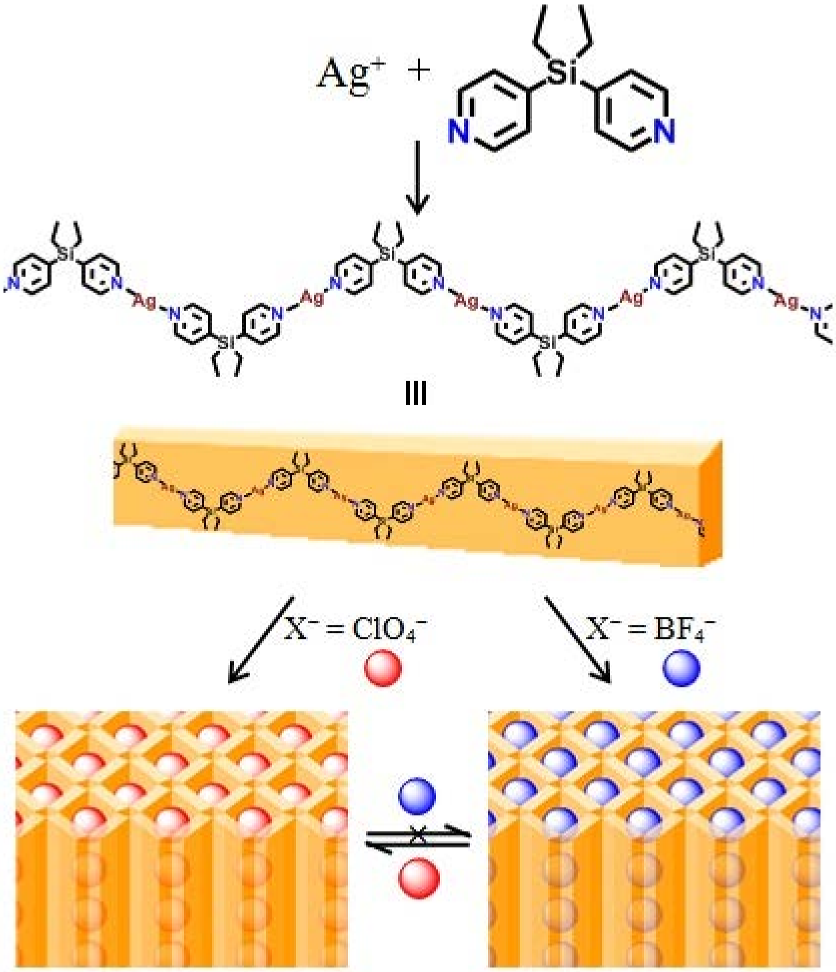
발표종류: 포스터, 발표일시: 수 16:00~19:00

Assembly of Supramolecular Channels consisting of Four 1-D Coordination Polymeric Single Strands

문소연 정옥상*

부산대학교 화학과

The reaction of AgX (X^- = ClO_4^- and BF_4^-) with bis(4-pyridyl)diethylsilane (L) produces crude solids. Vapor-diffusion of diethyl ether into the acetonitrile solution of the crude solids gives rise to a 1-D single strand consisting of $[Ag(L)](ClO_4)$ and $[Ag(L)](BF_4)$. We found that an unprecedented supramolecular channel motif is formed via the assembly of four 1-D single strand chains. The ethyl group attached to silicon atom weakly interacts with the pyridly group of the adjacent single strand. The counteranionic species, ClO_4^- and BF_4^-, are nestled in the supramolucular channels through the weak interactions with the silver(I) atom. The physiochemical properties including anion exchangeability were characterized by IR, TGA/DSC, and single crystal X-ray diffractometer.


Ag⁺ +
Si
N
N
Ag
X⁻ = ClO₄⁻
X⁻ = BF₄⁻

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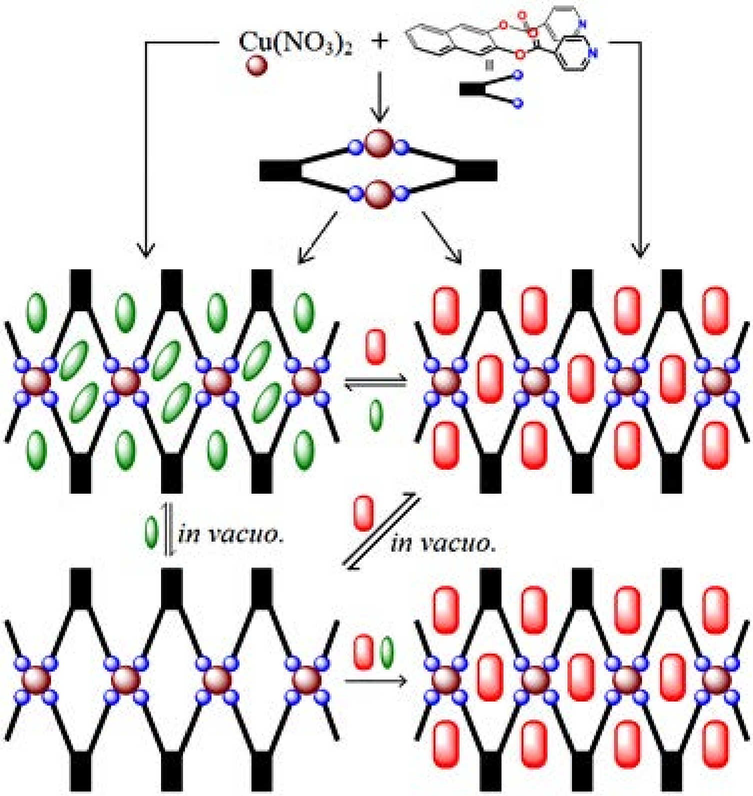
발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of Discrete Cyclodimer and 1-D Coordination Polymers of Copper(II) Compounds Containing 2,3-Bis(isonicotinoyloxy)naphthalene

조윤정 노태환 정옥상*

부산대학교 화학과

Self-assembly of copper(II) nitrate with 2,3-bis(isonicotinoyloxy)naphthalene (L) in a mixed acetonitrile/dichloromethane (CH_2Cl_2) produces a 30-membered discrete metallacyclodimer, $[Cu(NO_3)_2(L)]_2$, while the self-assembly in a mixed *N*,*N*-dimethylformamide (DMF)/CH_2Cl_2 and DMF/dioxane yields 1-D coordination polymers consisting of $[Cu(NO_3)_2(L)_2]\cdot 4CH_2Cl_2$ and $[Cu(NO_3)_2(L)_2]\cdot$3dioxane, respectively. Recrystallizations of $[Cu(NO_3)_2(L)]_2$ from DMF/CH_2Cl_2 and DMF/dioxane lead to $[Cu(NO_3)_2(L)_2]\cdot 4CH_2Cl_2$ and $[Cu(NO_3)_2(L)_2]\cdot$3dioxane, respectively. Construction of the metallacyclodimer versus the 1-D coordination polymer was affected with the reacting solvents rather than the synthetic methodologies. The removal/readsorption and exchange of the solvated molecules in the crystalline solids of $[Cu(NO_3)_2(L)_2]\cdot 4CH_2Cl_2$ and $[Cu(NO_3)_2(L)_2]\cdot$3dioxane were conducted and fully characterized by IR, NMR, TGA/DSC, and powder XRD. The 1-D coordination polymeric skeleton was able to discriminate between dioxane and CH_2Cl_2 molecules.


Cu(NO$_3$)$_2$
+
in vacuo.
in vacuo.

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Synthesis, Characterizations, and Their Catalytic Properties of Copper(II) Complexes Containing 1,3,5-Tris(isonicotinoyloxyethyl)cyanurate

홍우식 정옥상*

부산대학교 화학과

Studies of anion effects on the molecular construction of a series of CuX_2 (X_2^-= NO_3^-, BF_4^-, and ClO_4^-) complexes with 1,3,5-tris(isonicotinoyloxyethyl)cyanurate (L) have been carried out: the reactions of $Cu(BF_4)_2$, $Cu(ClO_4)_2$, and $Cu(NO_3)_2$ with L produce 1-D coordination polymer consisting of $[Cu(L)_2(H_2O)(BF_4)]BF_4\cdot 2H_2O$, 2-D coordination polymer consisting of $[Cu(L)(DMSO)_2(ClO_4)]ClO_4\cdot 2CH_2Cl_2$, and 3-D coordination polymer consisting of $[Cu(L)(O\text{-}NO_3)_2][Cu(L)(O,O'\text{-}NO_3)2(CH_3OH)]\cdot 2CH_2Cl_2\cdot CH_3OH\cdot H_2O$, respectively. The present compounds were fully characterized by IR, TGA/DSC, and single crystal X-ray diffractometer. In order to investigate the catalytic effects of the copper(II) complexes, a catechol oxidation was achieved.

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발표분야: 무기화학

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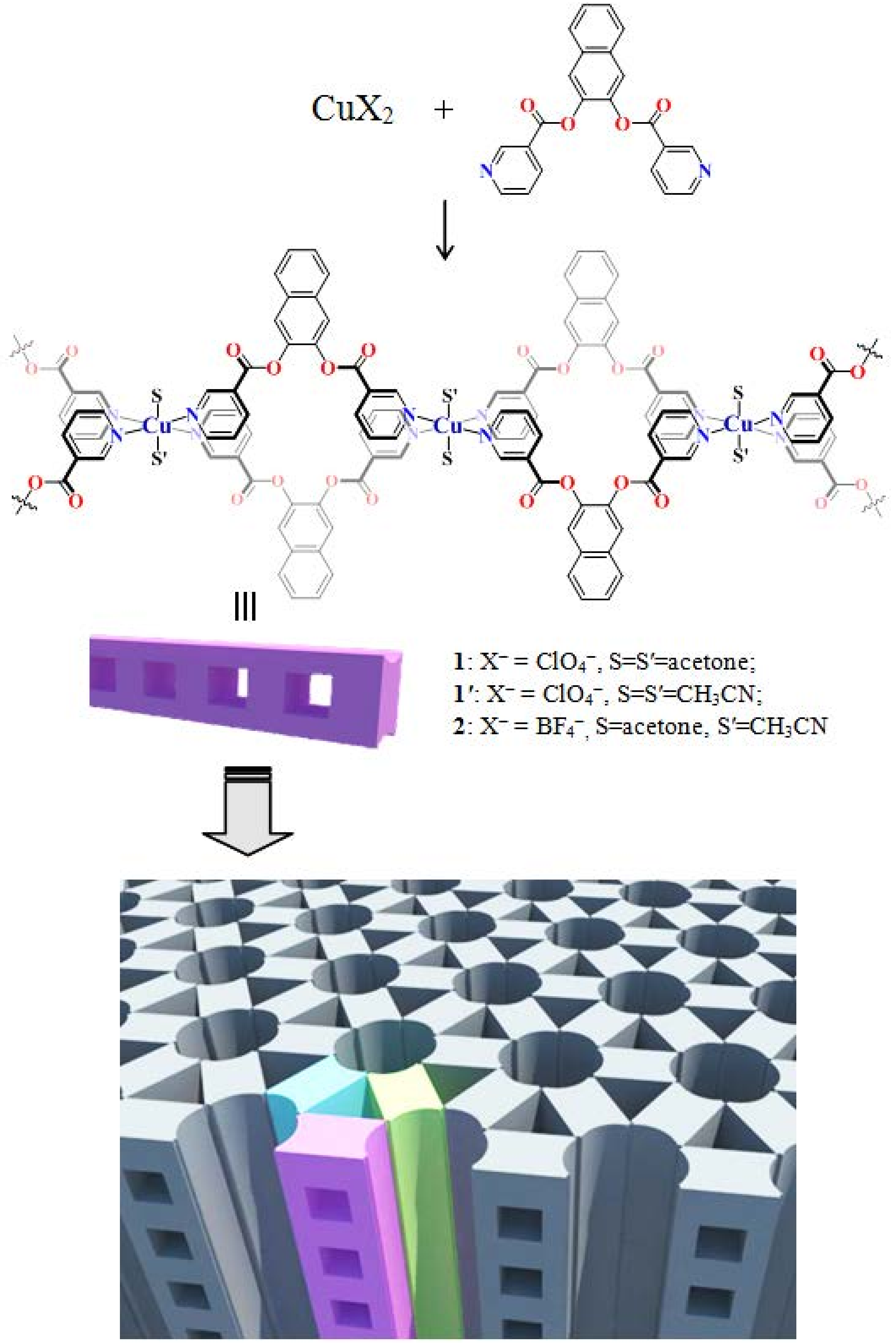
3-D Kagome-Type Supramolecular Channels via Molecular Array of 1-D Copper(II) Coordination Polymers

이해리 정옥상*

부산대학교 화학과

Self-assembly of CuX_2 (X^- = ClO_4^- and BF_4^-) with 2,3-bis(nicotinoyloxy)naphthalene (L) gives rise to 1-D loop-chain skeletons consisting of $[CuL_2(S)(S')](X)_2$ (1: S = S' = Me_2CO, X^- = ClO_4^-; 1': S = S' = MeCN, X^- = ClO_4^-; 2: S = Me_2CO, S' = CH_3CN, X^- = BF_4^-). The 1-D loop-chains weakly interact via two adjacent naphthyl groups (C-H···π interaction = 2.910 - 2.960), dihedral angle: 59.5(1) - 61.1(2)°) resulting in the formation of unprecedented 3-D Kagome-type channels consisting of large channels via six 1-D coordination polymers and small channels via three 1-D coordination polymers. The evacuated materials absorb carbon monoxide (CO) which coordinates to the copper(II) ion. The coordinated carbonyl moiety is dissociated under vacuum at 95 ºC, indicating that the carbonyl group reversibly coordinates and dissociates. The catalytic effects on the catechol oxidation of the present compounds were investigated.



1: $X^- = ClO_4^-$, S=S′=acetone;
1′: $X^- = ClO_4^-$, S=S′=CH_3CN;
2: $X^- = BF_4^-$, S=acetone, S′=CH_3CN

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Investigation of Fluorine Substituent Effect on Benzothadiazole Bridging Unit for Dye Sensitized Solar Cells

조나라 백상현 김철우 도광석 최혜주 임남우 고재중*

고려대학교 소재화학과

Introduction of fluorine atom is the simplest way to move short wavelength region factor in organic photovoltaic filed. Fluorine atoms have many influence on inter- and intramolecular interaction also give positive highest occupied molecular orbital. It will be have influence on the short circuit current and the fill factor even the open circuit voltage for dye sensitized solar cells. Herein, we report our photovoltaic performance investigation of fluorine effect on 5- and/or 6- position of 2,1,3-benzothiadiazole bridging group for dye sensitized solar cells. Further investigation for understanding of fluorine effects is currently underway.

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Synthesis and photovoltaic properties of TIPS-substituted benzo[1,2-b:4,5-b0]dithiophene-based small molecule material for Organic Photovoltaic.

임남우 김철우 백상현 조나라 고재중

고려대학교 소재화학과

Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV). Recently, polymer solar cell based on triisopropylsilylethynyl (TIPS) group anthracene-based copolymers have been applied toward improving the power conversion efficiencies (PCEs) (5-6%) of PSCs. TIPS have been shown lower energy level between lowest unoccupied molecular orbital (LUMO) and highest unoccupied molecular orbital (HOMO) than alkoxy substituent. In this work, we modified TIPS in small molecule field are based on a core acceptor/donor/acceptor (A/D/A) framework. The structures with containing benzo[1,2-b:4,5-b0]dithiophene based on chalcogenophenes have given good performance and several advantages for BHJ devices because of conjugated donor backbone and electron-withdrawing terminal with coplanar ring systems within slipped π-stacks for high open circuit voltage. We herein report these small molecules exhibit the properties of solution processability, large charge transporting capabilities and high voltage. Moreover, TIPS as a donor in small molecule substitutes improving the solubility, π-π stacking, and stability of acene molecules ,π-bridge Trithiophene with hexyl and methylene-malononitrile, acceptor hexyl cyanoacetate.

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Development of Organic dyes for Aqueous Dye-Sensitized Solar Cells

최혜주 임남우 백상현 박소진 고재중*

고려대학교 소재화학과

The photovoltaic technology has been considered as an effective way to solve the current energy and environmental crisis. Dye sensitized solar cells (DSSCs) are currently attracting wide-spread interest as low-cost alternatives to conventional solid-state photovoltaic devices. Organic based electrolyte with I-/I3- redox couple is one of main part of a typical DSSCs consists. However, organic based electrolytes with volatility and flammability degrades the durability and safety of the cell. Water electrolyte based DSSC is environmental friendly alternative and more feasible for indoor usage since it do not contain toxic volatile organic solvents. Therefore, in our study, we introduced water-based electrolyte using the novel organic sensitizers for DSSCs.

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Triphenylamine-Based unfused and fused Molecules: Design, Synthesis, and Their Application in Bulk Heterojunction Organic Solar Cells

도광석 김철우 임남우 박소진 고재중*

고려대학교 소재화학과

Organic solar cells (OSCs) fabricated by versatile printing methods such as the doctor blade, inkjet, and roll-to-roll methods are inexpensive, lightweight, and highly solution-processable. Over the past few years, considerable effort has been focused on improving the OSC performance, with the aim of achieving a power conversion efficiency (PCE) of 10%. The following strategies have been adopted for this purpose: (1) development of photoactive materials such as π-conjugated semiconducting polymers and fullerenes, (2) use of functional layers for buffering, charge transport, optical spacing, etc., and (3) tuning the morphology of the photoactive film by postannealing, solvent drying, or using processing additives. We synthesized a new type of organic sensitizers incorporating a unfused and fused triphenylamine unit and demonstrated to be a highly efficient sensitizers in OSC. Organic solar cells fabricated with fused molecule and [6,6]-phenyl C71 butyric acid methyl ester (PC71BM) by spin-coating from solution demonstrate similar fill factor (FF) but larger short circuit current density (Jsc) and open circuit voltage (Voc) in comparison with solar cells fabricated with corresponding unfused molecule and PC71BM. A PCE of 4.04 %, with Jsc = 10.803 mA/cm2, Voc = 0.886 V, and FF = 0.42 was achieved with TiOx treated fused molecule.

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Solution processable using new compounds of small molecule in organic solar cell

백상현 조나라 도광석 최혜주 임남우 김철우 고재중*

고려대학교 소재화학과

Organic solar cells (OPV) have been widely investigated recently due to their potential for light-weight, low-cost, and large-scale roll-to-roll processing. Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. Solution processable small molecule-based donor material has been also attempted as attractive alternative of donor in organic solar cell due to its facile synthesis, purification, and low batch-to-batch variation compared to polymeric materials. The synthesis and photovoltaic characteristics of new organic semiconductors are reported. 3,3'-Dihexylsilylene-2,2'-bithiophene have low-lying LUMO and stabilized HOMO level compare to the carbon counterpart. We think that to incorporate the broad absorption spectrum and good hole transport property of final compound. Also, we introduced 3-hexylthiophene as donor to increase solubility in organic solvents and extend the conjugation length. We introduced donor such as fluorene and triphenyl amine and accepter such as cyanoacrylate and malononitrile. We expected that malononitrile have much higher Voc than cyanoacrylate owing to they have lower HOMO. When we use fluorene donor moiety, it obtained much better current than triphenyl donor moiety because of fluorene increased molar extinction coefficient in the short wavelength. We gave efficiency of 2.34% with a short circuit photocurrent density (Jsc) of 7.31, an open circuit voltage (Voc) of 0.806, a fill factor 0.39.

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Organic Sensitizers Featuring a Planar Indeno[1,2-b]thiophene for Efficient Dye-sensitized Solar Cells

임기민 도광석 최혜주 박소진 고재중*

고려대학교 소재화학과

We already synthesized and announced sensitizers based on Indenothiophene derivative. In this paper, an efficient organic sensitizer (JK-306) featuring a planar indeno[1,2-b]thiophene as the π-linker of bridging unit for dye-sensitized solar cells (DSSCs) was synthesized. The dye has a strong molar absorption coefficient and a red-shifted absorption band compared with JK-305, resulting in a significant increase in the Jsc. Under standard global AM 1.5 solar conditions, JK-306 sensitized cells in the presence of CDCA and HC-A as coadsorbents afforded an overall conversion efficiency of 8.37% and 8.52%, respectively. Upon changing the electrolyte from I?/I3? electrolyte to CoII/CoIII redox couple, the cell gave the significantly improved conversion efficiency (η) of 10.02% when used multifunctional HC-A, which is the highest value reported for DSSCs with cobalt-based electrolyte.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Reactions of S_3 trapped in a porous coordination network

최완욱 Hiroyoshi Ohtsu Masaki Kawano*

포항공과대학교 첨단재료과학부

Sulfur has been extensively investigated over more than 200 years. However, small sulfur allotropes like S_2, S_3, S_4, and S_5 have not been studied well because they exist only in a gas phase. Therefore, we aimed to encapsulate such a small sulfur in a porous network to investigate the reaction of small sulfur allotropes that may show unique reactivity. We utilized crystalline powder of thermally stable porous network, $[(ZnI_2)_2(TPT)_3]$ (TPT: 2,4,6-tris(4-pyridyl)triazine), and successfully trapped S_3 in a pore of network that structure was solved by *ab initio* powder X-ray structural analysis. Here, we report the versatile reactivity of small sulfur in a porous coordination network. The S_3 in a pore is quite inert to many organic alkenes that usually react with small sulfur allotropes. This reactivity suggests that the S_3 in a pore is well isolated and significantly stabilized even though S_3 itself is normally so reactive. On the other hand, benzonitrile induced structure rearrangement from sulfur encapsulated network, $[(ZnI_2)_2(TPT)_3](S_3)_{0.5}$ to the benzonitrile@$[(ZnI_2)_3(TPT)_2]$, implying unique reaction occurred in the pore. Moreover, the S_3 in a pore reacted with acetylene to produce a polymer material that was confirmed by GPC, IR, UV/Vis, MALDI-MS, and NMR.

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Evidence for an Oxygen Rebound Mechanism in C-H Bond Activation by Non-Heme Fe^{V}O Complex

권은지 홍승우[1] 서미숙 CHO KYUNG BIN MICHAEL 이용민[2] 남원우[3,*]

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The hydroxylation of alkanes by heme Fe^{IV}O π-radical cation species (formally Fe^{V}O) occurs via the hydrogen atom abstraction/oxygen rebound mechanism. However, recent report shows that in the case of non-heme Fe^{IV}O species, the dissociation of the substrate radical formed via hydrogen abstraction from alkanes is more favorable than the oxygen rebound and desaturation processes. Here is an open question whether the hydroxylation of alkanes by nonheme Fe^{V}O proceeds via oxygen rebound mechanism as proposed in heme Fe^{IV}O π-radical cation species. We hypothesized that non-heme Fe^{V}O species follows the heme Fe^{V}O paradigm in C?H bond activation reactions. Herein we provide theoretical and experimental evidence that C?H bond activation of alkanes by synthetic non-heme Fe^{V}O complex occurs via oxygen rebound mechanism. We demonstrated for the first time the feasibility of oxygen rebound in the reaction between Fe^{V}O and alkanes by means of DFT calculation. This theoretical mechanistic insight was supported by analyzing products formed in the C-H bond activation reaction by non-heme Fe^{V}O complexes.

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Synthetic Control Over Photoinduced Electron Transfer in Phosphorescent Sensors of Zinc

조소민 유영민[1,*] 남원우[2,*]

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A series of iridium(III) complexes bearing cyclometalating ligands with various bandgap energies and electron densities have been prepared and evaluated for the phosphorescent response to zinc ion. The zinc sensors are comprised of two anionic cyclometalating ligands and a neutral 1,10-phenanthroline ligand that tethers a di(2-picolyl)amine (DPA) zinc receptor. To elucidate photoelectrochemical mechanism, mechanistic studies including variable-temperature steady-state and transient photoluminescence spectroscopy, electrochemical measurements, and computational calculations based on time-dependent density functional theory were performed. The studies allowed for assessment of the influence of the molecular factors underlying the phosphorescence zinc response, which are excited-state electrochemical potentials and the Coulombic barrier in the photoinduced electron transfer (PeT) from DPA to Ir^{IV} species. We further calculated the driving force for PeT by employing the Rehm-Weller equation, and the results were compared with the experimental phosphorescence dynamic ranges. As a useful demonstration, zinc biosensing utility was demonstrated through the phosphorescence visualization of mobile zinc ions in HeLa cells using confocal laser-scanning microscopy and photoluminescence lifetime-imaging microscopy.

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Characterization and Reactivity of Mn(IV)-Peroxo,Mn(V)-Oxo and Redox-Inactive Metal Ion Adduct Mn(V)-Oxo Complexes.

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Manganese-oxygen adducts, including manganese-peroxo [Mn(O_2^{2-})] and manganese-oxo [Mn(O)] species have been invoked as central intermediates in catalytic oxygen atom transfer (OAT) reactions as well as in photosynthetic oxygen evolution. Herein, Mn(IV)-peroxo, $[Mn^{IV}(O_2)(TAML)]^{2-}$, Mn(V)-oxo, $[Mn^{V}(O)(TAML)]^{-}$ and scandium ion adduct Mn(V)-oxo, $[Mn^{V}(O\text{-}Sc^{III})(TAML)(OTf)_3]^{-}$ were thoroughly synthesized and characterized with various spectroscopic methods such as UV-vis, electrospray ionization mass, EPR and resonance Raman spectroscopic methods, and X-ray crystal structure. Mn(IV)-peroxo was capable of carrying out nucleophilic reactions by reacting with aldehydes and O_2 transfer reaction to other Mn(II) complex. On the other hand, Mn(V)-oxo has very low reactivities in oxygen atom transfer and C-H bond activation reactions. However, scandium ion-bound Mn(V)-oxo exhibited much greater reactivities in the reaction with triphenylphosphine and electron transfer reactions with ferrocene derivatives.

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Crystal-to-Crystal Transformations of Isostructural Metal-Organic Frameworks of a 3-connected srs net topology

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울산과학기술대학교(UNIST) 친환경에너지공학부 [1]울산과학기술대학교(UNIST) 나노생명공학부/첨단화학공학과

A series of isostructural 3-D metal?organic frameworks (MOFs), [Zn2(BTC)(A)(S)3] (where BTC = 1,3,5-benzenetricarboxylate; A = OH?, NO3?; S = EtOH (1), DMF (2), DMA (3), or DEF (4)), of a 3-connected srs net topology have been prepared in the presence of serine as a template. All of the frameworks are stable under N2; however, at ambient conditions and in the presence of water molecules, they ultimately transform into the thermodynamically most stable 1-D chain structure, [Zn3(BTC)2(H2O)12]. While 1, 3, and 4 with a ligated NO3? anion change directly to the 1-D chain structure without the formation of any intermediate structures, 2 with a ligated OH? anion transforms to the 1-D chain structure via either an unidentified intermediate at ambient conditions or via the 2-D layer structure ([Zn3(BTC)2(H2O)8]) in the presence of sufficient water molecules added to the sample. A single crystal of 2 is stable in Mg(II) and Co(II) DMF solutions; however, it transforms into a single particle-like microcrystalline aggregate of Cu-HKUST-1 with the tbo net topology in Cu(II) DMF solution.

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Geometric isomerism of mononuclear nickel(II) complexes with H_2pmide ligand (H_2pmide= *N*-(2-pyridylmethyl)iminodiethanol)

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경북대학교 화학과 [1]경북대학교 사범대학 화학교육과

N-(2-pyridylmethyl)iminodiethanol (H_2pmide) ligand having an amine, two hydroxyl groups and a pyridine is considered to have the potential to form interesting metal complexes with transition metals. Recently, two isomers of mononuclear nickel(II) complexes, $[Ni(H_2pmide)_2](NO_3)_2$ (1) and $[Ni(H_2pmide)_2]Cl_2$ (2) have been synthesized using H_2pmide and $Ni(NO_3)_2{\cdot}6H_2O/NiCl_2{\cdot}6H_2O$, respectively. In complexes 1 and 2, nickel(II) ions are coordinated with two H_2pmide ligands; one O atom of hydroxyl group and two N atoms in each H_2pmide ligand and has a distorted octahedral geometry. Compounds 1 and 2 have violet and blue color in the solid state, respectively, due to the different coordination geometry depending on the anions (NO_3^- and Cl^-). In this poster, we will present the detailed preparation of the ligand and nickel complexes as well as crystal structures.

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New iron(II) spin crossover frameworks (SCOFs); synthesis, structure, magnetic property and gas adsorption

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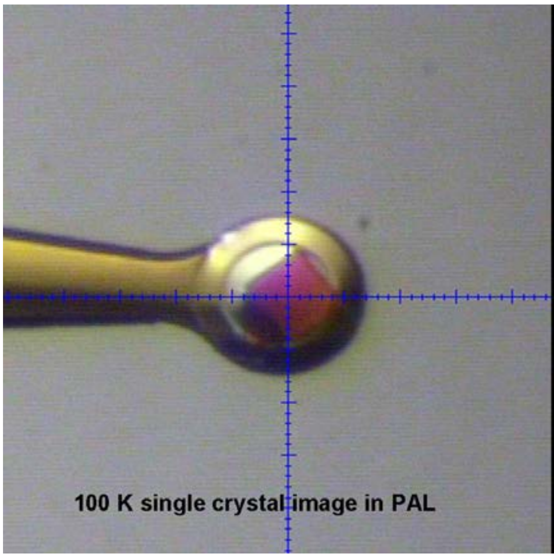
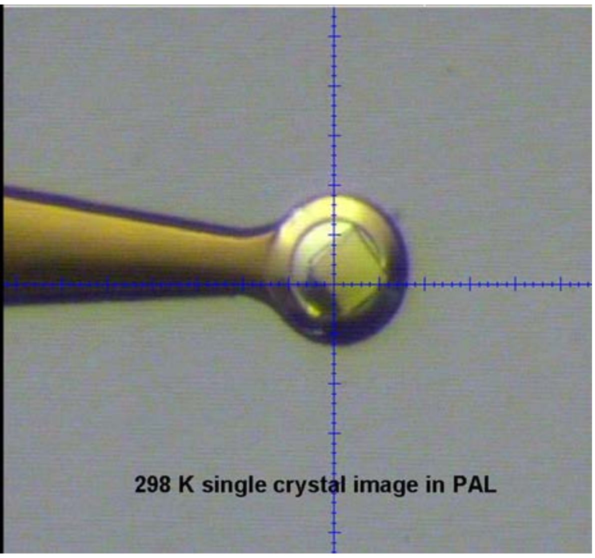
경북대학교 화학과 [1]경북대학교 사범대학 화학교육과

The development of porous framework materials having spin crossover (SCO) centers leads to new functional solids that display a range of interesting and potentially useful physical properties. Recently, new spin crossover frameworks (SCOFs) of iron(II) complex, $[(tpmd)_2Fe_2(NCBH_3)_4]_n\cdot$xguest (1) , has been prepared by the self-assembly of Fe(II) species and $NCBH_3$ counterions with *N*,*N*,*N´*,*N´*-tetra-4-pyridyl-methylenediamine (L, tpmd) in an oxygen-free dry box. The structure of 1 was determined by using single crystal X-ray diffraction at 100 and 298 K, Each Fe(II) ion has a distorted octahedral geometry with the four nitrogen atom of tpmd ligand and two nitrogen atom of $NCBH_3$ anions. At 100 K and 298 K, the average Fe-N distances are 1.976(1) and 2.185(2) Å and related to low spin and high spin states, respectively. The cell volume increases by 1013 $Å^3$ upon warming from 100 to 298 K. To confirm the porosity of 1, the gas sorption isotherms were measured for N_2 gas and exhibited 1054 m^2g^{-1} as BET surface at 77 K. 1 displays spin crossover behaviors about 240 K with thermal hysteresis (10 K). In addition to thermal spin crossover, 1 exhibits large hysteresis (30 K) by LIEEST (Light-induced excited spin-state trapping) effect. In this poster, we will present the detailed preparation of the ligand and iron compound, crystal structure, magnetic properties as well as interesting coordination chemistry.


100 K single crystal image in PAL


298 K single crystal image in PAL

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Kinetic Assembly of a Thermally Stable Porous Coordination Network Based on Labile CuI Units

<u>Hakuba Kitagawa</u> Hiroyoshi Ohtsu Masaki Kawano*

포항공과대학교 첨단재료과학부

The advantage of porous coordination network synthesis can be designable by changing metal sources and ligands. Therefore, not only many commercially available ligands but also newly synthesized ones were used for networking. On the other hand, most of metal sources are common reagents or stable metal moieties because they can be more predictable as a metal connector. So far there is no report focusing usage of labile metal sources. One of the promising methods to produce unique networks with such labile metal sources is kinetic control.Here we first report selective syntheses of thermally stable porous coordination networks using a labile CuI cubane cluster and a rigid T_d symmetry ligand by kinetic and thermodynamic control. From rapid cooling of hot solution of CuI cubane and T_d-tetradentate ligand, we obtained porous coordination network composed of novel CuI helical chain and this network is thermally stable even though this is kinetically controlled one. On the other hand, from slow cooling of the solution, we obtained more stable porous coordination network composed of CuI dimer. The CuI helical network crystal shows iodine chemisorption to make covalent bond with iodine that face to a pore. In contrast, the CuI dimer network crystal shows efficient iodine physisorption. In this poster presentation, we will report on the detail of the syntheses, the reaction mechanism of network formation, and the difference of the iodine sorption behavior between these two networks based on each structure of these network crystals.

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Zinc selective chemosensors based on the flexible dipicolylamine and quinoline

김현 송은주 박경진 조현용 김 철[1]

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Zinc sensor molecules containing quinoline have been synthesized, which show fluorescence in the presence of Zn^{2+}. The nitrogen in quinoline is critical to fluorescence and fluorescence enhancement is promoted by deprotonating the sensor’s amide. One of the sensors is highly selective for Zn^{2+} over Cd^{2+} and other cations such as Hg^{2+}, Fe^{2+}, Mn^{2+} and Ca^{2+}. This selectivity can be attributed to the increased absorption of the sensor in the presence of Zn^{2+} and the strong binding of Zn^{2+}. Structural studies, including X-ray and NMR, show the ability of dipicolylamine (DPA) to bind in facial and meridional manners to Zn^{2+}. Crystal structures of different compounds show Zn^{2+} coordinating to three, four, and five nitrogens from the compounds. They also indicate that the selectivity of DPA containing compounds towards Zn^{2+} may originate from Zn^{2+} being stable in different coordination environments.

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Synthesis and Characterization of New Volatile Strontium Precursor

조지쉐비메리 박보근 김창균 정택모[1,*]

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A new heteroleptic strontium complex was synthesized by treating the corresponding ligands in 1:1 ratio with SrI_2 to yield desired complex. The highly substituted ligand mixtures stabilize the central strontium metal ion and eventually prevent from undergoing oligomerization. The compound was characterized using NMR spectroscopy, FT-IR and Elemental Analysis. The thermo gravimetric analysis was carried out to measure the decomposition character and volatility of the complex, which displays temperature stability and a steady loss of mass in the temperature region of 125?350 ºC with 7% residue at the end. The studies to explore this compound as a possible strontium precursor for the growth of thin films of $SrTiO_3$ (STO), and $Ba_{0.5}Sr_{0.5}TiO_3$ (BSTO) using ALD techniques are in progress.

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Synthesis and Characterization of Novel Lead Sulfide Precursor

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Lead sulfide (PbS) has been utilized in optoelectronic applications, such as IR detectors and solar cells, because of its small bandgap (∼0.41 eV). Recently, high quality lead sulfide thin films have been explored using ALD/CVD technique. Suitable precursors are needed to deposit thin films of inorganic materials. However, lead sulfide precursors available for ALD/CVD process are very limited to lead complexes with dithiocarbamate and alkanethiolate ligands. Therefore, it is essential to prepare novel lead sulfide suitable for ALD/CVD precesses. Herein we report on the synthesis and characterization of new lead sulfide complex with designed aminothiolate ligand. The novel complex has been characterized by means of ^{1}H-NMR, elemental analysis, thermogravimetric analysis (TGA), X-ray Diffraction (XRD) and scanning electron microscope (SEM).

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Novel Tin Precursors for SnO2 Thin Films Deposition

정은애 박보근 김창균 정택모[1,*]

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Studies of metal oxide semiconductors have been widely reported due to their advantages of electronic and chemical properties. Particularly, these materials are applied for optoelectronic device such as light-emitting diodes (LEDs) and thin film transistors (TFTs) over the decades. Tin oxide with n-type conductivity due to oxygen vacancies and/or metal ion interstitials has been widely researched due to its wide band gap of 3-4 eV, its high optical transparency in the visible light range, and its good chemical stability. Recently, tin-based oxide semiconductors have been reported as feasible for use as the active channel material in the transparent TFTs, light-emitting diodes, and flexible displays.Novel Sn(II) complexes were synthesized by treating tin amide [Sn(NR2)2] with 2 equivalents of new oxime ligands (L1H, L2H). Compound 1 and 2 have been characterized by 1H, 13C nuclear magnetic resonance (NMR), FT-IR spectroscopy, elemental analysis and thermogravimetric analysis. The molecular structure of 1 and 2, determined by X-ray single crystallography are dimeric with oxygen-bridged four-membered ring and nitrogen atoms of ligands in the compound 1 bond the central tin metal.

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Photoactive NO-Releasing Ruthenium(III) Nitrosyl Complexes with Tetradentate N4 bis-Pyridyl/bis-Carboxamide Ligands

조장훈 이홍인

경북대학교 화학과

Since the discovery of Nitric Oxide (NO) as one of the major signal-transduction molecules in cells, there have been many attempts to devise acute NO-delivering systems for the purpose of developing disease therapies as well as studying cell functions. Metal-nitrosyl complexes are often releasing NO by light activation. This ability is applicable for killing cancer cells with high specificity because high concentration of NO in cells induces apoptosis. Ru-NO complexes have been studied for the usages of these photodynamic therapy (PDT) agents for a time. We have developed a new Ru-nitrosyl bis-pyridyl/biscarboxamide compound, [Ru(ebpp)(Cl)(NO)], where H_2ebpp = N,N’-(ethylene di-p-phenylene)bis(pyridine-2-carboxamide) to be tested as a model NO-releasing agent. The crystallographic analysis of the complex revealed that the ebpp ligand is tetradentately bound to Ru(III) and the remaining two cis sites of the octahedral geometry are occupied by NO and Cl-. Electronic absorption spectrum of the complex showed two absorption bands are 280 nm and 380 nm. Under the normal room light, 560 nm bands were growing. Simultaneous EPR (electron paramagnetic resonance) experiments at 110 K found that diamagnetic properties of the complex solution changed to a paramagnetic (S =1/2) species. These UV-VIS and EPR data can be interpreted as that the diamagnetic $[Ru\text{-}NO]^6$ (Enemark-Feltham notation) electronic state of the complex becomes low-spin Ru(III) (d^5, S=1/2) state upon losing NO by photoactivation. In this study, we have developed a series of [Ru(ebpp-X)(Cl)(NO)], where X is an electron-donating or withdrawing group for investigating the changes of their photosensitivities.

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Confined Growth of Highly Uniform Metal/Graphitic-Shell Nanocrystals in SBA-15

김다정 서원석*

서강대학교 화학과

We have synthesized highly uniform and single bcc-phased FeCo/graphitic carbon shell (FeCo/GC) nanocrystals with an average diameter of 5.7±0.3 nm by thermal decomposition of metal precursors in SBA-15 and subsequent methane CVD. Small-angle XRD data and N2 adsorption-desorption isotherms of the SBA-15 before and after loading with FeCo/GC nanocrysals clearly demonstrate that the structure of SBA-15 was retained during the nanocrystal growth and most of the channels of the mesoporous silica were stucked by the FeCo/GC nanocrystals. The nanocrystal sizes of 5~6 nm are consistent with the pore diameters of the SBA-15. The yield of nanocrystals in silica has increased 6-fold and the Fe/Co ratio of the FeCo/GC nanocrystals has been improved from 34:66 to 46:54 by using SBA-15 instead of fumed silica. The FeCo/GC nanocrystals exhibit superparamagnetism with high saturation magnetization of 209 emu/g metal at room temperature.

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Reaction mechanism of thermal hydrosiyilation studied by computational calculation.

정대로 정영애[1] 유복렬[2] 강윤경*

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Trichlorosilane undergoes a variety of interesting and useful Si-C bond formation reactions with unsaturated organic compounds, which give rise to the formation of many useful organosilanes important for the silicon industry. The thermal hydrosilylation reaction between allylchloride and trichlorosilane at temperatures ranging from 150 to 250C produces a number of products that include allyl trichlorosilane, trichloro(3-chloropropyl)silane, 1,3-bis(trichlorosilyl)propane, (2-(5-(trichlorosilyl)-2-(trichlorosilylmethyl)pentyl) propane-1,3-diyl)bis(trichlorosilane) and propene. The detailed reaction mechanisms of these reactions either through a singlet or a triplet manifold were calculated by using a density functional theory (DFT). The calculation results indicate that the reactions via pathways involving an ionic or a radical intermediate are unlikely due to the more than 150 kcal/mol of reaction barriers. All the reactions undergo concerted pathway with maximum ~65 kcal/mol of activation free energy. The calculation results give insight into the reactivities of thermal hydrosilylation reactions.

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Covalent Functionalization of Metal/Graphitic-Shell Nanocrystals

김다정 서원석*

서강대학교 화학과

We have produced covalently functionalized FeCo/graphitic carbon shell (FeCo/GC) nanocrystals using 1,3-dipolar cycloaddition of azomethine ylides generated by condensation of sarcosine (N-methylglycine) and glucose. The functionalized FeCo/GC nanocrystals are highly uniform, discrete and soluble in water and organic solvents, depending on the functional groups introduced. The resulting nanocrystals were characterized by FT-IR, UV-vis spectroscopy, XRD, and TEM. We expect the functionalized FeCo/GC nanocrystals to be useful for biomedical applications including magnetic cell separation, bio-detection, drug delivery, and magnetic-resonance imaging.

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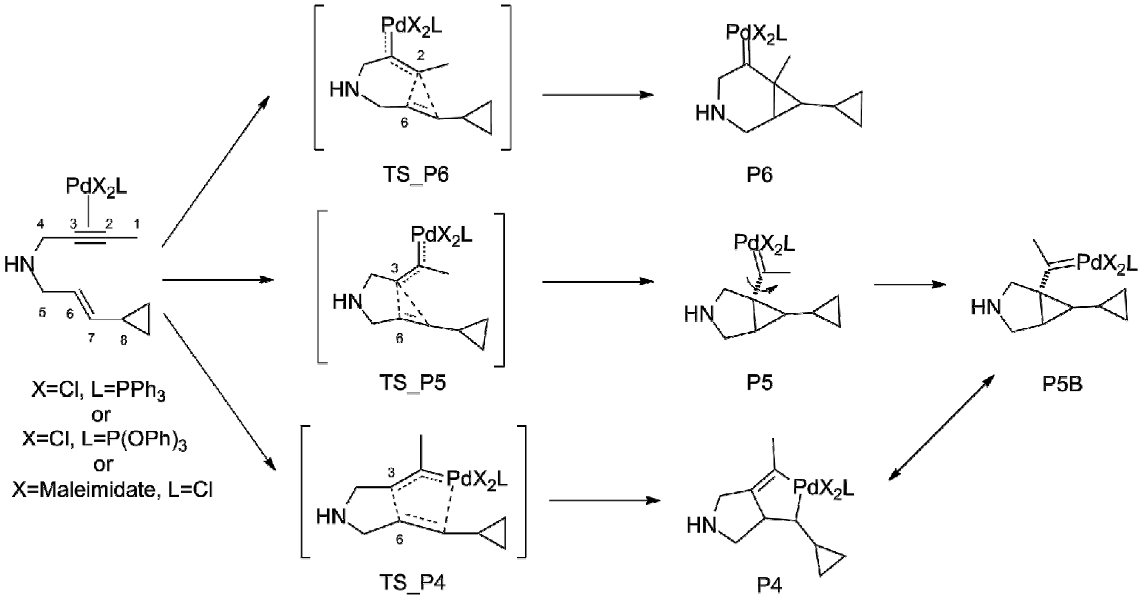
Reaction Mechanism of Palladium-Catalyzed Cycloisomerization of 1,6-Enyne Studied by Computational Calculation.

박지은 정영근[1] 강윤경*

상명대학교 화학과 [1]서울대학교 화학부

Transition metal-catalyzed cycloisomerization reactions provide polyfunctional cyclic compounds in a simple and easy manner. The palladium-based cycloisomerization of 1,6-enynes, in particular, have been proved to afford a wide variety of cyclic compounds that include the Alder-ene type products of either dialkylidene cyclopentanes or alkenyl alkylidene cyclopentanes, the enyne metathesis products of vinylcyclopentenes, the hydroxy- or alkoxycyclization products, the bicyclo[3.2.0]heptenes, and cyclopentenylbicyclo[3.1.0]hexanes. The transformation of 1,6-enynes to bicyclo[4.1.0]heptene type compounds in the presence of palladium catalysts, however, has not been reported until the recent discovery by Chung and coworkers. Here, we present the results of computational calculations that rationalize the experimental results. We performed a density functional theory (DFT) calculation using the B3LYP hybrid functional; three catalytic systems, PdCl2(PPh3), PdCl2{P(OPh)3}, and PdCl(maleimidate)2 were modeled without any structural modifications. Solvent effects were taken into account by CPCM method. With the (E)-N-(but-2-ynyl)-N-(3-cyclopropylallyl)-amine substrate, computational calculations indicate that the reaction is highly sensitive to the subtle difference of the catalysts. The 6-endo-dig cyclization pathway with PdCl2{P(OPh)3} catalyst in toluene shows significantly lower transition state relative to 5-exo-dig counterpart. The pathway toward metallacyclopentene was found unlikely. Current efforts are directed at gaining a deeper understanding of the fundamental principles dictating the reactivity of the substrates, as well as extending their utility by expanding the substrate scope.


PdX$_2$L
HN
4 3 2 1
5 6 7 8
X=Cl, L=PPh$_3$
or
X=Cl, L=P(OPh)$_3$
or
X=Maleimidate, L=Cl
TS_P6
TS_P5
TS_P4
P6
P5
P5B
P4

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Metal oxide-Hollow carbon Nanocomposites as Anode materials of Li-Ion Batteries

김다정 서원석*

서강대학교 화학과

Cobalt oxide-hollow carbon nanocomposites have been synthesized by using a simple chemical vapor deposition (CVD) method. Mesoporous silica spheres with an average diameter of ~150 nm are used as templates for the synthesis of the cobalt oxide-hollow carbon nanocomposites. The nanocomposites exhibit high reversible capacity and good cycle performance attributed to their beneficial features such as hollow structure and porous shell. The as-prepared materials were characterized by X-ray diffraction (XRD), TEM, BET and TGA. The resulting nanocomposites have a potential application as anode material for Li-ion batteries due to their simple method and excellent electrochemical performance

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Synthesis and Application of Metal-meso Carbon Yolk-Shell Nanocomposites

홍용훈 서원석*

서강대학교 화학과

We have synthesized metal-meso carbon yolk-shell nanocomposites by a chemical vapor deposition (CVD) method. The metal-meso carbon yolk-shell nanocomposites are composed of Au nanoparticles and mesoporous carbon shell embedded with FeCo-graphitic carbon shell (FeCo/GC) nanocrystals. The nanocomposites were characterized by XRD, TEM, BET, UV-Vis spectroscopy, and TGA. We expect the nanocomposites to be useful for recyclable catalyst due to the catalytic ability of gold nanoparticles in the reduction of nitro compounds and the presence of FeCo/GC nanocrystals that can be attracted to an external magnetic field.

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Chromium Complexes with N,N'-(ethylenedi-p-phenylene)bis(pyridine-2-carboxamide)

김유정 조장훈 **shuranjan sarkar** 이홍인

경북대학교 화학과

Among the first-row transition metal ions, Cr(III) is the most controversial in terms of the biochemical functions. Previously, a trace amount of Cr(III) has been considered to be a nutrient for human body, however, the role of Cr(III) has been questioned for several decades and it has been often reported that Cr(III) was an inducer of abnormalities in biological systems. It is known that Cr(III) interacts with proteins, but the details of the interactions and the safety or the toxicity of Cr(III) are yet to be explored. We have synthesized chromium complexes using a tetradentate ligand, called H_2EBPP (= N,N '-(ethylenedi-p-phenylene)bis(pyridine-2-carboxamide)) containing carboxamide groups, as a model for investigating chromium-protein binding mechanism. In the present poster, we present the synthesis, structures, and physical properties of the complexes.

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Synthesis, IR Spectroscopy and Crystal Structure of 5,16-Diethyl-2,6,13,17-tetraazatricyclo(16.4.0.0^{7,12})docosanium Dichloride

최종하* 홍용표[1] 유건상[1]

안동대학교 화학과 [1]안동대학교 응용화학과

The structure determination of title salt, $C_{22}H_{46}N_4^{2+}.2Cl^-.4H_2O$, reveals that protonation has occurred at diagonally opposite amine N atoms. The cyclohexane ring that is fused to the 14-membered ring exists in a chair conformation whereas the ethyl substituent occupies an axial site. The 14-membered macrocyclic molecule adopts the pseudo trans-III configuration. Intramolecular N-H..N hydrogen bonds stabilize the unusual conformation of the cation. There are four molecules in the unit cell. The Cl- and hydrate molecules are involved in hydrogen bonding. The IR spectral properties and assignments of main absorptions are also discussed.

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Crystal Structure and Modern Ligand Field Analysis of *cis*-[Cr(cyclam)(NCS)$_2$]SCN

최종하* 유건상[1] 심훈[1] 홍용표[1]

안동대학교 화학과 [1]안동대학교 응용화학과

The chromium atom is in a slightly distorted octahedral environment with four N atoms of the macrocyclic ligand and two N-bonded isothiocyanate in *cis* position. The cyclam adopts the folded cis-V configuration with six- and five-membered chelate rings in chair and gauche conformation, respectively. The average Cr-N(cyclam) and Cr-NCS bonds are 2.0850(14) and 1.9957(14) Å, respectively. The pure electronic origins due to spin-allowed and spin-forbidden transitions are assigned by analyzing the absorption and excitation spectroscopy. The angular positions of ligating six atoms and adjacent two carbons were taken from the X-ray crystal structure. Using the observed transitions, a ligand field analysis has been performed to probe the ligand field properties of coordinated atoms in the chromium(III) complex.

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Synthesis and structure studies of *s*-tetrazine silver(Ⅰ) complexes

김동현 강필재 최문근[*]

연세대학교 화학과

The *s*-tetrazine silver(Ⅰ) complex framework has been investigated. With Ag$^+$ as central metal, 1D, 2D and 3D coordination polymers with *s*-tetrazine have been synthesized and determined by single crystal x-ray diffraction studies. By using different anions, such as BF_4^-, ClO_4^-, PF_6^- and $CF_3SO_3^-$, the framework forms 1D, 2D and 3D network which show anion-π interaction, π-πinteraction of tetrazine rings and hydrogen bonding. The detailed structural feature will be presented.

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Synthesis of $Cu_2ZnSnSe_4$ nanoparticles through a simple sonochemical method

이원영 박종필 김영권 김항근 심일운*

중앙대학교 화학과

$Cu_2ZnSnSe_4$(CZTSe) is a promising material as absorber in thin film solar cells owing to its direct band gap of 1.44eV, high optical absorption coefficient and p-type electrical conductivity.Synthesis of CZTSe nanoparticles through a simple sonochemical method were performed under the multibubble sonoluminescence (MBSL) conditions. CuCl, $ZnCl_2$, $SnCl_2$, and Se powder were used for synthesis. Properties of CZTSe nanoparticles were measured with XRD, SEM, UV-vis spectrophotometer, HR-TEM, and etc.

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Preparation of PbTe/PbS core-shell nanostructure by simple sonochemical method

박종필 이원영 김영권 김항근 심일운

중앙대학교 화학과

PbTe nanocrystals are a promising material for thermoelectrics. Core-shell nanostructures such as PbTe/Pbs are attractive for n-type thermoelectric materials. Here, PbTe/PbS core-shell structure which has a form of core/shell structure nanoparticles which is of great interest for thermoelectric devices. Firstly, PbTe nanoparticles were synthesized using $Pb(NO_3)_2$ and Na_2Te in water. And then, PbTe/PbS core-shell nanocrytals were synthesized in ethylene glycol using PbTe NPs, $Pb(NO_3)_2$, and Thioacetoamide by sonochemical method. These core-shell nanocrytals were characterized by UV-vis spectrophotometer, near-infrared spectroscopy, X-ray diffraction, and high solution-transmission electron microscopy analyses.

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Hydrogenation at ambient temperature in Composited Material, Pt-MWCNT-MOF5, investigated by in Situ Raman Spectroscopy

강승기 조인화 이희주 최용남*

한국원자력연구원 중성자과학연구부

Highly porous MOFs (metal-organic frameworks) have been considered as promising hydrogen storage materials expected to satisfy the DOE’s (U.S. Department of Energy) requirement. MOF, however, shows its limitation in hydrogen adsorption properties for on-board application; high capacity at low temperature and low capacity at ambient temperature. To enhance the hydrogen uptake at ambient condition, composited MOFs with platinum (Pt) nanoparticles and defective multi-walled carbon nanotube (MWCNT) were investigated. Diatomic hydrogen molecules are dissociated into hydrogen atoms by Pt nanoparticles, and then chemisorbed by the defects on the MWCNT. The hydrogen atoms may hop from one defect site to nearby sites owing to a reduction of activation energies caused by oxygen group defects1, and finally will arrive at the hydrogen receptors in MOF5. Raman spectroscopy, which is a sensitive tool to a change in the vibrational modes, is employed to differentiate the change of spectra after the H2 exposure at several temperatures (30 K ~ 350K). Experimental results and discussion will be presented.

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Transition-metal Mediated Late-Stage Fluorination for Molecular Positron Emission Tomography (PET) Imaging

이은성 Jacob M. Hooker[1] Tobias Ritter[2,*]

Harvard University 화학과 [1]Athinoula A.Martinos Center for Biomedical Imaging, Massachusetts General Hospital and Harvard Medical School, Charlestown,MA 02129, United States [2]Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, Massachusetts 02138, United States

Positron emission tomography (PET) is a non-invasive imaging technique used to probe biological processes in vivo and requires synthesis of PET tracers which contain positron-emitting isotopes, such as 11C, 13N, 15O, and 18F. The 18F isotope is used most widely in clinical PET applications due to its longer half-life of 110 minutes, which allows synthesis and distribution of radiotracers for PET imaging. But C-F bond formation is challenging, especially with 18F. Here we present practical late-stage fluorination reactions with high-specific activity 18F fluoride to make aryl and alkenyl fluorides from organometallic palladium and nickel complexes. The late-stage fluorination reactions enable the synthesis of conventionally unavailable positron emission tomography (PET) tracers for anticipated applications in pharmaceutical development as well as pre-clinical and clinical PET imaging.

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Benzyl-functionalized MOF-205 and its gas adsorption properties

심재웅 노영수 오유진 김자헌*

숭실대학교 화학과

MOF-205 formulated as $Zn_4O(BTB)_{4/3}(NDC)$ is a mixed-ligand metal-organic framework exhibiting a large BET surface area of 4460 m^2/g. By replacing NDC with 1,5-dibenzyloxynaphthalene-2,6-dicarboxylate, an analogue of MOF-205 termed MOF-205Bn has been successfully synthesized and its crystal structure was determined by single crystal X-ray diffraction. Its porosity and gas adsorption measurements at both low and high pressures have been examined to evaluate the effect of the introduced benzyloxy groups.

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Connection of UiO-66-NH_2 crystalline particles through covalent bonds

유래경 조은희 김자헌*

숭실대학교 화학과

UiO metal-organic frameworks (MOFs) are composed of Zr-oxo clusters and aromatic carboxylates, and have larger chemical stability than common MOFs. An amine-functionalized UiO-66 (UiO-66-NH_2) has been prepared, and post-modified by succinic anhydride to give UiO-66-AMSuc. The coupling reactions took place on the surfaces of particles. Depending on solvent polarity, the post-modified particles showed different aggregation behaviors. The porosity of both the as-prepared and post-modified UiO-66-NH_2 particles has been investigated and compared using gas adsorption measurements.

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Synthesis of amine-functionalized UiO-67 metal-organic framework and its carbon dioxide adsorption

고낙은 노경규 김자헌*

숭실대학교 화학과

A new Zr-MOF (UiO-67-NH_2) was synthesized by a solvothermal reaction between amine functionalized biphenyl dicarboxylic acid and zirconium chloride. UiO-67-NH_2 is isostructral with that the well-known UiO-67 formulated as $Zr_6O_4(OH)_4(BPDC)_6$ (BPDC = biphenyl-4,4'-dicarboxylate). Activated UiO-67-NH_2 showed a BET surface area of 1190 m^2/g, and resulted in an increased isosteric heat of carbon dioxide adsorption by about 20 percent compared with that of more porous UiO-67. Post-synthetic modification of UiO-67-NH_2 was also explored for tuning its carbon dioxide selectivity.

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Controlled hydrolysis of Metal-organic frameworks

최상범 김태민[1] 김자헌[*]

숭실대학교 화학과 [1]숭실대학교

Partial and controlled hydrolysis of M-MOF-74s (M = Zn, Ni, Mg) were conducted with basic aqueous solutions. Interestingly, amorphous samples were still porous and could maintain significant portion of micro-porosity. In the case of M-MOF-74s, the porosity change pattern was depended on the sort of framework metal ions. We used to make mixed-metal MOF-74 for selective dissolution of frameworks. After hydrolysis, the collected samples were investigated by measuring X-ray power diffraction patterns and gas adsorption isotherms.

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CO_2 separation using metal-organic framework with adjustable portal dimensions

한승완 나명수*

울산과학기술대학교(UNIST) 친환경에너지공학부

A microporous MOF, $H_{1/3}[(Co^{II}_{13/2}(BTB)_4(OH)_{4/3}(DMA)_3]?2DMA?4H_2O$ (1) (where H_3BTB = 4’,4’’-benzene-1,3,5-triyl-tribenzoic acid; and DMA = *N,N’*-dimethylacetamide) was synthesized via solvothermal method. *1a*, activated under methylene chloride at 250 °C, is microporous and most of its pores are accessible for CO_2 with suitable kinetic diameter. However, other adsorbates such as N_2, CO, and CH_4 can partially access to the pore of *1a*. In this regard, equilibrium uptake amounts were dependant on the kinetic diameters of the adsorbates. Excellent breakthrough separation was performed for binary gas mixtures such as CO_2/N_2 and CO_2/CH_4. The structural characteristics, PXRD patterns and sorption behaviors of the three MOFs will be discussed in the presentation.

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In situ observation on dehydrogenation of LiBH$_4$ mixed with modified MWCNT: in-situ neutron diffraction and Raman scattering experiments

조인화 이희주 강승기 최용남*

한국원자력연구원 중성자과학연구부

LiBH$_4$ is a promising candidate for the hydrogen storage material due to its extremely high theoretical hydrogen capacity (18 wt.%, 121 kg m-3). However, its practical application has not been easy because of the high reaction enthalpy (~75 kJ mol-1 H2) and the slow hydrogen dissociation kinetics. Addition of catalyst such as MWCNT (multi-walled carbon nanotube) is one of the various tries to overcome these problems, since the additives can destabilize LiBH$_4$, which may reduce reaction enthalpy and increase the surface area of LiBH$_4$ confining it to nano-sized structures of MWCNT. In order to elucidate the role of MWCNT, it is very important to observe decomposition processes of LiBH$_4$ with varying temperatures. A composite system, LiBH$_4$ mixed with ball-milled MWCNT, was chosen to investigate the effect of additives on the dehydrogenation behaviors. High resolution neutron powder diffractometer (HRPD) installed at the research reactor HANARO in KAERI and a customized Raman spectrometer were employed with dedicated sample environments to monitor changes in dehydrogenation kinetics in related with the MWCNT addition. Experimental results and detail analysis will be discussed.

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A Highly Selective Fluorescent Chemosensor for Cu^{2+} Based on 7-(Diethylamino)coumarin

안경룡 신종일[1] 신승림[1] 박수열[1] 박균하 이상오[2] 고선덕[3] 전근[1,*]

충남대학교 화학과 [1]한국화학연구원 계면재료공정연구그룹 [2]충남대학교 [3]성균관대학교 화학과

A new Cu^{2+} fluorescent sensor (7-(diethylamino)-3-((E)-((E)-3-(2-hydroxyphenyl)allylidene)amino) -2H-chromen-2-one), derived from coumarin, was designed and synthesized by Schiff base condensation of ‘3-Amino-7-diethylamino-chromene-2-one’ and ‘2-hydroxy cinnamaldehyde’. This coumarin derivative showed high selectivity for Cu^{2+} over other metal ions such as Ag, Ca, Cd, Co, Fe, Hg, K, Li, Mn, Ni, Zn cations in acetonitrile. Fluorescence enhancement and obvious color change (orange to clear) were observed.

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Gas Phase Coordination Network Crystal Formation

Kojima Tatsuhiro **Masaki Kawano**[*]

포항공과대학교 첨단재료과학부

In general, coordination networks, which consist of organic linkers and metal ions, are synthesized in solution state, e.g. hydrothermal synthesis, slow diffusion of a layered solution and so on. Most of coordination networks, which were obtained by using the conventional synthetic methods, contain solvents or guest molecules as spacers in their pores. Therefore, when a network crystal is heated up over the boiling point of guest molecule, easily it can be decomposed or decay crystallinity. In order to obtain a thermally robust structure, we need to change the crystallization condition drastically. In this research, we introduced a new method, crystallization via gas phase, to obtain coordination network. As a first target for networking, we selected TPHAP ligand and ZnI2. By heating HTPHAP and ZnI2 at reduced pressure, we obtained the network crystals composed of HTPHAP and ZnI2. To the best of our knowledge, this is the first example of coordination network via gas phase reaction. Interestingly, we found that one proton attaches to the N atom of one of three pyridyl groups and it forms hydrogen bond to nitrogen atom of the HAP (hexaazaphenalene) skeleton in the next sheet. This structure is unique in having a network formed by both coordinate bonds and hydrogen bonds. Even though this network is formed by weak intermolecular interactions, the crystal is thermally so stable that it can keep single crystallinity at 200 °C. Furthermore, we succeeded in obtaining single crystals of coordination networks using other metal source, Cu(I)I and Cu(I)Br. Especially, the TPHAP-Cu(I)I network has a quite unique structure, which contains a multinuclear cluster as a metal connector.In summary, via gas phase reaction we successfully obtained the thermally most stable products. This method can be applied to other coordination network chemistry and crystal engineering.

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3D Porous Coordination Network Composed of TPHAP and Cd(II)

<u>Yakiyama Yumi</u> Masaki Kawano[*]

포항공과대학교 첨단재료과학부

Porous coordination network has recently been the subject of explosive development because of their fascinating properties such as gas separation/storage, catalysis, molecular recognition, conductivity, magnetism, drug delivery, and so on. Especially, their application as a nano-sized crystalline flask for in situ X-ray study is quite fascinating and unique for the visualization of unstable intermediate species. For this purpose, the porous network is required to have high stability and enough wide pores for guest encapsulation and reaction. Recently, we succeeded in preparing a unique tripyridyl ligand named TPHAP and obtaining various kinds of porous coordination networks which can show interesting properties. In this presentation, we will report 3D porous coordination network composed of TPHAP and Cd(II) ion. The crystal was obtained by the mixing of TPHAP with $Cd(NO_3)_2{\cdot}4H_2O$ in solution state. The resulting crystal was stable under air and possesses wide channels with 8.5Å×8.5Å opening size. Noteworthy is that it is easy to access large π-planes of TPHAP skeleton in the pore. This feature is useful for the encapsulation of various guest molecules which have π-planar structure.

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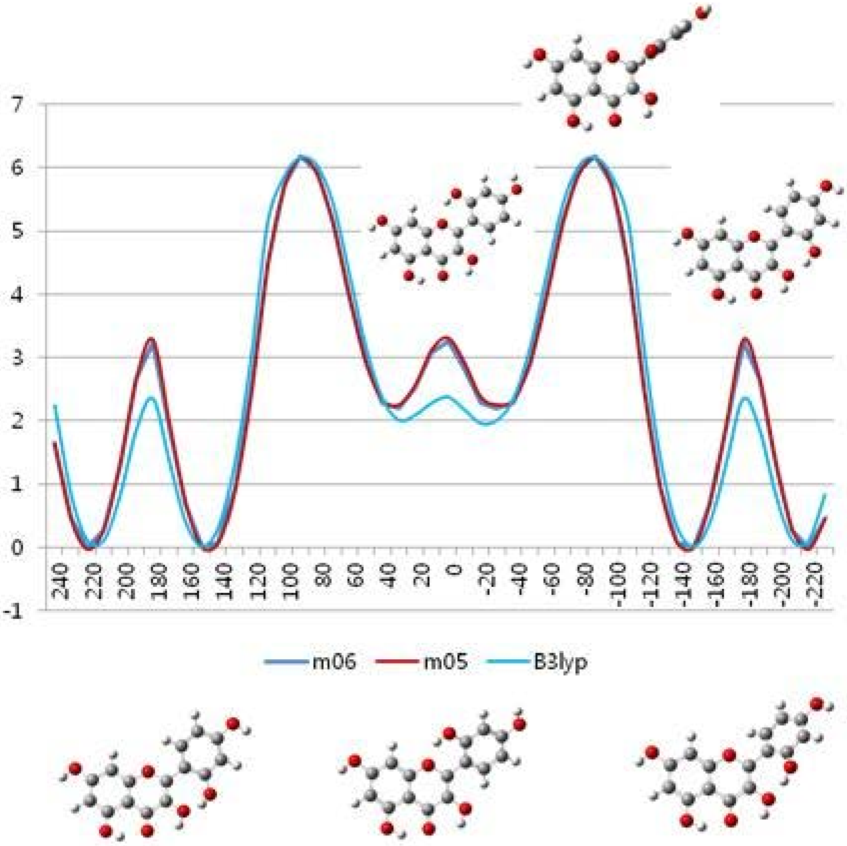
DFT studies of molecular structures and properties of metal complex with Quercetin and Morin

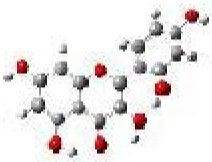
곽옥금 김수진 박기민 김봉곤*

경상대학교 화학교육과

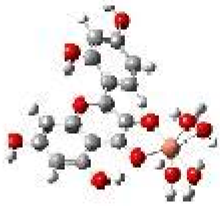
Flavonoids have long been recognized for their general health promoting properties, of which their antioxidant activity may play an important role. In this study, the molecular structure and vibration spectra and UV/Vis spectra of transition metal complexes(M=Cu^{2+}, Zn^{2+}) with Flavonoids such as Quercetin and Morin were investigated by the different density functional models(PBEPBE, PBE1PBE, B3LYP, M05-2x and M06-2x) using several basis sets including 6-311++G**, Lanl2dz, SDD, Lanl2mb.



DFT energies profile for rotation around the C2-C1’ bond of Morin in the gas phase.



Morin



[Cu(Morin)(H_2O)$_n$]$^+$

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Synthesis of half-metallocenes of thiophene-fused cyclopentadienyl ligands for ethylene/a-olefin copolymerization

전성해 이분열*

아주대학교 분자과학기술학과

Metallocene and bridged half-metallocene complexes constructed using thiophene-fused cyclopentadienyl ligands have been reported to exhibit enhanced polymerization activities, especially with a high molecular-weight polymer. Directed ortho-lithiation of the lithium carbamates generated from tetrahydroquinoline or tetrahydroquinaldine enables one-step preparation of thiophene-fused and tetrahydroquinoline-linked cyclopentadienes [2-R^1-3-R^2-4,5-dimethyl-6-(2-R^3-2,3,4,5-tetrahydroquinolin-8-yl)-4H-cyclopenta[b]thiophene (R^1, R^2, R^3 = H or methyl)], from which titanium(IV) and zirconium(IV) complexes are prepared. 2,3,4,5-Tetramethyl-4,5-dihydrocyclopenta[b]thiophen-6-one was prepared without chromatography purification on the 40-g scale in a laboratory setting, from which the ligand precursor for 2 was obtained in 65% yield on a 50g scale in a one-pot without the need for chromatography purification. Metallation was achieved in a high yield through reaction of the dilithiated compound with $TiCl_4$. Many derivatives were prepared by employing the same synthetic scheme. Also methylthiophene-fused or dimethylthiophene-fused trimethylcyclopentadienyl titanium trichloride complexes, (η^5-Me_4RC_7S)$TiCl_3$ (R = Me or H), are prepared, from which a chloride ligand is replaced with 2,6-diisopropylphenoxy, di(tert-butyl)ketimide, or tri(tert-butyl) phosphinimide ligand to yield (η^5-Me_4RC_7S)$TiXCl_2$.

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Gold nanoparticles coated with different silver shell thickness in imaging areas.

박지현 남좌민*

서울대학교 화학부

Nanoparticles showing different colors in dark field image can be useful material in imaging areas. We made silver coated gold nanorods that show different colors with different Ag shell thickness. Regardless of the gold nanorods' lengths, aspect ratios, the gold nanorod with within 5nm silver shell nanoparticles show red color in dark field microsopy. The gold nanorod with about 10nm silver shell nanoparticles show blue color. The gold nanorod with above 25nm silver shell nanoparticles show green color. Dark field microscopy is useful when imaging the unstained samples or live samples. Because the dark field microscopy shoots light to the sample and then the light scattered by the sample is collected and shown on the camera scan image. So the background is dark and only the place where the sample exist shows bright color. And the scattered light's colors can be changed because the plasmon made by each nanoparticles sample and the light shot by the dark field microscopy acts differently and produce different colors. So we made nanoparticles that show three accurately different colors in dark field image. And it can be applied to the areas when we need a discrete color material even when the materials surrouned by samples. For example, when we have to watch a materials in a amyloid beta, and the amyloid beta shows greenish bright color. And it's useful to use a gold nanoparticle with within 5nm silver shell showing red colors in the dark field microscopy to detect some materials in the amyloid beta. Therefore our interesting gold nanoparticles core with different thickness silver shell can be useful materials in imaging areas.

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Controlling kinetics of Au-Ag bimetallic nanoparticle synthesis and its structural dependence on SERS property

유명화 이정훈[1] 남좌민*

서울대학교 화학부 [1]서울대학교 화학과

Noble metal nanoparticles, like silver, gold and cupper have been extremely studied because of their rich localized surface plasmon resonance property. Each of the noble metal nanoparticles has its own property (i.e) high efficiency of plasmon excitation, chemical stability and biologically compatibility. Combining of two or more noble metal nanoparticles as a one mulimetallic nanoparticle is very important because it makes possible to enhance each of its own properties. For example gold and silver have strong electronic coupling, so the combination of both metals show greatly enhanced calalytic, electronic, optical properties relative to the monometallic components. The bimetallic nanocrystals have been successfully synthesized with versatile structures. However, it still remains a challenge to control the shape and spatial distribution of the secondary reduced metal on the surface of core nanocrystal. Here, we synthesized Au and Ag bimetallic nanoparticles by using the salt concentration as a kinetic controlling factor. The spherical Au-Ag core-shell particles are morphologically changed as Au-Ag 'nanosnowman' structure and disorderly multibudding particles, depending on the high to low salt concentrations. Further, surface-enhanced Raman scattering (SERS) studies have been performed with different shapes of synthesized bimetallic particles.

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Blue Phosphorescent Materials for Application to Organic Light-Emitting Diodes

강영진* 박정은[1] 오한국[2] 오시현[1] 김진호[1]

강원대학교 과학교육과 [1]강원대학교 화학과 [2]강원대학교 일반대학원 화학과

Three new Ir(III) compounds with deep blue phosphorescence have been synthesized. These molecules have the general formula of Ir(C∧N)2(L∧X) where C∧N = 2',6'-difluoro-2,3'-bipyridine (dfpypy), and L∧X = ancillary ligand such as 2-picolinate, pic (1), acetylacetonate, acac (2) or dipivaloylmethanoate, dpm (3). The ancillary ligands have been found to significantly destabilize both HOMO and LUMO level of the Ir(III) complexes, compared to Ir(dfpypy)3 without significantly changing the phosphorescence energy. Compounds 1 ? 3 emit brightly blue phosphorescence with λ_{max} = 440 ? 460 nm and quantum efficiencies of 0.60 ? 0.95 in solution and the solid state. Double-layer electroluminescent devices using compounds 1 ? 3 as the dopant, CDBP (4,4?-bis(9-carbazolyl)-2,2?-dimethylbiphenyl) as the host/hole tranporting layer, and TPBi (1,3,5-tris(N-phenylbenzimidazole-2-yl)benzene) as the electron transport layer have been fabricated. These EL devices show pure blue colour with high efficiency. The EL device of compound 3 at the doping level of 20 wt% has the best performance with EQE of 10% ? 15% at the brightness of 10 cd/m^2 ? 1000 cd/m^2 and the maximum current efficiency of 22 cd/A.

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Hydrogenation mechanism in Pt/Pd-infiltrated Na-X zeolites at ambient temperature

최용남[*] 이희주 윤경병[1]

한국원자력연구원 중성자과학연구부 [1]서강대학교 화학과

Zeolites, which belong to typical nano-porous framework materials, have been intensively studied for their useful applications as catalysts and gas adsorbents. Na-X is an aluminosilicate framework material, belongs to Faujasite class, having appropriate sodium ions as charge balancers. Platinum and palladium nano-clusters were infiltrated into the supercage (dia. ~ 11 ?) by a reduction method. Transmission electron microscopy was employed to characterize the nano-scale morphology of the samples. Physical and chemical properties of those samples, Na-X:Pt and Na-X:Pd, before and after the hydrogen exposure were investigated by PCT(sorption isotherm), in-situ neutron scattering, in-situ electron spin resonance, and ex-situ x-ray photoelectron spectroscopy measurements. Experimental evidences on the hydrogenation occurred at ambient temperature and possible model of its mechanism will be discussed.

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[발표취소] Mn(III)-porphyrin Based Nano- and Micro-sized Porous Coordination Polymer and Their Morphology Modulation and Catalysis

이경연 이석중*

고려대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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Single Crystalline FET based on Semiconducting Porphyrin and Its Anisotropic Carrier Transport Behavior

채승현 이석중*

고려대학교 화학과

In recent years, Organic Field-Effect Transistors (OFETs) are the most promising electronic devices fabricated using either well-defined single crystals or thin films as the charge-transporting layers. In particular, porphyrins have attracted as active materials for electronic devices due to their structural and electronic properties. Therefore, we have synthesized a series of novel π-extended Zn-porphyrin derivatives containing phenyl and thiophene substituents. Particularly, FETs using single crystals of porphyrin derivatives as active layers have been fabricated by slow solvent diffusion method. And their electrical, optical and charge transport properties are observed. In this presentation, unique anisotropic charge transport behavior with the position of sigle-crystalline porphyrin transistor will be demonstrated.

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Spin dynamics of nanostructured M_xZnO (M=Mn, Co)

김동훈 이계행[1] 김선희[*]

한국기초과학지원연구원 물성과학연구부 [1]한국기초과학지원연구원

Diluted magnetic semiconductors (DMS) are considered as an ideal system for spintronics, in particular, M_xZnO-based DMS with properties such as ferromagnetism at room temperature. Understanding basic physical properties and key factors for spin-relaxation of paramagnetic ion species are essential to develop better materials for spintronics. Thus, we employed multi-frequency pulsed EPR to measure spin-lattice relaxation (T_1) and spin-spin relaxation (T_2) of nano-structured M_xZnO. Temperature-dependent T_1 measurement allow in favorable cases the determination of the energy separation Δ between the ground and the first excited electronic states. We present size and transition metal ion effect on the dynamics of energy relaxation in these nanoscale materials. In addition, pulsed EPR spectroscopy, such as ENDOR and ESEEM, was utilized to further characterize the local structure of paramagnetic ions.

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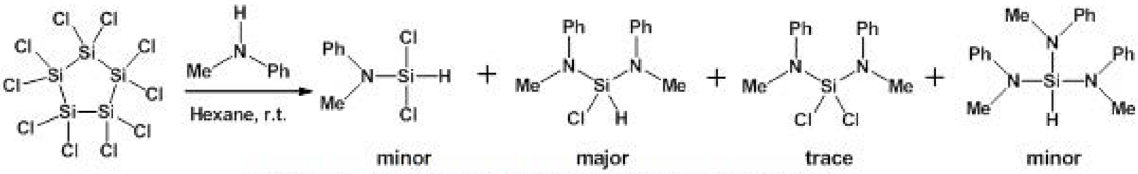
N-Methylaniline Promoted Si-Si Bonds Cleavage Reaction of Perchlorosilanes

최종민 송준현

연세대학교 화학과

Si-Si bond cleavage reaction can be occurred using alkali metal or UV radiation. For example, 1,5-dilithiodecaphenylpentasilane was prepared from decaphenylcyclopentasilane through a reductive Si?Si cleavage reaction with lithium. And a few examples of amine supported Si-Si bond cleavage were reported. For instance, neopentasilane was synthesized from Si-Si bonds cleavage of hexachlorodisilane through amine-induced disproportionation. Now, we wish to report Si-Si bonds cleavage of decachlorocyclopentasilane to give amino-substituted monosilanes in the presence of N-methylaniline.The reaction of decachlorocyclopentasilane with an excess amount of N-methylaniline gave (NMePh)SiHCl_2, $(NMePh)_2$SiHCl, $(NMePh)_3$SiH and trace of $(NMePh)_2SiCl_2$. We obtained $(NMePh)_3$SiH as a crystal by recrystallization in hexane. This reaction occurred through Si-Si bonds cleavage and nucleophilic substitution of *N*-methylaniline (Scheme 1). The products were identified by GC/MS, ^{1}H NMR, ^{29}Si NMR spectroscopy and X-ray crystallography. Octachlorocyclotetrasilane and neopentasilane in the presence of *N*-methylanline also afforded Si-Si bonds cleavage product in similar condition. Detailed results will be described in poster.



Scheme 1. Overall scheme of Si-Si bond cleavage of decachlorocycloprutasilane

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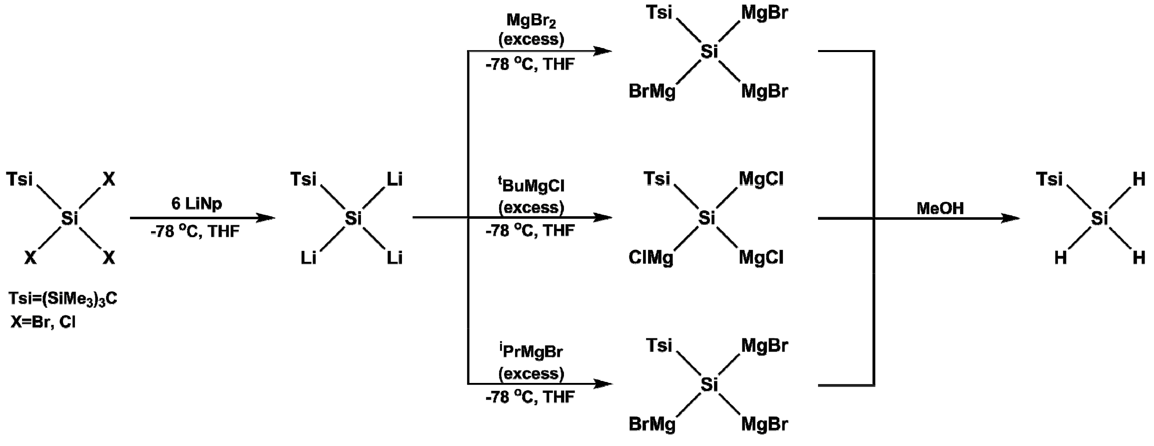
Preparation and Stabilization of Trimetallosilanes

송준현

연세대학교 화학과

The syntheses and structure of organosilicon lithium compounds have been the subject of much interest. Recently a few dilithiosilyl compounds including their synthetic applications and ab initio calculation, etc. were reported. However, trilithiosilane has not been reported yet. Last ten years we have synthesized stable halosilylenoids and dilithiohalosilanes formed from the reduction of trihalosilanes with strong reducing agents. These results prompted us to investigate a synthesis of trilithiosilanes.The reaction of trihalo[tris(trimethylsilyl)methyl]silane ($TsiSiX_3$, $Tsi=C(SiMe_3)_3$, X=Br, Cl) with more than 6 equivalents of lithium naphthalenide (LiNp) in THF at -78 ℃ gave trilithiosilane together with halodilithiosilane and halolithiosilane which are indirectly monitored by GC/MS after adding excess MeOH into reaction mixture. Transmetalation of lithiosilanes with $MgBr_2$, ^{t}BuMgCl, ^{i}PrMgBr and their thermal stability were also investigated. In this presentation, synthesis of trilithiosilane and its transmetalation will be discussed in detail.



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Synthesis and assembly of Anisotropic Au-Ag nanosnowmen

이정훈 남좌민[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Although monometallic nanoparticles have been demonstrated to control their interesting properties by changing the size or shape, multimetallic nanoparticles may offer the multifunctional properties when mutimetallic phases and surface modification of functional groups are combined within confined one nanoparticle. By combining different materials in a limited domain, it is expected to provide unusual optical and chemical properties such as plasmonic hybrid, chemical affinity. Here we report a straightforward and effective approach to synthesize the Au-Ag heterometallic dimers by kinetic control using DNA modification and salt concentration at mild aqueous condition. In this work, we focused on the asymmetric growth mechanism. We found out that gold nanoparticles should have modified with DNA strand for surface passivation and we could control the reaction rates and nucleation site through salt concentration and the reduction of silver component was preferentially occurred on the one side of DNA-modified AuNPs. Further, we showed that this can be used as a building block to assemble complex structures with orientation. Importantly, we show that the oriented assemblies of various anisotropic nanostructures are readily possible by using nano-snowmen with asymmetrically modified DNA as building blocks.

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Origin of ferromagnetic coupling of Kagome lattice YCa3(MnO)3(BO3)4: Density functional analysis

이창훈* 심지훈 **Myung-Hwan Whangbo**[1]

포항공과대학교 화학과 [1]North Carolina State University

A new borate compound YCa3(MnO)3(BO3)4 derived from the mineral gaudefroyite adopts a hexagonal space group P63/m with cell parameters of a =10.5726 ? and c=5.8576 ?. It is constituted of edge-sharing chains of MnO6 octahedra along c, the chains being interconnected by triangular BO3 groups to form a kagom? lattice in the ab plane. Although this system has three magnetic ions sit at the vertices of a triangle and experience antiferromagnetic (AFM) interactions, overall magnetic property of YCa3(MnO)3(BO3)4 is can be explained by ferromagnetic chain. In this study, we evaluated spin exchange interaction of YCa3(MnO)3(BO3)4 by performing relative energy-mapping analysis based on density functional calculations to find why they undergo a ferromagnetic ordering at low temperature and to reveal origin of ferromagnetic ordering. As a consequence, in-plane hidden exchange J2 and J6 interaction play an important role to take place ferromagnetic ordering YCa3(MnO)3(BO3)4. .

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The Effect of the Post-synthetic Cation Exchange on the Gas Sorption Properties in an Anionic MOF

박혜정 백명현[1,*]

포항공과대학교 첨단재료과학부 [1]서울대학교 화학부

The post-synthetic cation exchange with various metal ions such as Li^+, Mg^{2+}, Ca^{2+}, Co^{2+}, Ni^{2+}, and Cu^{2+} in an anionic MOF, $[Zn_3(TCPT)_2(HCOO)][NH_2(CH_3)_2]$ (SNU-100') significantly affects the gas sorption properties of the MOF. The impregnation of various metal ions in the pores enhances isosteric heat, selectivity, and uptake capacity of CO_2 adsorption in the MOF, while the replacement of framework metal ions in the MOFs affords stepwise sorption isotherms for N_2, O_2, and CO_2 gases.

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Water Purification by using Poly-N-Phenylglycine Nanofiber

도지훈 신구*

세종대학교 화학과

물은 생명 현상과 화학 반응에 있어 매우 중요한 역할을 하는 물질로서, 고효율의 물정화 내지는 수처리 기술은 환경 뿐만 아니라 인류의 건강에 필수적이다. N-Phenylglycine 은 Aniline 과 유사한 화학적 구조를 가지는 단량체로, 질소-카르복실기 functional group 구조를 포함하고 있다. 따라서 카르복실기의 극성도를 이용하면 정전기적 인력을 통해 물 속에 함유되어 있는 중금속 이온들을 처리할 수 있는 능력을 가지게 된다. 본 발표에서는 표면적이 극대화된 nanofiber Poly-N-phenylglycine 의 우수한 중금속 포집 능력을 보고하고자 한다. Poly-N-phenylglycine nanofiber 를 구리와 니켈 수용액에 일정시간 장입하여 금속 제거 효과를 고찰하였다. 잔류 금속 이온양은 Beer-Lambert 법칙으로 산출되었고, 구리 수용액의 경우 99% 이상의 높은 금속 이온 제거율을 나타내었다. 본 연구를 통해 Poly-N-phenylglycine 이 우수한 수처리 능력을 보이는 새로운 고분자 물질임을 논증하고자 한다.

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Synthesis of core/gap/shell gold nanorods for multimodal molecular imaging and photothermal therapeutic applications

김민호 임원규 남좌민*

서울대학교 화학부

The noble metal (Au, Ag or Cu) nanoparticle can enhance absorption and scattering of electromagnetic radiation by its unique optical property, surface plasmon resonance (SPR). Especially, gold nanorods are easily tuned their optical properties from visible to near-infrared (NIR) region by controlling aspect ratio, and can be applied NIR deep tissue molecular imaging or photothermal cancer therapy. For diagnostic application, NIR radiation is useful because it penetrates native tissue deeply due to its less absorption by water, blood, and intrinsic chromophore. Furthermore, the suitably engineered gold nanorods heat up temperature at targeted cancer region locally because of strong absorption of NIR radiation, so engineered gold nanorods can be used for noninvasive photothermal therapeutic application.Here, we fabricated core/gap/shell gold nanorods structure for multimodal molecular imaging (fluorescence, SERS, and radionuclide) probe, and applied efficient photothermal cancer therapeutic agents. Firstly, we synthesized gold nanorods and attached dye-linked DNA onto surface of gold nanorods. Then, we formed silver shell onto gold nanorods and carried out galvanic replacement between silver shell and additionally added gold precursor to generate core/gap/shell structure. The gap distance and SPR properties are tuned by controlling degree of galvanic replacement. In these structures, the dye molecules located between core and shell showed enhanced SERS signal. In addition, we linked radionuclides to prepared nanostructure for radiological imaging. And we also investigated photothermal properties of prepared nanostructure for hyperthermia therapy.

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Cobalt Sulfide film for use in Photovoltaic devices

안도영 한성환*

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Various metal sulfide have been studied.Cobalt sulfide has the advantage of low cost, simple fabrication.In this experiment, It is grown on the FTO surface.It forms hexagonal rod structure.Compare Co_4S_3 electrode with platinum electrode.Cobalt sulfide film shows very high conductive. It is as good as platinum electrode.We can use this film for photo voltaic devices.In this experiment, it was characterized with use of 4-point probe, XRD(X-ray diffractometer), SEM(scanning electron microscope)We can improve Co_4S_3 film's performance by control the condition.

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Fabrication and characterization of nickel telluride thin film

김은경

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Metal chalcogenides and their mixtures are attractive and useful systems for solar energy conversion studies by photoelectrochemical means. This materials meet the requirements of the band gap energy matching for solar spectrum and the competitiveness of production cost.

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$AgIn_5S_8/ZnS$ core/shell 양자점의 silane 표면개질을 통한 나노군집체 형성 개발

김상엽 윤성호[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

양자점은 높은 색순도, 발광효율, 넓은 색 재현성과 사이즈에 따라 에너지 밴드갭을 조절할 수 있는 장점으로 LED 의 색 전환물질로 많은 연구가 진행되고 있다. 양자점을 이용하여 Color Converting Material(CCM)을 제조시 양자점사이의 거리가 가까워져 에너지 전달에 의해 광효율이 떨어지고 열이 발생하는 quenching 현상이 발생하게 된다. 이를 방지하기 위하여 $AgIn_5S_8/ZnS$ core/shell 양자점을 plum pudding model 형태의 구조체를 형성하였다. 이를 통한 양자점 사이의 거리 조절과 양자효율 변화에 관한 내용을 발표하고자 하다. 양자점의 표면개질은 둘러 싸고 있는 alkyl group 유기리간드를 hydroxyl group 으로 개질 후, 3-aminopropyltriethoxysilane (APTES)와의 silanization reaction 을 통해 나노군집체를 합성하였다.

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Hydrogen Permeation of Lanthanum Nickel Oxide Composite Membrane

박도경 정미원*

성신여자대학교 화학과

The Ruddlesen-Popper series, $La_{n+1}Ni_nO_{3n+1}$ has perovskite structure which has been known for good proton conductor [1]. The proton conductors can make selective hydrogen transport possible and hence are much attractive in application to hydrogen separation [2]. And also the RP series has drawn interest as cathode for SOFCs for intermediate temperature range [3]. Recently, trials for developing perovskite oxide that conduct protons for hydrogen separation are being made in that temperature range. This is the attempt to connect these two issues. It was tried to make thin film on the membrane surface through the dip coating with the precursor sol solution. And the differences of the surface and hydrogen permeation were compared when the membrane was dip coated or not. The fine Lanthanum Nicikel Oxide powder was prepared via sol-gel process from nitrate compounds and molded into disc by hydraulic press. After annealing the membrane, the surface of the membrane was characterized by XRD and FE-SEM and porosity by the BET. Hydrogen permeation test was carried out at various temperature through H_2 and CO gas, respectively. The objective of this study is to enhance the selectivity and hydrogen permeation flux. We will discuss about the effect of $La_{n+1}Ni_nO_{3n+1}$ which has perovskite structure.

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Synthesis and magnetic properties of copper(II) complexes with 3,5-dichloro-2-((quinolinylimino)methyl)phenol.

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A new ligand derived from 3,5-dichloro-2-hydroxybaenzaldehyde and quinoline, 3,5-dichloro-2-((quinolinylimino)methyl)phenol (dcqmpOH) and its copper(II) complexes were synthesized and characterized. Two complexes, [Cu(dcqmpO)(CH_3OH)(ClO_4)] (1) and [Cu_2($dcqmpO)_2$($NO_3)_2$] (2) have been investigated by X-ray crystallography and magnetochemistry. Complex 1 has a square pyramidal geometry and shows monomeric structures. 2 exhibits a dimeric structure with bridging nitrato anions, and the copper(II) ions have a pyramidal geometry. In case of 2, a weak antiferromagnetic interaction between the copper(II) ions via nitrato anions occurs. In this poster, we will present the detailed preparation of the ligand and properties of the copper(II) complexes.

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Titanium Complexes Containing Bidentate Benzotriazole Ligands as Catalysts for Ring Opening Polymerization of Lactide

고민정 박가현 이준승

전남대학교 화학과

The selective syntheses of titanium complexes containing 2-(2H-benzo[d][1,2,3]triazol-2-yl)-4,6-di-tert-pentylphenoxide (LH) ligand such as [LTiCl2(μ-Cl)]2 (1), LTiCl3(THF) (2), L2Ti(NMe2)2 (3), L2TiCl2 (4), and L2Ti(O-i-Pr)2 (5) were unprecedentedly achieved by changing the solvents or metal precursors. Their solid structures of 1 ? 5 were revealed by single-crystal X-ray analyses. Complexes 2 and 5 showed the fast thermal exchange process of benzotriazole ligand L. Among 1 ? 5, complex 5 was proven as a highly effective catalyst for the controlled ring opening polymerization (ROP) of lactide (LA) as shown by the linearity of molecular weight versus [LA]/[Ti] ratio as well as very narrow PDI values of PLA polymers obtained.

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Fe(III) Complexes Using Bidentate Two Type of Tetrazole Ligand For Selective binding with Metal

박가현 고민정 이준승

전남대학교 화학과

The syntheses, characterizations and alkali metal recognition studies of iron complexes containing tetrazole ligands, which form high dimensional coordination polymers in the solid status, are investigated. From the reaction of iron(III) perchlorate, {5-(2-hydroxy) phenyl}tetrazole (LH2) and 2,2’-bipyrimidine(bpym) in H2O, high dimensional mixed metal coordination polymers, [Li3(bpym)1.5FeL3(H2O)6]n (1a), [Na3(bpym)1.5FeL3(H2O)7] n (2a), [K3(bpym)FeL3(H2O)7]n (3a) were synthesized with high yield and their solid structure were determined from X-ray diffraction studies. In all three structure, dual-tridentate iron anion fragment (FeL33-) was observed. As the ion sizes of alkali metals increased, more strong binding between alkali metal ion and iron fragment were observed. Because iron fragment has outstanding coordination ability, extremely short Fe - K distance, which is most short distance among reported in literature, was observed in complex 3a. When bpym was excluded in the reaction, 0-D [Li3FeL3(H2O)3] (1b), 2-D [Na3FeL3(H2O)7] (2b) and [K3FeL3(H2O)7] (3b) were synthesized and coordination between alkali metal ion and iron fragment (FeL33-) was stronger than bpym contained species. In particular, due to lack of binding sites, potassium binds to TzOH ligands with σ and π character in complex 3b. {2-(1-hydroxy-2-dimethylethyl)-5-(2-hydroxy) phenyl}tetrazole is tridentate ligand like scorpionates. we synthesized same method of using LH2 ligand but {2-(1-hydroxy-2-dimethylethyl)-5-(2-hydroxy) phenyl}tetrazole could not observe alkali metal in iron complexes.

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Substituent Effect on Electronic Energy of Methyl- Substituted Benzyl Radicals

이은혜 윤영욱 이상국

부산대학교 화학과

Substitution into benzene ring is expected to change physicochemical properties of aromatic compounds. The spectroscopic observation shows the substitutions of CH_3 into benzene ring of the benzyl radicals shift the origin bands of the electronic energy in the D1→D0 transition to red region in the decreasing order for o-, m-, and p-positions of mono-substituted benzyl radicals. However, multi-substituted benzyl radicals exhibit the substituent effects that depend on the positions and number of substituents. Recently we have found that the free electron molecular orbital theory of the π electronic states which is based on 'a particle-in-box' eigenfunctions could be excellent candidate for explaining the substituent effect on electronic energy of conjugated double bonded organic molecules. The theory assumes that the π electrons in a conjugated molecule can be separated from the σ electrons and that the σ framework is frozen. In this presentation, we will describe that the size and shape of two-dimensional box available for delocalized π electrons at a given electronic state can explain the observed substituent effect quantitatively.

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Formation of self-assembled model clusters and tubes of fluorine-substituted [16]annulene by DFT methods

장효원

순천대학교 화학과

One of the weakly interacting hydrocarbons, [16]annulene is shown to forms various clusters and tubes when half of the hydrogen atoms are replaced by fluorine atoms in DFT quantum chemical simulations.The bond properties in such models are analyzed by the Coulomb interactions between partial charges induced by the electropositive hydrogen and the electronegative flourine atoms. In addition, another class of polymers is idenitfied where covalent bonds bind annulene monomers. The stability ordering of two classes is transposed as the chain grows since the covalent bonding effect dominates the highly strained unsaturated-ends effect of the shorter oligomers in the latter class.In summary, electrostatic interactions hold the monomers in small clusters while carbon-carbon covalent bonds play major role in the long tubes.

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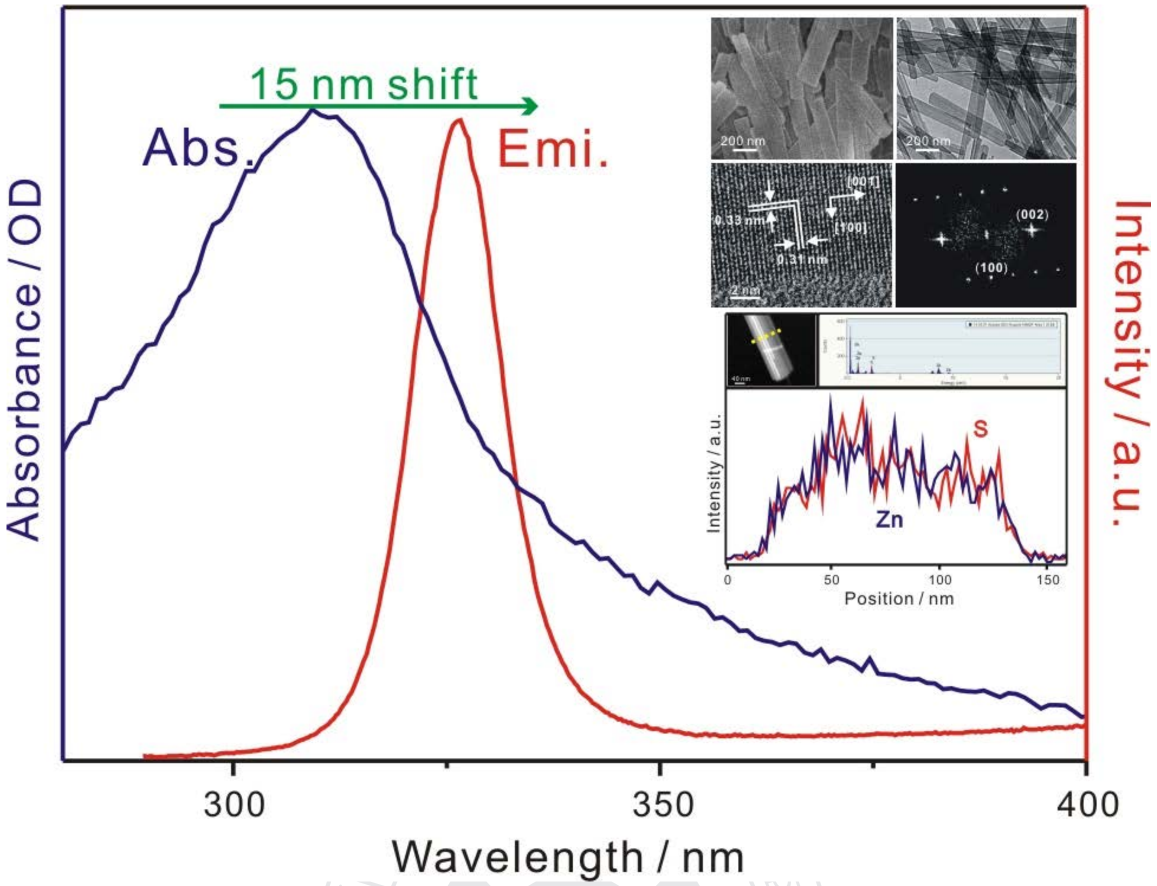
Hydrothermal synthesis of wurtzite ZnS nanoblades in ternary mixed solvent systems

김연호 장두전*

서울대학교 화학부

ZnS is well-known direct band gap II-VI semiconductor, and it attracts intense interest due to its excellent properties of luminescence which enable ZnS to have promising materials for optical, photonic and electronic devices. We have developed a facile and the effective one-step mild hydrothermal process for the synthesis of single-crystalline and pure-wurtzite ZnS nanoblades possessing sharp band-edge emission at room-temperature having diverse length-to-width (aspect) ratios. Each of nanoblades was composed of chemically pure, structurally uniform, single-crystalline, and defect-free ZnS. These features suppress trap or surface states emission, which enhance ultraviolet band-edge emission of ZnS nanoblades possible at room temperature. The reaction medium consisting of mixed solvents such as hydrazine, en, and water has played an important role in the crystallinity and optical properties of ZnS nanoblades. The unique ZnS nanoblades possessing sharp band edge emission obtained via a single-step simple hydrothermal process guarantee high potential for both fundamental research and technological applications.


15 nm shift
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Catalytic properties of Ag-Au alloy nanoboxes@SiO_2 synthesized via galvanic replacement

이재원 장두전*

서울대학교 화학부

Nanoscale noble-metals have attracted attention from researchers in various fields of study because of their unusual optical properties as well as novel chemical properties. It is well-known that nanoparticles of noble-metals show strong absorption bands in the visible region due to their surface-plasmon oscillation modes of conductive electrons. Silver nanocubes stand out from various types of Silver nanostructures due to their superior performance in a range of applications involving localized surface plasmon resonance, surface-enhanced Raman scattering, and biosensing. In addition, extensive efforts have been devoted to the investigation of Gold-based nanocomposites to achieve high catalytic performances and utilization efficiencies. Furthermore, hollow nanospheres possess structurally tunable features such as shell thickness, interior cavity size, and chemical composition, leading to relatively high surface areas, and low densities compared with their solid counterparts. Silver nanocubes dispersed in water have been transformed into Ag@Au nanoboxes, which show highly enhanced catalytic properties, by adding $HAuCl_4$. By using this concept, SiO_2-coated Ag@Au nanoboxes have been synthesized via galvanic replacement of SiO_2-coated Ag nanocubes. SiO_2-coated Ag@Au nanoboxes have been found to catalyze the degradation of 4-nitrophenol efficiently in the presence of $NaBH_4$. By changing the amount of the added noble metal salt to control the molar ratio Au to Ag, we could tune the catalytic properties of the nanostructures in the reduction of the dyes. Catalytic performances were affected noteworthily by the metals, sizes, and shapes of noble-metal nanostructures.

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Study of Reaction Mechanism of Benzoyl Chloride Derivatives

고한중

전주교육대학교 과학교육과

The ortho-effect of substituents upon the kinetics of reactions taking place at a reaction center attached to an aromatic ring has long been a topic of interest. For benzoyl chloride solvolyses, it was shown by Bentley and co-workers that the 2,6-dimethyl-derivative followed an ionization pathway with characteristics very similar to those for the solvolyses of p-methoxybenzoyl chloride. We have carried out a Grunwald-Winstein equation treatment of the solvolyses of 2,6-dichlorobenzoyl chloride, with similar size chlorines replacing the methyl groups but now with an overall electron-withdrawing influence of the ortho-substituents. In this way the reactivity is moderated and the study can be extended to the important fluoroalcohol-contaning solvents. For the 30 solvents studied, an ionization pathway with a moderate nucleophilic solvation component is indicated. For comparison purposes, the treatment has also been applied to the 2,4-, 3,4-, and 3,5-dichloro-derivatives. For the 2,4-dichloro-derivative, the two reaction channels are clearly visible and the solvents included for each channel are consistent with their solvent properties.

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Direct Observation of Valence Band Mixing in CdS Hollow Submicrospheres Prepared via Microwave Irradiation

김연신 김형배 장두전*

서울대학교 화학부

A new synthesis method of CdS hollow nanostructures via microwave irradiation has been explored, resulting in hollow spheres with diameters ranging in the submicrometer scale but with a shell thickness within the quantum confinement range. CdS, a semiconductor material with a band gap of 2.42 eV, is our material of interest due to its direct band gap and its ability to absorb a wide range of visible light. CdS has recently shown much interest in displays, solar cells, and optoelectronic devices due to its unique photophysical and photochemical properties. With the assistance of microwave irradiation, we have developed a facile method of preparation of uniform CdS hollow submicrospheres with a shell thickness of about 10 to 15 nm. Compared to the polystyrene template or the template-free synthetic methods of preparing CdS hollow spheres, our method of preparation allows for much more control and results in highly uniform and well-defined hollow structures. Other advantages of this method are that it has very few steps, it gives us control over the size of the submicrospheres, it is easily scalable, and that it does not require an inert environment. The physical characteristics of these CdS hollow structures have been studied with data extracted from HRTEM, HRXRD, and XPS, revealing a cubic zinc blende crystal structure with a crystallite sizes ranging from 4.7 to 6.2 nm. The photophysics of the CdS hollow spheres was then studied in detail with the absorption and photoluminescence spectra, revealing valence band mixing due to strong quantum confinement effects.

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Structural, Optical, and Photocatalytic Properties of CdSe·(ethylenediamine)$_{0.5}$ Nanorods

김형배 장두전

서울대학교 화학부

Solvothermal synthetic routes have attracted great attention to produce highly crystalline nanostructure. And there are so many CdSe nanocrystals synthesized by solvothermal methods. However, the structure of CdSe·(ethylenediamine)$_{0.5}$ synthesized by solvothermal routes has been veiled yet due to the lack of reports and systematical analysis. In this poster, we have demonstrate structural, optical, and photocatalytic properties of CdSe·(ethylenediamine)$_{0.5}$ nanorods as well as their post hydrothermal treatment results for removal of ethylenediamine. As prepared inorganic-organic-layered CdSe·(ethylenediamine)$_{0.5}$ nanorods possess strong quantum confinement effect and unique porous structure was obeserved through HAADF STEM imaging system. And CdSe·(ethylenediamine)$_{0.5}$ nanorods have been successfully decorated with platinum under microwave irradiation. Our CdSe·(ethylenediamine)$_{0.5}$ decorated with Pt have been found to have highly enhanced photocatalytic efficiency under visible light irradiation. This information will contribute the manipulation in semiconductor photocatalyst design.

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Solvent effects on the spectroscopic behavior of Quercetin and Apigenin

박형련* 임서은 박기민[1]

전남대학교 화학과 [1]경상대학교 화학교육과

Quercetin(QCT) and apigenin(API) are the polyphenolic compounds which have received much attention because of the biological effects attributable to their antioxidant activity. These substances consist of many OH functional groups in the molecules. Since OH group is affected by the characterization of the solvent systems, their solvent effects on the spectroscopic properties were investigated in methanol-water and acetonitrile-water mixtures. The UV-vis absorption spectrum of qucertin reveals two maximum peaks at around 257 nm and at around 370 nm in methanol. This of apigenin reveals at around 280 nm and at around 320 nm. According as the contents of water increased in the methanol-water mixtures, a remarkable change in the absorption spectrum of qucertin is not observed. On the other hand, the maximum peaks in the UV-vis absorption spectra of apigenin are shifted according as the contents of water increased in the acetonitrile-water mixtures. All of the emission bands of QCT and API are broad and the intensity decreases quickly as the H2O composition in the solvent increases. When the amount of H2O exceeds 50%, all of the fluorescence emission disappears. The reason of these might be related with the intermolecular hydrogen bonding as well as intramolecular hydrogen bonding caused by the polarity of the solvent systems.

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Synthesis and Spectroscopic Study of Organic/Inorganic Hybrid Poly(3-hexylthiophene)-Au Nanoparticles.

이동기 장두전*

서울대학교 화학부

Conducting polymer/nanoparticle hybrid films are of high interest due to their novel properties such as photoluminescence and semiconducting behaviors and their applications in field effect transistors (FETs), light-emitting diodes (LEDs), and photovoltaic cells. The synthesis of organic/inorganic hybrid nanoparticles in an organic medium is important due to their enormous applications. Thus, we have synthesized thiol-terminated poly(3-hexylthiophene) (P3HT) following the Grignard metathesis (GRIM) and the Mitsunobu reaction. Organic/inorganic hybrid poly(3-hexylthiophene)-coated Au nanoparticles (P3HT-Au NPs) have been prepared using the “grafting-to” approach. Thin films of P3HT and P3HT-Au NPs were prepared by spin-coating the above homogeneous solutions at 2000 rpm. Transmission electron microscopy (TEM) images indicate that Au NPs in the P3HT matrix are distributed homogeneously. Differential scanning calorimetry (DSC) and high resolution X-ray diffraction (HRXRD) have been employed for structure analysis. A blue shift of the luminescence band of the P3HT-Au NPs film is observed probably due to the coupling of plasmon vibrations with the electronic levels of P3HT.

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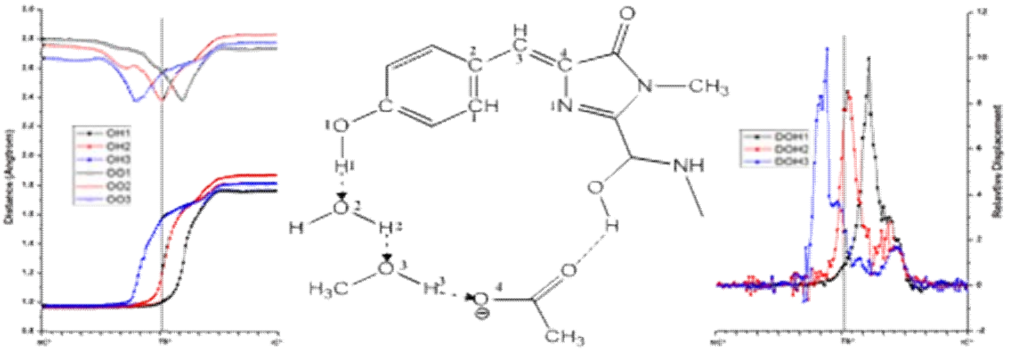
Concerted Asynchronous Proton Transfer in H-Bonding Relax Model: An Implication to Green Fluorescent Protein

Kang baotao 이진용*

성균관대학교 화학과

Multiple proton transfer of GFP model was investigated in the ground state and the first excited singlet state. It was found that both the forward and reverse GSPT reaction, which is strongly affected by the protein environment, can take place due to the small energy barrier (~3 kcal/mol) and small difference (~0.5 kcal/mol) in relative stability between the reactant and the product. Upon excitation, the forward ESPT reaction can occur with an energy barrier of 13.19 kcal/mol. And IC* becomes more stable in energy than NC* upon proton transfer by 4.96 kcal/mol. Both of the GSPT and ESPT reactions take place via single barrier without any stable intermediate, they must be concerted process. Meanwhile, the protons show asynchronous character. Concerted/stepwise and synchronous/asynchronous are two different concepts. Concerted/stepwise means that the reaction takes place via single/multiple barrier with/without stable intermediates. However, synchronous process means that a chemical process takes place in a synchronous fashion. Thus, both GSPT and ESPT are considered as a concerted and asynchronous process. For the forward GSPT and ESPT, the first proton to transfer is the methanol proton (H3) to acetate, and the chromophore proton (H1) is the last one to transfer. While for the reverse GSPT, H1 should be the first, while H3 should be the last to move.



Concerted and Asynchronous

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Scaling Factor of Intramolecular Magnetic Coupling Constants for Organic Diradicals

고경철 조대흠 이진용*

성균관대학교 화학과

The intramolecular magnetic coupling constants (J) of 9 diradicals (i?ix) coupled with an aromatic ring were investigated by means of unrestricted density functional theory calculations [B3LYP/6-311++G(d,p)]. For those diradicals, the remarkable linear relationship was found between the calculated (x-axis) and experimental (y-axis) J values on the basis of results of the linear regression analysis. In this study, we suggest that the value of slope (0.380) of linear regression line can be used as scaling factor for estimating the accurate J values. By applying this scaling factor to the calculated J values, we can predict the reliable J values of four DTDA driadicals (x?xiii) coupled with an aromatic ring for the first time. It also found that certain scaling factors have a restricted application depending on the length of a coupler. In conclusion, this approach, which uses a scaling factor, can be used to estimate the accurate J values for diverse diradical systems coupled with a particular coupler using DFT calculations.

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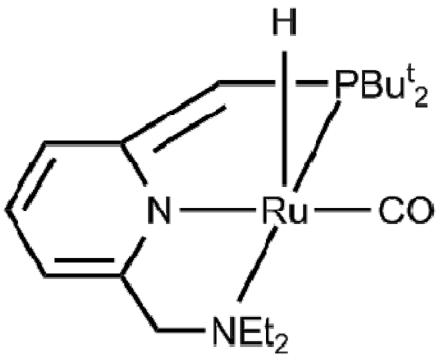
Catalytic Mechanism for the Ru-Complex Catalyzed Amidative Coupling of Alcohols and Amines and Design of a New Catalyst: A DFT Study

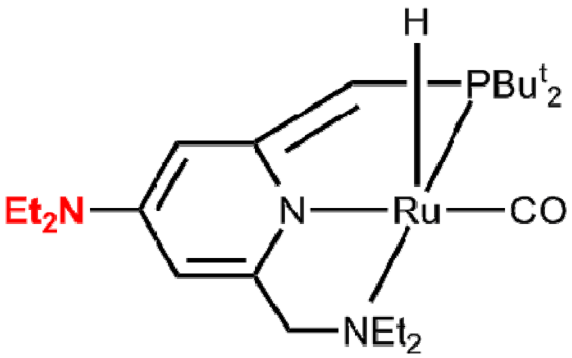
조대흠 고경철 이진용*

성균관대학교 화학과

In spite of its importance, synthetic methods for preparing amides have a number of difficulties, which include intricate reaction procedures and acidic or basic derivatives as reagents or catalysts. Surprisingly, Milstein and coworkers recently succeeded in synthesis of amides in mild condition utilizing pyridine based Ru-PNN pincer ligands (Science 2007, 317, 790-792). In this study, we tested their proposed mechanism by M06 density functional theory (DFT) calculations, and the free energy barriers of this reaction were calculated to be not so large that the reaction could occur under an experimental condition. Based on the analysis of NBO charges and orbital interactions of the intermediates species, we designed a new functionalized catalyst introducing an electron donating substituent to the Milstein's catalyst. Electron donating substituent increases charge density of sp^2-C of the C-P(t-Bu)$_2$ moiety, hence, facilitates hydroxyl hydrogen transfer to this carbon. Moreover, softness of Ru atom was raised with functionalized catalyst, which results in enhancement of hemi-lability of amine ligand. The newly designed catalyst was expected to have higher catalytic efficiency than the Milstein's catalyst as noted from the lowered energy barriers and relative energies.



Milstein's Catalyst



Functionalized Cat.

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A Novel Strategy to Heal Monovacancies and Eliminate Epoxy Groups from Graphene-like Nanostructures

Liu Hongguang 이진용*

성균관대학교 화학과

Using first-principles DFT calculations, we have systematically explored the CO adsorption on the pristine graphene flake and the defective one by taking the external electric field into account. It is found that the electric field can increase the CO adsorption energy and there is a barrier for CO?vacancy recombination that is mostly believed to remerge instantaneously when they come close to each other. Also, we propose a mechanism for the subsequent healing of a monovacancy on a graphene flake by interaction with CO molecules, leading to the restoration of a pristine hexagonal carbon network. To the best of our knowledge, the electric field mediated graphene oxide (GO) reduction has not yet been systematically investigated. Herein, we provide a novel strategy to eliminate the epoxy group from the basal plane of graphene flakes as well. Given that the current reduction methods are unsatisfactory to clean the epoxides or sometimes cause undesirable structure deformations. The proposed scenario would permit the improvement of existing GO reduction methods and assist in the fabrication of high-quality graphitic materials.

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A Mechanistic Study of Fluorination of Graphene

이성식 이성렬[1,*]

경희대학교 국제캠퍼스 화학과 [1]경희대학교 응용화학과

We describe the mechanism of graphene fluorination by XeF_2 calculated by using the plane wave basis and periodic boundary condition. We find that fluorination of graphene proceeds by simultaneous bonding of F, via transition states that interact a bit asymmetrically with the graphene surface. Several different mechanisms are proposed and compared. We also elucidate the origin of experimental observations that only 25 % of carbon bond with F when only one side of graphene is exposed to XeF_2 whereas 100 % of saturation with F is obtained when both sides are allowed to react with XeF_2. We find that fluorination at ortho or meta position on the same surface is extremely difficult (with very high barrier), but fluorination at one side facilitates the bonding of F at ortho or meta position at the other side of graphene by lowering the activation barrier of fluorination. We also calculate and compare the DOS for various structures of fluorinated graphene.

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Comparison of ultraviolet-ozone and O_2-plasma surface treatment of Indium tin oxide anode in organic light emitting diodes

김정호* 강헌

서울대학교 화학부

Indium tin oxide (ITO) has been popularly used as an anode in organic light emitting diodes (OLEDs) due to its good conductivity, high work function and transparency in visible range. For more enhanced hole injection, the ITO anode has been treated with simple physical pretreatments such as ultraviolet-ozone (UVO) cleaning and plasma surface treatments for as much as high possible work function of ITO. Both UVO and plasma treatment probably largely remove the ambient contaminants but do not affect the surface morphology. However, the best one physical treatment must be clarified and chosen for the industrial application of OLED. Here the effects of UVO and O_2 plasma treatment on the OLED device performance were compared each other. While the OLED device treated with UVO shows relatively low turn-on voltage, the device life time is shorter than that treated with O_2 plasma, which is in the contrast to the general belief that the lower turn-on voltage is also beneficial for longer lifespan. Therefore the origin of the discrepancy between enhancement trends of turn-on voltage and life time is to be further discussed in conjunction with surface analysis techniques.

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Theoretical Study on Electron Transport in Conjugated Molecular Junction with Silicon Electrodes

최진규 Pham Thu Hien 정현담*

전남대학교 화학과

Research attention on the transport behavior of electrons through a single molecule has recently been much encouraged due to its fundamental scientific importance as well as being accompanied with recent prototype-advances on molecular electronics, at which individual molecule can act as a functional building unit. The electron transport properties through a molecule are not only dependent on the molecule itself but also interaction with electrode. To date, gold (Au) electrode has been mostly used as the metal electrode due to its conducting characteristics and good adhesion property with sulfur atom of a molecule. In this study, electron transport properties through simple conjugated molecules; dithiolbenzene (DTB) and dithioldiphenylethyne (DDE), with metallic Au as well as semiconducting silicon (Si) electrodes, in which the molecules would have interestingly unique interaction with the Si electrode, were theoretically investigated using nonequilibrium Green’s function/density functional theory (NEGF-DFT) formalism in Atomistix ToolKit (ATK) package.

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Synthesis and Characterization of Thioacetic Acid-Capped PbS Quantum Dots

HAFEZMAHMOUDELSAYEDMAHMOUDAHMED Dao Duy Tung Hassouna M.E.M.[1] 정현담*

전남대학교 화학과 [1]Department of Chemistry, Faculty of Science, Beni-Suef Unevirsity, Egypt

Lead sulfide quantum dots capped by oleic acid (PbS QDs-OA) were synthesized and their sizes were controlled by a typical *hot injection method* using OA as stabilizing agent. The OA was replaced by thioacetic acid (TAA) via ligand exchange in order to obtain TAA-capped PbS quantum dots (PbS QDs-TAA) which were confirmed by decrease in the intensity of aliphatic C-H peak in FT-IR spectra. The TAA ligand on the surface of QDs is very short molecule and is expected to undergo *condensation reaction* upon post thermal annealing, by which the QDs within the QD thin films are connected each other through very short linker ?S?, resulting in the improvement of current through the PbS QD-TAA thin film. By curing at 200 oC, we found the current through the PbS QD-TAA thin film is about 2-4 orders of magnitude higher than that of PbS-OA thin film.

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Solution-Processed Indium Zinc Oxide Nanocrystal-Embedded Zinc Oxide Thin-Film Transistors

Pham Thu Hien 최진규 정현담*

전남대학교 화학과

Nanocrystal of inorganic semiconductors is of interest for a large range of electronic devices. A method for the synthesis of indium-doped zinc oxide (IZO) nanocrystal was developed using hot injected method in a noncoordinating solvent 1-octadecene (ODE). Structural, optical and elemental analyses clearly indicated the doping of indium into the host ZnO lattice. Here a solution route to fabricate IZO nanocrystal-embedded ZnO TFT is presented. A simple double layer spin-coating process, in which a dense IZO nanocrystal was formed then ZnO precursor solution was spin-coated, was investigated. The n-channel TFT exhibits mobility of up to 0.07 cm^2/V.s and low threshold voltage of about -15.3V.

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Solution-Processed High?*k* ZrO_2-SiO_2 Hybrid Gate Insulator for Organic Thin-Film Transistors

고예슬 최진규 정현담[*]

전남대학교 화학과

Solution-processed high-*k* ZrO_2-SiO_2 hybrid gate insulator was prepared by sol-gel method from metal alkoxide monomers, followed by spin-coating onto Si-wafers. The properties of ZrO_2-SiO_2 hybrid thin films according to the Zr-Si ratio and curing temperatures were investigated. The dielectric constant (*k*) and leakage current of the hybrid thin films were measured from capacitance-voltage (C-V) and current-voltage (I-V) curves in metal-insulator-semiconductor (MIS) and metal-insulator-metal (MIM) structures, respectively. Pentacene semiconductor layers and Au electrodes (source and drain) were deposited by conventional vacuum deposition technique at low pressure of 10^{-6} torr on the hybrid gate insulator thin films to fabricate organic thin-film transistors (OTFTs) then the transfer and output characteristics were obtained using a semiconductor parameter analyzer, HP4145B, in which highly-doped p-type Si-wafers were used as substrate and gate electrode as well. In addition, the effect of polystyrene layer, which was synthesized from styrene monomer via thermally-initiated radical chain reaction, inserted between the ZrO_2-SiO_2 hybrid and pentacene layers on the OTFT properties was investigated.

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A Study on Electronic Structure of Silicon Quantum Dots using Cyclic Voltammetry

LETHUHUONG 정현담*

전남대학교 화학과

Silicon quantum dot (Si QDs) were synthesized by etching of silicon powder with aqueous hydrofluoric acid (HF) and nitric acid (HNO_3). By only controlling the etching time, the size of hydride-terminated silicon quantum dots (H-Si QDs) was tuned. Then, the H-Si QDs were functionalized by 1-octene (Oct). Using electronic structure of various sized H-Si QDs and Oct-Si QDs were investigated by cyclic voltammetry (C-V). The electronic structure such as conduction band edge, valence band edge, inter-band trap, and quasi-particle gap of Si QDs of various sizes were determined. The C-V results of Si QDs with different size were compared to spectroscopic results such as UV-vis absorption and photoluminescence (PL). The effects of surface chemistry and oxidation on the QD's electronic structure were investigated.

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Condensable InP Quantum Dot Solids

Mai Xuan Dung Dao Duy Tung 정현담*

전남대학교 화학과

Colloidal thioacetic acid-capped InP quantum dots (InP-TAA QDs) and their spin coated-films have been examined in comparison with those of myristic acid-capped InP (InP-MA) QDs. While the QDs are far away from each other in the InP-MA QD films, even in an InP-MA QD film cured at 250 ^{o}C, upon thermal annealing a film of InP-TAA QDs at 250 ^{o}C, the indium thioacetate groups on the surfaces QDs likely condensed, thus resulting in the QD film that consists of individual and proximally packed InP QDs. The structures of the films of InP-MA QDs or InP-TAA QDs were characterized by means of TEM, XRD, and XPS. The current through the film of InP-TAA QDs cured at 250 ^{o}C was about 2-5 orders of magnitude higher than that of the film of InP-MA film annealed by the sample conditions. We, newly in this letter, define this kind of materials architecture as the condensable QDs solid concept.

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InP Quantum Dot - Organosilicon Nanocomposites

<u>Mai Xuan Dung</u> 최진규 정소희[1] 정현담[*]

전남대학교 화학과 [1]한국기계연구원 나노기계연구본부

InP quantum dot (QD) - organosilicon nanocomposites were synthesized and their photoluminescence quenching was mainly investigated because of their applicability to white LEDs (light emitting diodes). The as-synthesized InP QDs, which were capped with myristic acid (MA), are incompatible with typical silicone encapsulants. We have introduced a new ligand, 3-aminopropyldimethylsilane (APDMS), which enables embedding the QDs into vinyl-functionalized silicones through direct chemical bonding. The exchange of ligand from MA to APDMS does not significantly affect the UV absorbance of the InP QDs, but quenches the PL to about 10% of its original value with the relative increase in surface related emission intensities, which is explained by stronger coordination of the APDMS ligands to the surface indium atoms. InP QD-organosilicon nanocomposites were synthesized by connecting the QDs using a short cross-linker such as 1,4-divinyltetramethylsilylethane (DVMSE) by the hydrosilylation reaction. The formation and changes in the optical properties of the InP QD-organosilicon nanocomposite were monitored by ultraviolet visible (UV-vis) absorbance and steady state photoluminescence (PL) spectroscopies. As the hydrosilylation reaction proceeds, the QD-organosilicon nanocomposite is formed and grows in size, causing an increase in the UV-vis absorbance due to the scattering effect. At the same time, the PL spectrum is red-shifted and, very interestingly, the PL is quenched gradually. Three PL quenching mechanisms are regarded as strong candidates for the PL quenching of the QD nanocomposites, namely the scattering effect, Forster resonance energy transfer (FRET) and cross-linker tension preventing the QD's surface relaxation.

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Newly Synthesized Silicon Quantum Dot-Polystyrene Nanocomposite Having Thermally Robust Positive Charge Trapping

Mai Xuan Dung 최진규 정현담*

전남대학교 화학과

Striving to replace the well known silicon nanocrystals embedded in oxides with solution-processable charge-trapping materials has been debated because of large scale and cost effective demands. Herein, a silicon quantum dot-polystyrene nanocomposite (SiQD-PS NC) was synthesized by post-functionalization of hydrogen-terminated silicon quantum dots (H-SiQDs) with styrene using a thermally induced surface-initiated polymerization approach. The NC contains two miscible components: PS and SiQD@PS, which respectively are polystyrene and polystyrene chains-capped SiQDs. Spin-coated films of the nanocomposite on various substrate were thermally annealed at different temperatures and subsequently used to construct metal-insulator-semiconductor (MIS) devices and thin film field effect transistors (TFTs) having a structure p-Si^{++}/SiO2/NC/pentacene/Au source-drain. Capacitance-voltage (C-V) curves obtained from the MIS devices exhibit a well-defined counterclockwise hysteresis with negative fat band shifts, which was stable over a wide range of curing temperature (50-250 ^{o}C). The positive charge trapping capability of the NC originates from the spherical potential well structure of the SiQD@PS component while the strong chemical bonding between SiQDs and polystyrene chains accounts for the thermal stability of the charge trapping property. The transfer curve of the transistor was controllably shifted to the negative direction by varying applied gate voltage. Thereby, this newly synthesized and solution processable SiQD-PS nanocomposite is applicable as charge trapping materials for TFT based memory devices.

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Tuning Optical Properties of Silicon Quantum Dots by π-Conjugated Capping Molecules

Mai Xuan Dung **Dao Duy Tung** **정소희[1]** **정현담***

전남대학교 화학과 [1]한국기계연구원 나노기계연구본부

The absorption and photoluminescence (PL) properties of silicon quantum dots (QDs) are greatly influenced by their size and surface chemistry. Herein, we examined the optical properties of three Si QD samples with increasing σ-π conjugation length: octy-, trimethylsilyl)vinyl-, and 2-phenylvinyl-capped SiQDs. The PL photon energy obtained from as-prepared samples decreased by 0.1-0.3 eV, while the photoluminescent excitation (PLE) extended from 360 nm observed in the octyl-capped Si QDs to 400 nm in the case of 2-phenylvinyl-capped Si QDs. A vibrational PL feature observed in all samples with an energy separation of about 0.192±0.013 eV was explained mainly due to the electron-phonon coupling. The σ-π conjugation induced an increase in the UV absorption cross-section near the band gap transitions. Effect of oxidation on the optical properties of Si QDs was also studied. After soft oxidation through drying the samples in open air, all samples showed blue PL with maxima at approximately 410 nm. A similar high-energy peak was observed with a bare Si sample. The changes in optical properties of Si QDs originate from additional states that are created due to the quantum dot oxidation or the σ-π conjugation. Numerical calculations showed that charges are extracted more at the organic capping layer by lengthening the σ-π conjugation, thus implying a faster charge transfer across the QD’s surface for fostering silicon nanocrystals based photovoltaics.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Plasmon Coupling of Compositionally Heterogeneous Core-Satellite Nanoassemblies

윤준희 윤상운*

단국대학교 화학과

Understanding plasmon coupling between compositionally heterogeneous nanoparticles in close proximity is intriguing and fundamentally important due to the energy mismatch between the localized surface plasmons of the associated nanoparticles and interactions beyond classical electrodynamics. In this presentation, our group explores surface plasmon coupling between silver nanoparticles (AgNPs) and gold nanoparticles (AuNPs), assembled in the form of core-satellite structures. A recently developed assembly method allows us to prepare ultrapure core-satellite nanoassemblies in solution, where 50 nm AgNPs are surrounded by 13 nm AuNPs via alkanedithiol linkers. Our group observes changes in the plasmon coupling between the AgNP core and AuNP satellites as the core-to-satellite gap distance varies from 2.3 nm to 0.7 nm. Comparison with theoretical studies reveals that the traditional hybridized plasmon modes are abruptly replaced by charge transfer plasmons at about a 1 nm gap. Changes with the number of satellites are also discussed.

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Probing the Bilayer Formation of Alkanedithiol on Au Substrates

차훈 윤준희 윤상운*

단국대학교 화학과

Alkanedithiol 의 자기조립단분자층(self-assembled monolayer, 이하 SAM)은 금속 기판에 나노입자를 고정시키거나 나노입자의 조립체를 만드는데 매우 유용한 구조이다. 하지만 thiol 기끼리 disulfide 결합을 만들어 bilayer, 나아가 multilayer 를 이룰 수 있으므로 이를 확인하는 것이 매우 중요하다. 지금까지 이러한 alkanedithiol 의 bilayer 형성 여부는 주로 분광학적인 방법으로 이루어져 왔다. Ellipsometry, IR, Raman, X-ray photoelectron spectroscopy 와 같은 방법은 SAM 을 직접 관찰하므로 매우 유용하지만, 감도와 재현성, 스펙트럼의 해석 등에 문제점을 노정해왔다. 우리는 이 발표에서, alkanedithiol layer 에 금나노입자를 흡착시키고 이를 disulfide 결합의 환원제인 TCEP(Tris(2-carboxyethyl)phosphine)와 반응시켰을 때 나타나는 변화를 전자현미경과 SERS 로 직접 관찰함으로써 alkanedithiol 의 bilayer 형성 여부를 감지할 수 있음을 보이고자 한다.

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Intermolecular energy flow and bond dissociation of vibrationally excited toluene in collisions with N_2 and O_2

이종백* 김성희 H. K. shin[1]

전남대학교 화학교육과 [1]Dept of Chem Univ of Nevada

Intermolecular energy flow and C-H_{methyl} and C-H_{ring} bond dissociations in vibrationally excited toluene in the collision with N_2 and O_2 have been studied by use of classical trajectory procedures. The energy lost by the vibrationally excited toluene 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, and the energy transfer in the collision with O_2 is larger than with N_2. While V-V transfer is nearly constant, V-T transfer increases as the total vibrational energy of toluene increases. When the total energy content E_T of toluene is sufficiently high, either C-H bond can dissociate. The C-H_{methyl} dissociation probability is higher than the C-H_{ring} dissociation probability, and that in the collision with N_2 is larger than with O_2.

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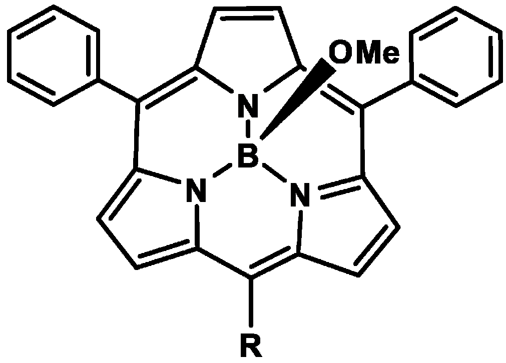
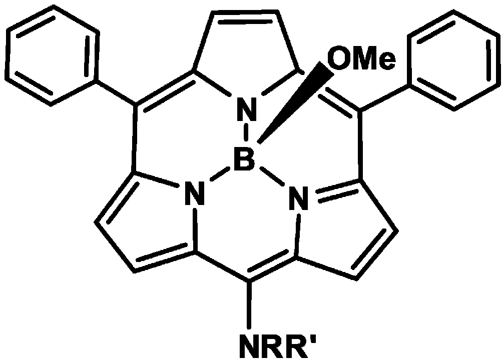
Charge Transfer Phenomena in Subporphyrins

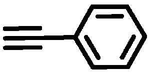
차원영 김동호*

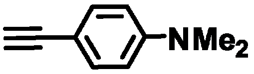
연세대학교 화학과

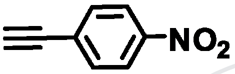
We prepared the two types of subporphyrins which are meso-phenylakynyl 1 and meso-arylamino substituted subporphyrins 2 to make a comparative analysis on photo-induced charge separation between subporphyrin core and meso-substituents with directivity of electron flow by using the electron donor and acceptor groups. Subporphyrins 1 have the triple bond between subporphyrin core and aryl substituents, which gives rise to expansion of π-conjugation with planar molecular structures. And subporphyrins 2 which are first synthesized molecules containing heteroatom substituents, except halogen atom at meso-position showed very special fluorescence properties. We have investigated the ICT and TICT phenomena of meso-phenylalkynyl and meso-arylamino substituted subporphyrins by time-resolved absorption and fluorescence spectroscopic analyses and computational calculations. Through the linear conjugation lines containing the triple bond of 1b and 1c, charge separations between subporphyrin core and substituents are well allowed in polar solvent. Especially, 2b and 2c revealed the fluorescence quenching regardless of solvent polarity due to charge separations involve the significant structural changes. Different with previous TICT studies with other molecular system, we blocked the possibilities of structural twist with the methods of low temperature and viscous-controlled experiments, which can be substantial evidences of TICT interactions and ultrafast fluorescence quenching.

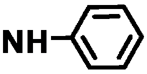


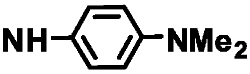


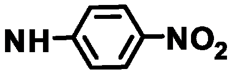
1a : R = 

1b : R = 

1c : R = 

2a : NRR′ = 

2b : NRR′ = 

2c : NRR′ = 

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Intra-cluster Energies and Fragmentation of $(Ar_2^+)Ar_{12}$

이종백* **H. K. Shin**[1]

전남대학교 화학교육과 [1]*Dept of Chem Univ of Nevada*

Intra-cluster energy flow and fragmentation of $(Ar_2^+)Ar_{12}$ with the embedded diatomic ion in a vibrationally excited state is studied in classical dynamics procedures using an analytic represention of the energy of all host ... guest and host ... host interactions. The total energy of $(Ar_2^+)Ar_{12}$, n = 1 - 12 formulated in a building-up procedure is in agreement with the literature values of an extended diatomics-in-molecules approach. Local translation of Ar_2^+ mediates collision-induced energy flow from Ar_2^+ to host atoms, most of energy flow occuring on a picosecond timescale. The time evolution of ion-to-host energy relaxation can be accurately modeled by a triexponential decay. Following energy flow, ~27% of host atoms dissociate and most of dissociations occur within a time period of ~100 ps. The extent of fragmentation occuring at nanoseconds is small but not insignificant. The size distribution of fragmentation products is peaked for $(Ar_2^+)Ar_9$, shifting to $(Ar_2^+)Ar_8$ when more intra-cluster energy becomes available. Relaxation timescales are weakly dependent on both temperature (50-300K) and initial vibrational excitation (v=1-4). The dependence of fragmentation size distribution on initial vibrational excitation is strong, especially for smaller clusters. The size distribution supports the fact that local translation is efficient in transferring energy flow from vibration to host atoms, which in turn, inducing fragmentation of host...host and ion...host interactions of $(Ar_2^+)Ar_{12}$

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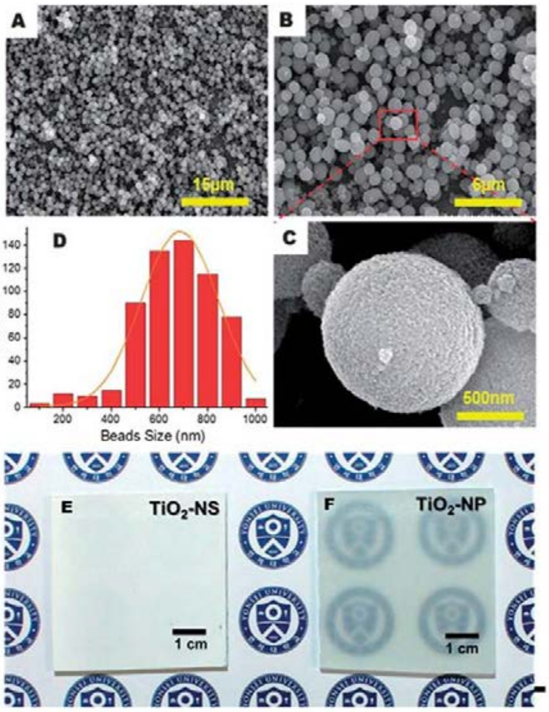
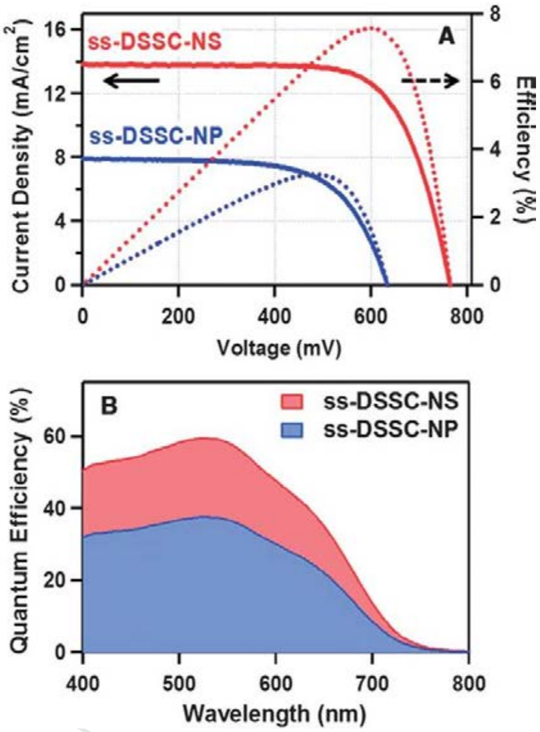
Superior photoelectrodes for solid-state dye-sensitized solar cells using amphiphilic TiO_2

황대섭 김동호*

연세대학교 화학과

Hierarchically structured TiO_2 nanospheres (TiO_2-NSs) were successfully prepared by an electrostatic spray (e-spray). The TiO_2-NSs were employed as photoelectrodes for solid-state dye-sensitized solar cells (ss-DSSCs), in which a novel plastic crystal/polymer blend based solid-state electrolyte (PC-SSE) was used. The nanoparticles-in-sphere shape offered enhanced surface area, pore volume for high dye-loading, and beneficial solid-state electrolyte infiltration, while the submicron-scale of the spheres induced efficient visible-light scattering. The efficiency of the TiO_2-NS-based ss-DSSCs was >2 times higher than that of TiO_2-NP-based ss-DSSCs with notable concurrent improvement in the short-circuit current (JSC = 13.9 mA cm-2), open circuit voltage (VOC = 765 mV), and fill factor (FF = 71.6%). The optimized cell efficiency of 7.6% is thus far the highest reported efficiency for PC-SSE-based DSSCs.Figure 1. SEM images of the e-sprayed TiO_2-NSs. (A?C) SEM images of e-sprayed TiO_2-NS photoelectrode onto FTO/glass (uniform distribution over the entire substrate and nanoparticles-in-sphere structure is indicated); (D) size distribution of TiO_2-NSs used in this study (the line is the fitted result by Gaussian function) and photographs of photoelectrodes: (E) TiO_2-NSs (laminated) and (F) TiO_2-NPs.Figure 2. Photovoltaic performance of the ss-DSSCs. (A) J?V characteristics (straight line) and e?ciencies (dotted line); and (B) incident photon-to-current conversion e?ciency (IPCE) spectra.[1] *J. Mater. Chem. A*, 2013, 1, 1359-1367 D. Hwang, D. Kim*


A
15μm
B
5μm
D
Counts
0
20
40
60
80
100
120
140
200
400
600
800
1000
Beads Size (nm)
C
500nm
E
TiO2-NS
1 cm
F
TiO2-NP
1 cm


A
ss-DSSC-NS
ss-DSSC-NP
Current Density (mA/cm2)
0
4
8
12
16
Efficiency (%)
0
2
4
6
8
Voltage (mV)
0
200
400
600
800
B
ss-DSSC-NS
ss-DSSC-NP
Quantum Efficiency (%)
0
20
40
60
Wavelength (nm)
400
500
600
700
800

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STUDY ON THE WETTABILITY FOR NATURAL AND SYNTHETIC FIBERS WITH THE NATURAL COLOR PIGMENT

서현진 황기환[1] 부진효[*]

성균관대학교 화학과 [1]성균관대학교 물리 화학 통합과정

Tuning wettability is of importance in a wide range of technical applications. In this report we show that wettability of natural and synthetic fibers can be tuned by introducing a natural pigment that has been used for coloring food substrates, leathers, and natural protein fibers. We take wool and polypropylene which are inherently hydrophobic. Interestingly, we observed that the wettability turned hydrophobic into hydrophilic with coating a natural color pigment such as Brazilin or Al(III) complex Brazilein that extracted from Caesalpinia sappan Linn. We also demonstrate that the observed wetting tunability of the fibers is able to use for humidity and chemical sensing devices.

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The roles of the nitrogen bridges perturbing the photophysical properties in porphyrin framework

성영모 김동호*

연세대학교 화학과

Pyrrole replaced porphyrinoid research such as heteroporphyrins, vinylogous porphyrins, carbaporphyrins and triphyrins is spotlighted because these provide an inspiration for developing new fields and refreshing discussions. In this regard, Latos-Grazynski et al. reported synthesis of vacata and divacataporphyrin which can be classified as an annulene-porphyrin hybrid.1,2 These new compounds have potentials to reveal the nitrogen effects on the photophysical properties of porphyrin. The absorption spectra of vacataporphyrin systems show red-shifted and intensified Q-band with changing from TAPH2 to Vac2TAP. The fluorescence spectra show red-shifted with decreased fluorescence quantum yield and excited state lifetime. These aspects could be caused by various factors such as the molecular rigidity, structural distortion and perturbed electron structures. To confirm these factors, we have measured the spectrophotometric titration and temperature dependent experiment.

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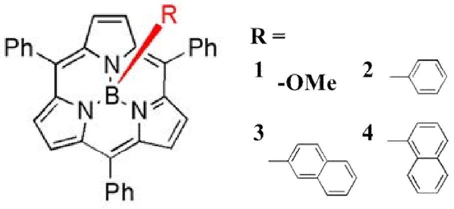
발표종류: 포스터, 발표일시: 수 16:00~19:00

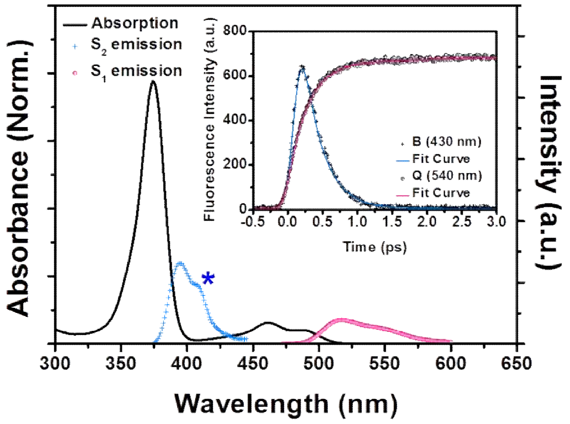
S2 Fluorescence Dynamics of meso-Aryl-substituted Subporphyrins

성주영 김동호*

연세대학교 화학과

Porphyrins represent one of the most widely and intensively studied macrocyclic ring systems since these systems have been recognized as key pigments in photosynthesis. On the other hand, the photophysical behaviors of subporphyrins, which are one of well-known synthetic analogues of porphyrins, are little known. In addition, the S2 fluorescence of subporphyrin has never been reported. Thus, the focus in the current investigation is whether the S2-fluorescence of subporphyrins can be detected or not. It is also intriguing to determine the S2 lifetimes of subporphyrins and to identify structural features that affect these lifetimes Besides S1 fluorescence, another fluorescence bands were observed for subporphyrins 1-4 upon excitation at the respective Soret-like band (Fig. 1). These fluorescence spectra have been assigned as S2 fluorescence on the basis of their mirror images of the S2-S0 absorption. To explore the intrinsic excited state relaxation dynamics of 1-4, fluorescence transients were recorded with our fluorescence up-conversion apparatus. Interestingly, we find that the S2-S1 IC rates of 1-4 are approximately five times faster than that of ZnTPP. Furthermore, despite different axial substituents such as methoxy, phenyl and naphthyl groups, the S2-S1 IC rates of 1, 2, and 4 are similar to each other. The p orbitals of B-axial substituent and the main π-system are orthogonally oriented. It seems to have no significant interaction between the central subporphyrin π-system and B-axial phenyl moiety. Hence we can expect that the S2-S1 IC rates of 1, 2, and 4 are almost identical in spite of different substituents.


Ph
R
Ph
N
B
N
N
Ph
R =
1
-OMe
2
3
4


Absorption
S$_2$ emission
S$_1$ emission
*
Absorbance (Norm.)
Intensity (a.u.)
Wavelength (nm)
300
350
400
450
500
550
600
650
Fluorescence Intensity (a.u.)
800
600
400
200
0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Time (ps)
B (430 nm)
Fit Curve
Q (540 nm)
Fit Curve

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The aggregation behavior of quinoxaline dendrimers at the air-water interface

최소영 김환규[1] 손대원[*] 김재헌

한양대학교 화학과 [1]고려대학교 신소재화학과

Molecular conformation and orientation of 2,3-bis(4-(2,3-bis(4-methoxyphe-nyl)quinoxalin-6-yloxy)phenyl)quinoxaline-6-carboxylicacid ([G2-DPQ]-CO2H: G2) and 2,3-bis(4-(2,3-bis(4-(2,3-bis(4-methoxyphenyl)quinoxalin-6-yloxy)phenyl)quinoxalin-6-yloxy)phenyl)quinoxaline-6-carboxylicacid ([G3-DPQ]-CO2H: G3) at the air-water interface have been investigated using surface pressure-area isotherms by Langmuir-Blodgett technique, Atomic Force Microscopy, UV-vis spectroscopy, and X-ray reflectivity.In the case of G2, the surface pressure-surface area isotherm shows a steep increase around 100 Å2/molecule. G2 experiences a direct transition from the gaseous phase to the solid phase, and molecules are compressed without complicated transitions. The monolayer of G2 is aligned straightly at 5 mN/m. At higher surface pressure near 20 mN/m, G2 molecules maintain their ordering and form a close-packed arrangement.In contrast to G2, the isotherm for G3 shows a gradual increase owing to the flexibility of G3 molecules. G3 molecules form circular domains at the surface pressure of 1 mN/m as a result of the difference in hydrophobicity between the core group and the peripheral end group. Upon further compression, G3 made many aggregate domains, size of ~ 40 nm.

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Fabrication of solid thin target arrays for laser-driven ion acceleration

박형주

한국전자통신연구원 바이오메드연구실

Laser-plasma acceleration of ions has made great progress during the past decades, because the developments may one day allow construction of compact tabletop proton therapy accelerator. Here, we reported the fabrication of solid thin target arrays for proton generation by using micro-electro-mechanical-system (MEMS) process and observed the high energetic protons on the backside of the solid thin target. After depositing silicon nitride thin films on both sides of silicon wafer (6 inch, 500 μm), the square window patterns were opened on the back of silicon wafer by photo lithography. And next, the thin membrane-type targets were successfully prepared by wet etching. The target layer thickness was defined by measuring deposited silicon nitride thin films, and the sort and number of target was determined by the photo-mask design.

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Green synthesis of Highly-luminescent ZnSe/ZnS:Mn/ZnS core/shell/shell Nanocrystals

윤수진 최종완 허윤중 김낙중*

한양대학교 화학과

New water-soluble and highly luminescent ZnSe/ZnS:Mn/ZnS core/shell/shell nanocrystals (quantum yield is upto 42.9%) with color-tunable emission range between 580 and 600 nm (from $^4T_1$ to $^6A_1$ transition) were synthesized via a multistep in single flask method by regulating feeding molar ratio [Zn]/[Mn] for electronic device. At the low enough Mn^{2+} dopant concentration ZnSe/ZnS:Mn core/(doped) shell and ZnSe/ZnS:Mn/ZnS core/(doped) shell/shell nanocrystals (NCs) emit white light in aqueous media with a quantum yield about 27.6% and 20.5%, respectively. Here in this work, white light emission of as-prepared NCs is a result of combined emission of blue light (emission from band gap of ZnSe core) and yellow/orange light ($^4T_1$-$^6A_1$ emission from Mn^{2+} ions doped in ZnS of the first shell). Especially, the green emission generated from surface defects was found as a key factor that affects the photoluminescence quantum yields of core/(doped) shell and core/(doped) shell/shell NCs.

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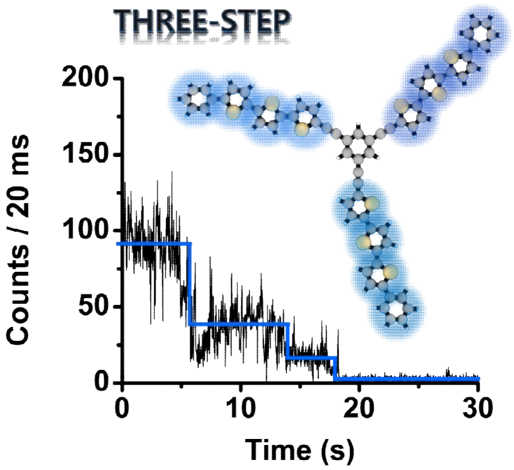
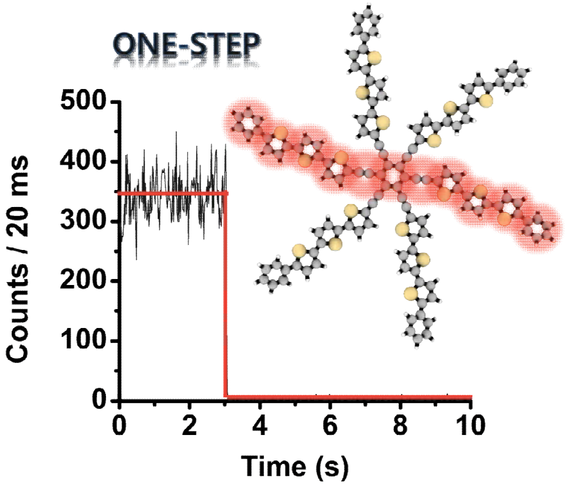
Structure-dependent Electronic Natures of Star-shaped OligothiophenesProbed by Ensemble and Single-molecule Spectroscopy

정희재 김동호*

연세대학교 화학과

We have investigated the photophysical properties of star-shaped oligothiophenes with three terthiophene arms (S3) and six terthiophene arms (S6) connected to the ethynylbenzene core to elucidate the relationship between molecular structure and electronic nature by a combination of ensemble and single-molecule spectroscopic techniques. We postulate the two different conformations for S3 and S6 on the basis of X-ray structure and manifest the coexistence of those conformers by spectroscopic methods. From the steady-state spectroscopic data, we could reveal that the exciton is delocalized over the core, but that the meta-linkage of S3 prevents the electronic communication between the arms. In single-molecule studies, however, we observed some molecules show long fluorescence lifetimes (~1.4 ns) in the fluorescence intensity trajectories, which indicates the π-electrons are delocalized along the meta-linker. Based on these observations, we suggest that the delocalized exciton is sensitive to the dihedral angle between the core and the adjacent thiophene ring as well as the substituted position of the terthiophene arms. Our results highlight that the fluorescence lifetimes of S3 and S6 are strongly correlated with their spatial location of excitons which are mainly affected by their conformations; whether the facing innermost thiophene rings exist or not in both S3 and S6.


THREE-STEP
Counts / 20 ms
200
150
100
50
0
0
10
20
30
Time (s)


ONE-STEP
Counts / 20 ms
500
400
300
200
100
0
0
2
4
6
8
10
Time (s)

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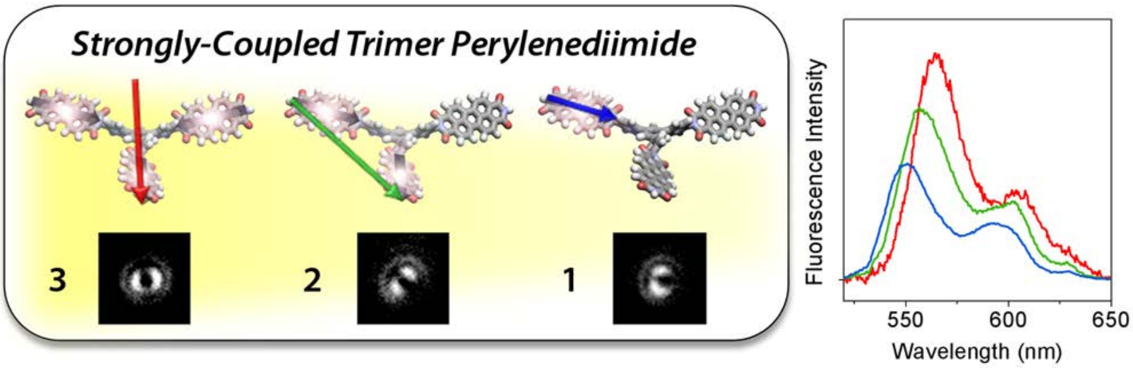
Excitonic Coupling in Linear and Trefoil Trimer Perylenediimide Molecules Probed by Single-Molecule Spectroscopy

유혜진 김동호*

연세대학교 화학과

Perylenediimide (PDI) molecules are promising building blocks for photophysical studies of electronic interactions within multichromophore arrays. Such PDI arrays are important materials for the fabrication of molecular nano-devices such as organic light emitting diodes, organic semiconductors and biosensors because of their high photostability, chemical and physical inertness, electron affinity and high tinctorial strength over the entire visible spectrum. In this work, PDIs have been organized into linear (L3) and trefoil (T3) trimer molecules and investigated by single-molecule fluorescence microscopy to probe the relationship between molecular structures and interchromophoric electronic interactions. We have found a broad distribution of coupling strengths in both L3 and T3, and hence strong/weak coupling between PDI units by monitoring spectral peak shifts in single-molecule fluorescence spectra upon sequential photobleaching of each constituent chromophore. In addition, we have used a wide-field defocused imaging technique to resolve heterogeneities in molecular structures of L3 and T3 embedded in a PMMA polymer matrix. A systematic comparison between the two sets of experimental results allowed us to infer the correlation between intermolecular interactions and molecular structures. Our results show how control of the PDI intermolecular interactions using suitable multichromophoric structures may serve to guide single-molecule device design.


Strongly-Coupled Trimer Perylenediimide
3
2
1
Fluorescence Intensity
550
600
650
Wavelength (nm)

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Time-resolved fluorescence anisotropy of coumarin-labeled amyloids in PBS buffer

이유민 이민영*

이화여자대학교 화학나노과학과

Coumarin 343 (C343) was labeled to amyloid-β consisting of 40 amino acid residues (Aβ40) to investigate the rotational motion of amyloid in PBS buffer. The rotational reorientation time of C343-Aβ was measured as a function of unlabeled Aβ40 concentration using time-resolved fluorescence anisotropy. The rotational reorientation time of free C343 in buffer has been measured as ca. 100 ps. By increasing the concentration of unlabelled Aβ40, the rotation time C343-Aβ was significantly increased due to aggregation, which falls into a nanosecond range. The monomeric Aβs are in dynamic equilibrium with dimers and trimers, where the relative ratios are dependent upon the overall concentration. It was attempted to discern the relative oligomer ratio by analyzing the time-resolved anisotropy data in the absence and presence of organic aggregation inhibitors. The method may provide an efficient way to access molecular interactions between amyloid oligomers and potential inhibitors.

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Studies on amyloid aggregation processes and amyloid-ligand interactions using AFM and FRET

고문지 이민영*

이화여자대학교 화학나노과학과

Atomic force microscopy (AFM) and fluorescence resonance energy transfer (FRET) have been widely used to investigate size determinations and molecular interactions, respectively, with a nanometer-scale spatial resolution. In this work, AFM was used to probe the amyloid aggregation processes in the presence of small molecule inhibitors such as curcumin, hemin, and azobenzene derivatives. They have drawn special interest as small molecules that bind to amyloid and show antiaggregation effect. In accordance with AFM, time-resolved FRET was also used to determine the binding affinity between amyloid and the inhibitors. For FRET, coumarin 343 (C343), a highly photostable dye, was labeled to Aβ and the fluorescence lifetime was obtained by time-correlated single photon counting. We present that AFM and FRET are excellent methods to detect the early stage of Aβ aggregation and to screen potential small molecule inhibitors.

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In search of early-stage amyloid aggregation inhibitors using pyrene fluorescence.

이휘인 이민영*

이화여자대학교 화학나노과학과

The aggregation of amyloid-β (Aβ) is known to be a primary cause of Alzheimer's disease. Aβ monomers associate progressively to form several self-assemblies such as dimers, oligomers, protofibrils, and fibrils. Recently, finding small molecule inhibitors that bind to amyloids at the early-stage becomes an important issue. We investigated amyloid-ligand interactions with a home-built two-channel fluorescence detection system, which can monitor simultaneously the energy transfer between pyrene-labeled Aβ42 (Py-Aβ) and a series of coumarins covering coumarin 6H, coumarin 102, coumarin 153, 7-(diethylamino)coumarin-3-carboxylic acid, coumarin 6, coumarin 7, coumarin 30, coumarin 314, coumarin 334, and coumarin 343. By analyzing the binding affinity data obtained from the ratio of pyrene/ligand fluorescence, we showed that the molecular structure of coumarin influences the specific binding mode to amyloid through mostly hydrophobic interactions.

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Persistence length of single-stranded DNA measured by FRET

강주연 정지원 김성근*

서울대학교 화학부

Single-stranded DNA (ssDNA) is an essential intermediate in many DNA metabolic processes such as replication, recombination, repair, and transcription. We investigated the mechanical flexibility of ssDNA by single-molecule fluorescence resonance energy transfer (FRET). By labeling both ends of DNA segments of different lengths with a pair of fluorescent probes and measuring their FRET efficiency, we were able to compare the degree of bending for ssDNAs ranging in lengths from 11 to 14 nucleotides. Our measurements yielded two distinct values of FRET efficiency with a clear and abrupt change at 13 nucleotides, which suggests that ssDNAs longer than this critical length moves rather freely in random fluctuation whereas those shorter than that should be so mechanically rigid as to exhibit a severely restricted motion.

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Tip Enhanced Raman and Fluorescence Spectroscopy with Single Nanoparticle Attached AFM Probe

김웅 이은별[1] 김지환[1] 박준원*

포항공과대학교 화학과 [1]고려대학교 화학과

Tip enhanced Raman spectroscopy (TERS) is analytical technique to detect a variety of chemical bond, biological and material sample. Especially, the best challenge to TERS field is how to make TERS tips. In this study, a single gold nanoparticle is attached at the apex of an AFM tip through a picking process. We were controlled by silver shell thickness of gold attached with edge of AFM tip to used various concentration of silver enhancing solution and time control. The optical signal is very enhanced by local electromagnetic field. Finally, TERS measurements on single-wall carbon nanotube were successfully performed and simulation data (FDTD) to calculate the electric field in the tip apex is well fitted of experimental results. Single nanoparticle attached AFM tip is working for tip enhanced fluorescence (TEF). Our investigation tips are suitable for single molecule fluorescence and our investigation tips break diffraction limit (FWHM > 100nm). Through investigation tips, We can understand unknown nano, material science.

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Self Powered Position Dependence Graphene Photodetector

최종완 윤수진 배정아 오진우[1,*] 김낙중[*]

한양대학교 화학과 [1]부산대학교 나노소재공학과

Reduced graphene oxide(rGO) is one of the candidates for optoelectronic application such as optical modulator photodetector, phototransistor and plasmonic devices due to exceptional physical and photonic properties. Furthermore rGO can be approached for fabrication of large areas and flexible / stretchable device. In this work, we prepared a free standing rGO sheet by vapor-phase reduction method with HI/acetic acid, and we also fabricated a large position sensitive photodetector with homogeneous electrodes structure. The photocurrent varied from positive and negative as the light illumination position from one electrode to another one at zero bias voltage. This proved that photocurrent is changed by schottky barrier at the graphene-metal contacts.

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Different Exciton Coupling Dynamics in Alkyl-bridged Zn(II) Porphyrin Dimers

이상수 김동호*

연세대학교 화학과

Recently, there are various efforts to realize molecular optoelectric devices due to their potential applications. A variety of covalently linked multichromophoric systems have been prepared as biomimetic models of photosynthethic systems, photonic materials, and functional molecular photonic devices.1 For these applications, it is important to understand exciton coupling dynamics among constituent units. To elucidate the relationship between exciton coupling and structural change upon photoexcitation, two types of Zn(II) porphyrin dimers were synthesized such as β-β singly linked (SLZn) and β-β, meso-meso doubly linked dimers (DLZn). 2 Based on X-ray crystallographic data, dihedral angles between two porphyrin moieties are determined to be 75° and 99° with center-to-center distances of 8.11 and 8.36 ? for SLZn and DLZn, respectively. In spite of these similar structures, large differences in their exciton coupling strengths were observed in steady-state absorption and fluorescence excitation spectra. Furthermore, we measured ultrafast depolarization times of 1.54 ps and 320 fs for SLZn and DLZn, respectively, by using femtosecond transient absorption anisotropy, which should be correlated excitation energy transfer time in each dimer. These exciton coupling strengths and transfer times are matched with theoretically expected values based on F?rstertype incoherent energy hopping model. These results will provide further understanding about relationship between structures and exciton coupling dynamics in the various multichromophoric molecular architectures.

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Synthesis and Properties of Solution-Processed ZnO Nanocrystals with Different Size and Shape for Thin Film Transistors

이돈성 최진규 정현담*

전남대학교 화학과

Semiconductor metal oxides such as In_2O_3, SnO_2, and ZnO have recently drawn much attention due to their high carrier mobility, transparency, environmental stability, and solution-processability. In this study, high-crystalline ZnO nanocrystals (ZnO NCs) of various size and/or shape were synthesized by forced hydrolysis in an organic solvent. The size and shape of ZnO NCs were tuned by controlling the hydrolysis ratio ($H=n_{H2O}/n_{Zn}{}^{2+}$). Then the synthesized ZnO NCs were etched by acetic acid (AC) to give transparent coating solution for thin films. The thin films were fabricated on quartz and Si-wafer substrates using spin-coating method followed by curing at various temperatures. It was observed from UV-vis spectra and XRD analysis that the surface of the ZnO NCs was etched by the AC, which causes reducing their size. ZnO NC thin film transistors (TFTs) were fabricated by deposition of aluminum electrode on the ZnO NCs/SiO_2/Si thin films, where highly-doped p-type Si-wafer was used as substrate as well as gate electrode. The effects of size and shape of the ZnO NCs on their TFT properties were investigated.

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Interaction between Cucurbit[6]uril and Spermine Measured by Atomic Force Microscopy

배영인 백강균[1] 김기문 박준원[*]

포항공과대학교 화학과 [1]기초과학연구원 복잡계자기조립연구단

Atomic force microscopy (AFM) has been widely used to study specific interaction between host-guest complexes as well as biomolecule pairs. At a single molecule level, we measured the unbinding force of a host-guest complex, cucurbit[6]uril (CB[6]) and spermine. To observe single unbinding event of the complex, a dendron was self-assembled on both an AFM tip and a substrate. Then, a dendron-coated tip was functionalized with spermine. And bovine serum albumin (BSA) was introduced on the dendron-coated substrate before the functionalization of CB[6]. Under the condition, we observed characteristic stretching in the force-distance (f-d) curve showing single unbinding force due to the elasticity of the protein. For bridging CB[6] and BSA, we introduced amine-reactive and homo-bifunctional linker. On the reaction of the linker, we used organic solvent and observed distinguishable stretching f-d curves. In this solvent, these are relatively more stable and shorter than in buffer solvent. Also, we measured the unbinding force depending on several pH. With these approaches, unambiguous sorting the specific unbinding event and distinguishing different behavior of stretching depending on the solvent were possible. Furthermore, we obtained the force map of CB[6] distribution on the BSA surface and the unbinding forces with dependence on pH.

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Porphyrin based dyes containing low band gap for dye-sensitized solar cells: A DFT/TD-DFT study

SUBRAMANIANKARTHIKEYAN 이진용*

성균관대학교 화학과

One of the most significant aspects in the development of dye-sensitized solar cells (DSSCs) is the exploration and design of high efficiency and low cost dyes. In the present paper, we have reported a theoretical design of porphyrin based dyes. The geometries, electronic properties, light harvesting efficiency, and electronic absorption spectra of these dyes are studied at density functional theory (DFT) and time dependent density functional theory (TD-DFT). The optimized geometries indicate that these dyes are nonplaner, which is very useful to inhibit the close intermolecular π-π aggregation effectively. The band gap of these dyes can be ensuring positive effect on the process of electron injection and dye regeneration. The trend of band gaps nicely compares with the predicted spectra data. Our calculated results of dyes show that the new dyes should have better performance than the existing efficient dye (YD2-o-C8) due to their improved optical properties.

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Carbon dioxide reforming of methane over mesoporous Ni/SiO_2 and effect of TiO_2 addition on the catalytic reactivity

김대한

성균관대학교 화학과

Mesoporous SiO_2 -supported Ni catalysts (Ni/SiO_2 and Ni/TiO_2/SiO_2) were fabricated by atomic layer deposition (ALD), and their catalytic activity and stability were investigated in carbon dioxide reforming of methane (CRM) reaction at 800 ℃. The Ni/SiO_2 catalysts showed high stability as a result of confinement of Ni particles with a mean size of ~10 nm within the pores of SiO_2 support. Besides, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM) results showed that the Ni nanoparticles were partially buried inside the SiO_2 support. The strong interaction between Ni and the SiO_2 support could also be advantageous for long-term stability of the catalyst. In case of the Ni/TiO_2/SiO_2 catalyst, it was found that the catalytic activity of 10 nm-sized Ni nanoparticles was not much influenced by TiO_2 addition.

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Carbon Dioxide Reforming of Methane to Syngas over a TiO_2 -Ni Inverse Catalyst

김대한

성균관대학교 화학과

TiO_2 -Ni inverse catalyst was fabricated using an atomic layer deposition (ALD) process, and catalytic carbon dioxide reforming of methane (CRM) reactions over the catalysts (either bare Ni or TiO_2 coated-Ni particles) were performed using a continuous flow reactor at 800 ℃. The TiO_2 -Ni inverse catalyst had a higher catalytic reactivity at the initial stage of the CRM reaction at 800 ℃ compared to that of bare Ni catalysts. Moreover, the high activity of the TiO_2 -Ni catalyst was maintained over 65 hrs of the CRM reaction at 800 ℃, whereas deactivation of the bare Ni surface began within 1 hr under the same conditions. Surface analysis using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy showed that deposition of graphitic carbon was effectively suppressed in the presence of TiO_2 nanoparticles on the Ni surface, thereby improving the catalytic activity and stability of the TiO_2 -Ni catalytic system. We suggest that utilizing the decorative effect of oxide nanoparticles on the surface of metal catalyst has great potential for the development of metal-based catalysts with high stability and reactivity.

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The photo-chemical reaction kinetics at indivisual junction using single molecule SERS

최한규 김지환[*]

고려대학교 화학과

We investigate the photoreduction of 4-nitrobenzenethiol (NBT) into 4,4'-dimercaptoazobenzene (DMAB) using the gap-plasmons at Ag nanoparticle and a Au thin-film junction. The individual gap-junctions are illuminated by a laser light (λ_{ex} = 632.8 nm) to induce photoreduction and to monitor the surface-enhanced Raman scattering (SERS) during the reaction. While the $\nu_s(NO_2)$ peak of the reactant shows continuous pseudo 1st-order decay kinetics of many (~200) molecules, the product bands (9b, 3, and 19b) show discrete steps of intensities. We also observe that the center frequency of $\nu_s(NO_2)$ (1350 cm-1) in the SERS spectra red-shifts by 10 cm^{-1} prior to the decay in intensity. This red-shift indicates that the decay kinetics is in fact the nitrobenzene anion radials ($R\text{-}NO_2^-$) formed by the metal to NBT electron transfer reaction, rather than the neutral NBTs. In addition, the dynamics of the product steps are strongly correlated to the decay of the $\nu_s(NO_2)$ peak. Furthermore, the sizes of the steps show remarkable consistency among different hot-spots. These, together with the statistical analysis of the trajectory confirm that the "quantized" steps of the products indeed represent the buildup of individual DMAB products. Also, we could identify isomer (o-NBT, m-NBT) dependent reaction kinetics. The result constitutes the first observation of photochemical reaction of unlabeled individual molecules.

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Influence of various NLO chromophores on the Photorefractivity in polysiloxane carbazole based polymer composites.

허윤중 최종완 윤수진 김낙중*

한양대학교 화학과

The photorefractive (PR) effect is a spatial modulation of the refractive index of a material upon illumination of a non-uniform beam through Photoconductivity and Electro-optic (EO) properties. When two coherent beams intersect a PR material, the internal space-charge field is formed due to the redistribution of the photogenerated charge carriers that subsequently modulate the refractive index via EO effect. The photorefractive composite is composed with several components such as photoconducting polymer, sensitizer, non-linear optic (NLO) chromophore and plasticizer. Photoconducting polymer and sensitizer related to charge generation, transport and trapping processes. NLO chromophore is an important factor to perform a good photorefractivity because orientational of NLO chromophore determines EO properties of the PR composite. Plasticizers are used in order to lower the glass transition temperature (Tg) of the composites down to the room temperature. We investigate the photorefractive properties such as photocurrent, birefringence and PR response time using several photorefractive composites. The composition of polymeric composite was photoconducting polymer (PSX-Cz) : NLO chromophores (PDCST, PNCST, DB-IP-DC or DME-IP-DC) : sensitizer (TNF) 69:30:1 by wt%.

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Synthesis of Tetragonal LaVO4 and Its Application to Downconversion Phosphor of Dye-Sensitized Solar Cell

김두경 강영수*

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Lanthanide orthovanadate crystals have two types of morphologies, those are tetragonal phase with zircon structure and monoclinic phase with monazite structure. Generally tetragonal LaVO4 is a better host for rare-earth activators. The charactericstic of downconversion phosphor enables to convert UV into visible light. This phenomenon is expected to enhance the efficiency of DSSC (dye-sensitized solar cell) and stability of dye which is easily photooxitized. LaVO4 was prepared using La(NO3)3?6H2O, Dy(NO3)3?6H2O, NH4VO3 and EDTA which was used as a capping agent for hydrothermal method.[1] The morphology of nanoparticle changes as the pH changes because of the different protonation of EDTA at each pH condition. Characteristics of nanoparticles have been checked by XRD, SEM, TEM and photoluminescence (PL).

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Synthesis of Single Crystalline TiO2 Particles with Various Shapes with Facet Selective Exposure

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TiO2 films with oriented anatase (001) facets and their photoelectrochemical property have been widely investigated because of its many promising properties as photocatalyst. The properties of anatase TiO2 crystals are largely determined by the largest exposure of the most photoactive facet. Many efforts have been made to improve the percentage of high-reactive facets like (001) facets of anatase TiO2 to enhance its photocatalytic properties. TiO2 films with oriented anatase (001) facets grown on transparent conductive fluorine-doped tin dioxide substrate were prepared via a facile rubbing method and hydrothermal route. The obtained TiO2 film as a photoanode shows efficient photoelectrochemical water splitting ability (photocurrent). The presence of high-energy facets in titania improves significantly its adsorption, electronic, and photocatalytic properties, making this material attractive for various environmental and energy-related applications.

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Upconverting Microparticles Synthesized by a Facile Hydrothermal Route and its Application into Dye-Sensitized Solar Cells

이재호 강영수*

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Upconversion is a process where low-energy photon is converted into a high-energy photon. By using upconverting microparticles, we can convert infrared light into visible light. These materials can be a possible candidate to overcome the spectral mismatch of dye-sensitized solar cells (DSSC). Upconverting microparticles such as β-NaYF4 doped with Yb3+, Er3+, Ho3+ are the possible candidates for application since they have excellent upconverting efficiencies along with emissions around ~550 nm, which can be efficiently absorbed by the N-719 dye. Different morphologies of β-NaYF4 doped with Yb3+ and Er3+ was synthesized by a facile hydrothermal route. By making these microparticles into a film, we can apply it to the external light reflection part of the DSSC, thus not disturbing its internal circuit and enhance its efficiency by using not only visible light, but also infrared light.

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ZnO and its Different Facets for Photocatalytic Application

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Research in artificial photosynthesis seeks to replicate the natural process of photosynthesis that converts water and carbon dioxide into carbohydrates and oxygen using sunlight as the energy source. The visible-light driven splitting of water into hydrogen and oxygen and the production of methanol from CO2 reduction are sometimes included in the definition. [1] ZnO with a direct wide-band gap (3.37 eV) and a larger excitation binding energy (60 meV) has been increasingly studied for many years due to its excellent physical properties and applications in various fields. It is widely reported that the main properties of ZnO nanostructures strongly depends on their morphology, crystalline structure, defect and impurity contents. In this sense, the ZnO preparation route affects in a significant way to those properties. For photocatalytic applications, the improvement of the photoactivity might be achieved by influencing those properties that control either the charge carrier dynamics (carrier generation, transfer and diffusion) or the surface catalytic process, which are the quality of the structure and the surface features. In this sense, here in poster presentation we describe the hexagonal, bilayer and rod type ZnO using solvothermal synthesis [2] would provide the adequate structural and surface properties for photocatalytic applications.

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Fabrication of Cu2O-WO3 p-n Junction Film to Enhance the Anodic Photocurrent

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The transparent WO3 film with the thickness of ca. 200 nm was fabricated on FTO by the facile spin coating method. The Cu2O films with different morphologies were prepared on WO3/FTO by electrochemical deposition of the same copper precursor solution with different pHs (pH 7, 9, 11). The morphologies of as-obtained films were characterized by scanning electron microscopy, which shows that the films composed of nano-sized particles were uniform. The crystallinity of films was characterized by XRD. Compared with the WO3/FTO film, the anodic photocurrent of Cu2O-WO3/FTO prepared at pH 7 was enhanced by construction of p-n junction.

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Electrochemical Synthesis and Characterization of Anodized TiO2 Nanotube Arrays/ZnO composite Electrode

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TiO2 nanotubes arrays (TNTA) synthesized by electrochemical anodization of Ti foil using ammonium fluoride and glycerol (electrolyte) at constant anodization potential of 60 V for 10 h. Self assembled titania nanotubes carry many advantages as compared to conventional nano particulate film in term of better electron transport properties and higher electron diffusion length. Photo electrochemical properties of TNTA can be tuned by tailoring wall thickness, pore diameter and length of channels on the basis of electrochemical anodization parameters i.e applied voltage, anodization duration and electrolyte composition. Beside several strong points of titania nanotubes arrays, there are also certain shortcomings of this material limiting efficiency of photo conversion efficiencies. Recombination of large amount of photo generated charge carriers is the key hindrance to attain maximum theoretical efficiencies of titania. Solid- solid interface is useful methodology to separate electron/hole pair from undesired recombination. Here in this work we have coupled ZnO with titania nanotubes arrays by electrochemical route as a viable methodology to control the amount of secondary material deposit. Based on the variation of deposition time we have investigated morphology of the deposited ZnO as well as photoelectron chemical properties of resultant composite electrode have been discussed in detail.

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Controlling Morphosynthesis of Semiconductor Nanomaterials for Photoactivity

van thanh khue 강영수*

서강대학교 화학과

Taking advantages of selective adsorption of each particular crystal facet of semiconductor nanomaterials, the morphology-controlled synthesis of various shapes was done by using surfactants or foreigner chemical species that benefit to photoactivity. As the results, by using cetyltrimethylammonium bromide (CTAB) which acts as surfactant, dispersed CdS single crystals were obtained via a hydrothermal condition. The strong interaction between the cationic head group of CTAB and the (001) plane of CdS hexagonal crystals results in a single-crystalline growth along the [100] direction. On the other hand, uniform and single-crystalline α-Fe2O3 polyhedral nanoparticles in hexagonal crystal system named truncated hexagonal bipyramid (THB) were fabricated. Under hydrothermal condition, carboxymethyl cellulose (CMC) and hydrazine molecules play roles such as dispersant and capping agents, respectively, during the crystallographical growth. The optical and magnetic properties of the hematite particles were investigated as well.

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Synthesis of Single-Crystalline Monoclinic BiVO4 by the Seed Layer Assisted Growth on FTO Glass

손영석 강영수*

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Recently, semiconductor photocatalysts on a nano-structure scale have become more and more attractive because of their different physical and chemical properties from bulk materials. The surface structure of photocatalysts plays an important role to their photocatalytic activities because the photocatalytic reaction or photoelectron conversion takes place only when photoinduced electrons and holes are available on the surface.BiVO4 has been received much interest as a promising photocatalyst for oxygen evolution from water, but little is known about the factors that limit its performance as a photoanode. BiVO4 has been widely reported with controlled morphology from spherical particle to pyramidal shape. However few researches have been reported about single crystalline BiVO4. Moreover it is very few to report BiVO4 films as photoanode. In this study, we report BiVO4 nanoparticle film on the FTO by hydrothermal method. Using seed layer by spin-coating, BiVO4 nanoparticle film with various morphologies with facet selective exposure to solar light was grown on the seed layer. We demonstrated growth of single-crystalline monoclinic BiVO4 on FTO. The structure and optical properties of BiVO4 film have been well characterized and displayed a strong photo response in the visible region.

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Sol- Gel Followed by Reduction-Diffusion Method to Synthesize Nd2Fe14B Hard Magnet

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서강대학교 화학과

Nd2Fe14B hard magnetic nanoparticles were synthesized by chemical synthesis techniques. In my case, we use the process of sol-gel followed by reduction-diffusion (R-D). The common metal salts (chlorides) was used as precursors and citric acid was used as chelating ligands of metal ions and ethylene glycol was used as as a cross-linking to form a polymeric resin on molecular level. This process can reduce segregation of particular metal ions and ensure compositional homogeneity. Besides, we used the CaH2 as reducing agent in the R-D process. It is easy to remove the residue Ca(OH)2 by washing out in the final step. In this method, it offers several advantages such as ease of elemental substitution, ease of obtaining nanoparticles and the relatively low temperature required for synthesis.

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Synthesis of Well-aligned ZnO Nanotubes

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Photocatalytic devices by simulating the photosynthesis of plant can be designed as photoelectrochemical cell (PEC cell), which can split the water into oxygen gas and hydrogen gas. These gases can be used for clean fuels which can solve the lack problem of fossil fuels. The ZnO is a good photoanode which can be applied in many ways because of its various morphologies. In addition, ZnO nanotubes has high surface area so they can be applied in many ways such as formation of high-efficient junction with other chemical materials.

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A novel biocompatible fluorescent probe for glucose uptake

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We developed a novel, inexpensive, biocompatible fluorescent probe for glucose uptake in the human body. This compound can be readily produced by UV irradiation of a common natural product, which yields a photoproduct that has a large Stokes' shift, high fluorescence quantum yield, and large two photon absorption cross section. Unlike typical organic fluorophores, this new compound has little cytotoxicity and full biocompatibility, while its glucose group makes it a powerful imaging probe for cancer cells that tend to have over-expressed glucose transporters (GLUTs) on the cell membrane that enhances cellular uptake of glucose.

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Kramers restricted complete active space self-consistent field theory: Implementation and applications

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한국과학기술원(KAIST) 화학과

We report an implementation of the relativistic two-component complete active space self-consistent field theory in Kramers restricted formalism (KRCASSCF) in the framework of the relativistic effective core potential. As a multi-configurational approach, this method can effectively treat static electron correlation, which differs from dynamical correlation by arising from the (nearly-)degenerate states and becomes more important for molecules containing heavy atoms owing to the spin-orbit coupling as relativistic effect. The theory has been revised by means of adding time-reversal symmetry in the expressions of gradients and Hessians resulting from the employment of elementary spinor excitation operator so as to complete the course of theoretical development and reduce computational overhead, and is fully implemented to the relativistic two-component *ab initio* electronic structure program KPACK. In the implementation, the two-step approach is employed; the configurations are first optimized with fixed spinor space followed by the rotation of the spinor space with the pre-optimized configurations, and the same procedure is iterated until the convergence. The KRCASSCF method was applied to atoms and diatomics of the 7*p* series of superheavy elements for calculating various atomic and molecular properties.

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Coverage Dependent Variation of Adsorption Structure of 2-Thiophenecarboxaldehyde on the Ge(100) Surface

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숙명여자대학교 화학과

Coverage dependent variation of the adsorption and electronic structure of 2-thiophenecarboxaldehyde (C5H4SO) on the Ge(100) surface using core-level photoemisiion spectroscopy (CLPES) and density functional theory (DFT) calculation. Analysis of S 2p, C 1s, and O 1s core-level spectra reveals three distinct adsorption geometries, which we assigned to a Ge-S dative bonding state, a [4+2] cycloaddition bonding state, and a [2+2] C=O cycloaddition bonding state as a function of coverage. At low coverages, the kindetically favorable dative bonding state (Ge-S) is initially formed at room temperature. As the molecular coverage is increased, thermodynamically stabel [4+2] cycloaddition reaction products are additionally produced. In addition, we found that as the coverage was further increased, the [2+2] C=O cycloaddition reaction product is additionally observed. We systematiclly elucidate the changes in the bonding states of adsorbed 2-thiophenecarboxaldehyde on the Ge(100) surface according to the 2-thiophenecarboxaldehyde coverage.

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Theoretical study on the molecular structure and boding properties of C3SiNH species

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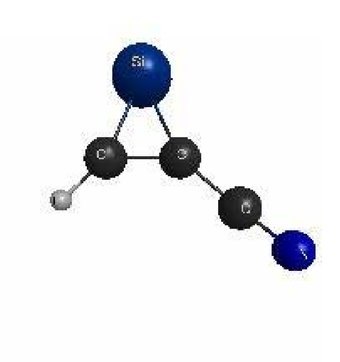
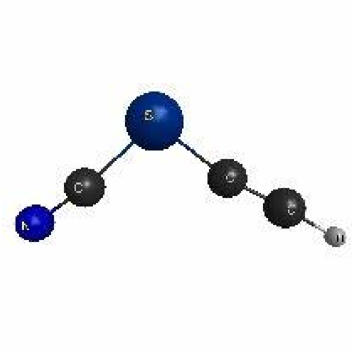
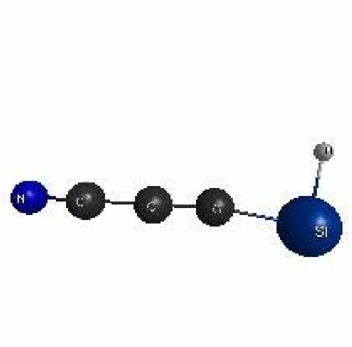
An astro-chemical species, C_3SiNH, is precisely investigated by using an ab initio method and the density functional theory. The bonding behavior for various structural isomers in various electronic states are scrutinized with the MP2 and B3LYP calculations. It turns out that the structural features of singlet state molecules are the linear, bent and three-membered ring structures. The energy differences among various singlet isomers are predicted to be within 50 kcal/mol. The triplet states lie at least about 20 kcal/mol above the singlet states. The electron affinities and proton affinities are also estimated in order to understand the first step of the mechanism growing up to much bigger molecular system. The electron affinities of all singlet isomers are computed to be within 50 kcal/mol, whereas the proton affinities are predicted to be about 150~200 kcal/mol.







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Fluorescent Optical Biosensor based on ZnO Nanoplates in Living Cells

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Fluorescent quantum dots of semiconductor such as CdSe and CdTe have intensively been explored due to their photo-stability and size-controllable tenability of colors as compared with organic fluorophores for medical diagnostics and therapies using various optical methods. However, these conventional fluorescent quantum dots are biohazards and aggregative, and their biological application is limited. Recently ZnO nanostructures have received considerable attention as new biosensor materials because they are biocompatible and nontoxic. They have been used to immobilize low IEP DNA or proteins by electrostatic interaction for the electrical biosensor because of their high isoelectric point (IEP)(9.5), but they have been little used as a direct fluorescent biosensor. This may be because the conventional ZnO nanostructures do not absorb visible light due to the large band gap energy (Eg=3.37 eV) corresponding to UV light energy which is toxic to biological molecules.Thus, in the present work, the visible light-sensitive single crystalline ZnO nanoplates are synthesized by sol-gel method through formation of liposome-ZnO nanocomposites with hydrothermal reaction and they were characterized by measurements of XRD, SEM, and TEM. The UV-Visible absorption spectra of the nanoplates were observed to exhibit high absorption of visible light from 400nm to 600nm as compared to that of ZnO nanoparticles. The confocal fluorescent images of living cells are measured with ZnO nanoplates upon visible light excitation at 410 nm. The ZnO nanoplates are observed to be effectively penetrated into the cells, exhibiting strong intracellular red emission. These results demonstrate that visible light-sensitive ZnO nanoplates are promising optical biosensor in vivo by visible light excitation.

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Thermodynamic Discrimination for Aggregation-Prone Protein by Water

정성호 함시현*

숙명여자대학교 화학과

The tendency of proteins to aggregate rather than to remain soluble has been a central problem to address in preventing protein aggregation diseases in human. What are the intrinsic molecular factors distinguishing aggregation-prone proteins from soluble ones in aqueous environments? Here we have identified "biomolecular hydrophobicity" defined by the solvation free energy of a protein as a major determinant of protein aggregation propensity through the structural and thermodynamic investigation on various mutants of amyloid-beta protein associated with Alzheimer's disease. A combination of extensive molecular dynamics simulations with the liquid integral-equation theory allows us to compute the solvation free energy of a protein, which properly takes into account protein structure as well as its hydration structure. From detailed analyses on factors contributing to the biomolecular hydrophobicity, a remarkable role of hydration structure discriminating positively charged residues from negatively charged ones on protein surface is clarified. We find that this originates from the modification of the orientational hydration structure at a long-distance regime by flanking charged residues on protein surface. Biomolecular hydrophobicity is also largely affected by protein conformational changes, such as salt-bridge formation between oppositely charged residues on protein surface, through the expulsion of hydration water at a short-distance regime. Our results provide a unique insight to the biomolecular hydrophobicity for predicting the protein aggregation propensity upon mutation in aqueous environments, and open a new avenue to design aggregation-resistant proteins as biotherapeutics.

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Conformational Entropy of Intrinsically Disordered Protein

정성호 함시현*

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Intrinsically disordered proteins (IDPs), though lacking stable tertiary structures, are known to possess certain amount of residual structure. Conformational disorder plays a crucial role through the conformational entropy in regulating protein-protein and protein-ligand interactions involved in signaling and regulation, and also modulates protein aggregation and amyloidogenesis associated with a number of human diseases. Yet, a direct and quantitative connection between the residual structure and the conformational entropy remains to be established. Here we show using a novel computational approach that the conformational entropy of amyloid-beta protein, an IDP whose aggregation is associated with Alzheimer's disease, is significantly correlated with the contents of residual helical structure, beta-sheet structure, and salt-bridge network. Identification of the thermodynamically significant residual structure is of fundamental importance for a comprehensive understanding of the relationship between the functional conformational disorder and the protein activity regulation, and will also serve the thermodynamic basis of the amyloid polymorphism.

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Accurate rotamer population in exposed residues of protein L determined using statistical torsion angle potential (STAP)

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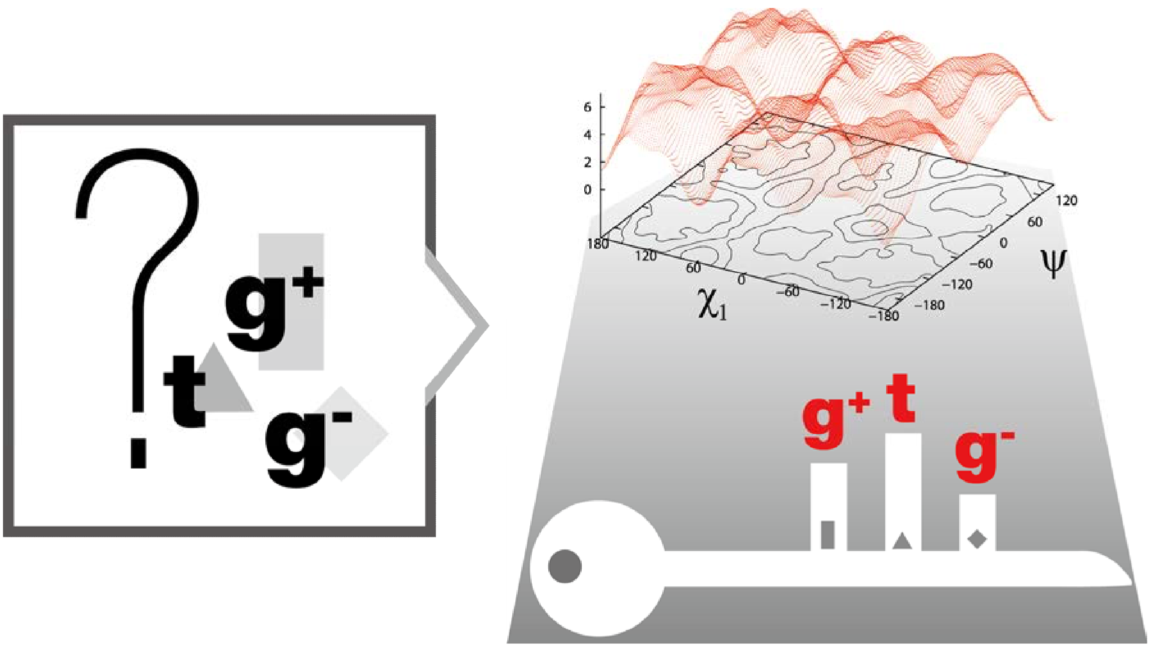
한국생명공학연구원 생명정보센터

Accurate prediction of the rotamer population is crucial to understanding protein-protein and protein-ligand interactions in biological systems. The rotamer population is associated with side-chain conformational entropy, and the conformational entropy can be evaluated on the basis of the methyl- and methylene order parameter (C_β-C_γ) or the dipolar coupling (C_β-H_β) determined through Nuclear Magnetic Resonance (NMR) experiments. In this study, the prediction of three χ_1 rotamer populations is performed for 11 exposed residues of the B1 immunoglobulin binding domain in peptostreptococcal protein L (PDB ID: 1HZ6). The protein L is a challenging target because theoretical studies of this protein rarely produced any satisfactory results. We used the newly developed Statistical Torsion Angle Potential (STAP) to predict three populations. Compared with Clore's Torsion Angle DataBase Potential (TADBP), the STAP yields a smaller average root-mean-square deviation (RMSdev) of the three populations and better correlations with experimental results for the residue-wise conformational entropy and order parameter. This study demonstrates that computational analysis with well-defined knowledge-based potentials can be used to characterize the χ_1 conformation of exposed residues. The results of these computational studies may help us understand side-chain motion with high precision.


?
t
g⁺
g⁻
6
4
2
0
180
120
60
0
−60
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χ1
120
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−180
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g⁺
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Elucidating the Molecular Origin of Hydrolysis Energy of Pyrophosphate in Water

홍주연 함시현*

숙명여자대학교 화학과

The molecular origin of the energy produced by the ATP hydrolysis has been one of the long-standing fundamental issues. A classical view is that the negative hydrolysis free energy of ATP originates from intramolecular e?ects connected with the backbone P?O bond, so called “high-energy bond”. On the other hand, it has also been recognized that solvation e?ects are essential in determining the hydrolysis free energy. Here, using the 3D-RISM-SCF (three-dimensional reference interaction site model self consistent ?eld) theory that integrates the ab initio quantum chemistry method and the statistical mechanical theory of liquids, we investigate the molecular origin of hydrolysis free energy of pyrophosphate, an ATP analogue, in water. We demonstrate that our theory quantitatively reproduces the experimental results without the use of empirical parameters. We clarify the crucial role of water in converting the hydrolysis free energy in the gas phase determined solely by intramolecular e?ects, which ranges from endothermic, thermoneutral, to highly exothermic depending on the charged state of pyrophosphate, into moderately exothermic in the aqueous phase irrespective of the charged state as observed in experimental data. We elucidate that this is brought about by di?erent natures of solute?water interactions depending on the charged state of solute species: the hydration free energy of low-charged state is mainly subjected to short-range hydrogen-bonds, while that of high-charged state is dominated by long-range electrostatic interactions. We thus provide unambiguous evidence onthe critical role of water in determining the ATP hydrolysis free energy.

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Improving PEC Efficiency of Hematite Thin Film for Water Splitting

강명종 강영수*

서강대학교 화학과

DA (Deposition and Annealing) method is one of the facile methods for synthesizing hematite thin film. To improve photoelectrochemical (PEC) efficiency of hematite film synthesized by this method, thin silica layer has inserted between fluorine doped tin oxide (FTO) coated glass substrate and hematite layer. The determination of the efficiency has been performed in several ways. IPCE (Incident Photon to Current conversion Efficiency), EIS (Electrochemical Impedance Spectroscopy) and photocurrent density has measured for it.

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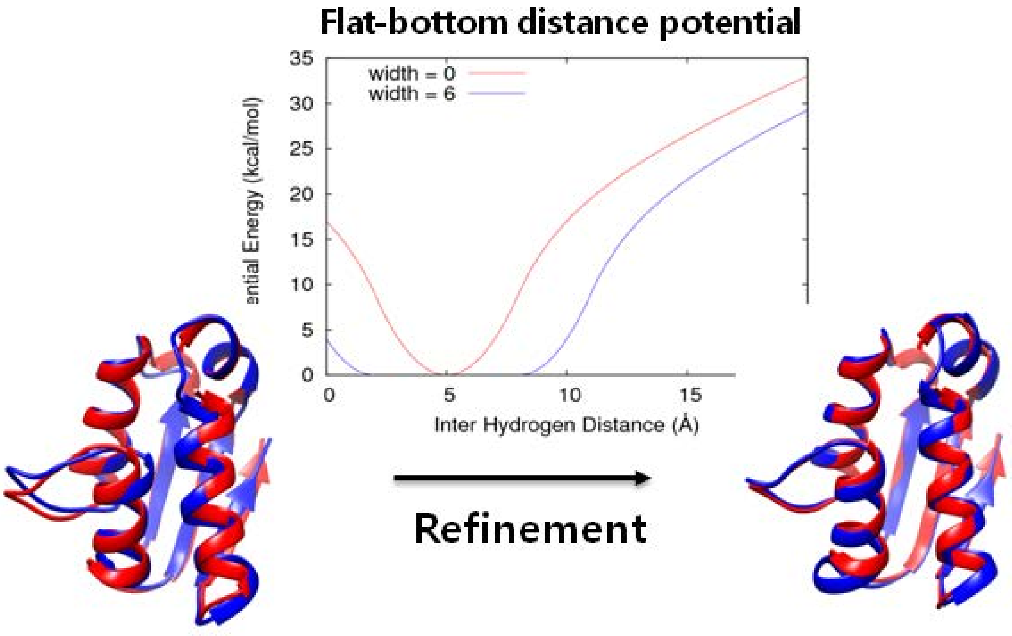
NMR structure refinement using flat-bottom distance potential and STAP

유효정 지선영[1] 이진혁[1]

한국생명공학연구원 유전체의학연구센터 [1]한국생명공학연구원 생명정보센터

In this study, simulated annealing methods with two developed energy potentials, flat-bottom distance potential and statistical torsion angle potential (STAP) is used to refine NMR structures in Protein Data Bank (PDB). One of test sets consists of 396 NMR structures and is used to optimize “width” parameter in the flat-bottom distance potential functions. Based on 12 quality assessment scores (TM-score, NOE distance violation, protein-like scores, and etc.) of the refined structures, we evaluated the generated structures and compared them with the original NMR structures. From that, we found the optimal width of 6.0 indicating that the developed structures has higher total evaluation score, weight averaged score in 12 quality assessment scores . Another test set is a validation set and is consisted of 108 NMR structures, coexisting in X-ray structures. We refined 108 structures with the optimal width of 6.0. Our refinement protocol provided us with improved quality scores (TM-score, protein-like scores, and etc) except NOE distance violation.


Flat-bottom distance potential
width = 0
width = 6
ential Energy (kcal/mol)
35
30
25
20
15
10
5
0
0
5
10
15
Inter Hydrogen Distance (Å)
Refinement

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Photoexcitation Dynamics of the Anionic Ligand Complexes of the Heme Proteins Probed by Time-resolved Vibrational Spectroscopy

박성철 박재홍 임만호*

부산대학교 화학과

The dynamics of the anionic ligand, NCO^- and NCS^- complexes of the heme proteins such as hemoglobin and myoglobin upon Q-band excitation has been investigated by femtosecond time-resolved vibrational spectroscopy. After Q-band excitation of the NCO^- complexes, the transient spectrum shows a bleach in the stretching band of OCN near 2160 cm^{-1} and a red-shifted new absorption. The red-shifted absorption band increases with a time constant of 0.5－0.8 ps and decays with a time constant of 5－7 ps. The absorption is initially broad but narrows while shifting toward the fundamental band. The time-resolved spectra on the NCS^- complexes also display a bleach in the stretching mode of SCN near 2010 cm^{-1} and two new absorption bands. One absorption is at lower energy than the fundamental band and the other absorption is at higher energy. The absorption band at lower energy increases with a time constant of 1－2 ps and decays with a time constant of 8－10 ps, which is a similar to the behavior of the new absorption in NCO^--bound heme complexes. The absorption band at higher energy decays with a life time of 1－2ps and its extinction coefficient is about 3 times weaker than that of the bleach signal. The red-shifted new absorption can be attributed to a thermally excited fundamental band that evolves as the molecule thermally relaxes. The blue-shifted absorption at the SCN^- complexes is attributed to the CN mode in an electronically excited state where the CN bond is weakened with a lowered extinction coefficient. Evidently, NCO^- and NCS^- bound heme complexes are photostable upon Q-band excitation and they rapidly relaxes toward the ground state without photodeligation.

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Carrier Mobilities of Semiconductor Quantum Dot Arrays

최완 심은지*

연세대학교 화학과

We investigated carrier mobilities of semiconductor quantum dot(QD) arrays with respect to the properties of QDs and capping ligands. On account of recent development in granular electronic material for potential applications in electronic and optoelectronic devices, it has become critical to understand electronic properties of QD arrays. In particular, synthesis and size regulation of QDs led to focus on understanding the transport and optical properties of these arrays. Experimentally, as the size of its individual dot becomes larger, the carrier mobility has been known to increase. However, in a recent experiment, the electron mobility of PbSe showed non-monotonic trend with respect to QD diameter. In this work, QD size dependent trend of the carrier mobilities is investigated using the on-the-fly filtered propagator functional path integral method, which evaluates time-evolution of the density matrix to extract charge transfer rates and carrier mobilities. We discuss various factors that define the crossover QD diameter where the carrier mobility reaches its maximum.

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Single-molecule fluorescence study for the effects of DNA methylation on the binding and dissociation kinetics of restriction endonuclease and DNA

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서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

DNA methylation plays a crucial role in epigenetic gene regulation, which in turn affects cellular development and differentiation. To understand DNA methylation at the molecular level, we investigated the effects of DNA methylation on DNA-protein interaction by single-molecule fluorescence assay. We measured the association and dissociation rates of native vs. methylated DNA and type II restriction endonuclease, and found that DNA methylation hinders the interaction between DNA and protein. In addition, we observed that restriction endonuclease exhibits signs of dimeric binding and dissociation with native DNA but not with methylated DNA, which may lead to molecular understanding of the mechanism of epigenetic gene regulation.

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Spontaneous Nanotubule Formation based on Frustrated-Aggregate Assembly

한민우 현정인 심은지*

연세대학교 화학과

The driving force of spontaneous sheet-to-tubule transformation phenomena is investigated by introducing the frustrated aggregate rearrangement model. Building blocks assemble into aggregates due to non-directional and non-specific intermolecular interactions such as stacking or amphiphilicity and often, subsequently, rearrange within the aggregate to attain ordered and free energy minimized equilibrium structures. Such rearrangements may require a large amount of energy to overcome kinetically trapped barriers for structurally inhomogeneous building blocks. In particular, for building blocks that include rigid segments and intermolecular H-bonding sites, not all molecules have the right orientation for H-bonds within the initial aggregates. When molecules form two-dimensional sheet structures, such partial H-bond fractions lead to an overall anisotropic sheet that undergoes spontaneous transformation into curved structures including nanotubules. By using molecular dynamics and density functional theory approach, we have confirmed that inhibition of the directional H-bonds owing to the rigid moiety is the key to form spontaneous curvature. Controlling internal cavity of tubule may also be possible by the regulation of H-bond fractions.

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Membrane Penetration and Translocation of Nanoparticles

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연세대학교 화학과

Understanding interactions between nanoparticles and lipid bilayer membranes is of great importance due to the potential applications in bio-nanotechnology such as drug deliveries, carrying genes, and utilization of integral membrane proteins. To investigate the dynamics of nanoparticle penetration and translocation into membranes, we performed dissipative particle dynamics simulations which use simple and intuitive coarse-grained models yet effectively describe hydrodynamic interactions in cell environment. We discuss the influence of the shape and the volume of nanoparticles as well as the properties of membranes including large membrane-embedded proteins that are found to significantly affect orientation of nanoparticles within membranes and, in turn, the minimum force required to translocate nanoparticles.

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Controlled and Reversible Transformations of Helices and Nanotubules based on Heterosurface Nanosheets

현정인 한민우 심은지*

연세대학교 화학과

Higher-order chiral structures such as helices and twisted ribbons are of enormous interests for their wide area of applications, however, fabrication and characteristics of such structures have not been fully understood. In particular, most of helices and twisted ribbons are metastable and can be formed only at certain conditions. In this work, we introduce a novel scheme to construct stable helices and nanotubules. Using dissipative particle dynamics simulations, we show that the design and control of the helical morphology such as radii and pitch angles are possible utilizing heterosurface nanosheets by manipulating surface grafts. We also present that, while the structures can be kept stable at a given condition, controlled and reversible transformation from a helix to a nanotubule can also be induced by external stimuli such as temperature and solvent compositions.

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Self-Assembly and Conformational Changes of Surface Grafted Nanocomposites

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연세대학교 화학과

We investigate self-assembly of surface grafted nanoparticles and their spontaneous structural transformations induced by external stimuli such as pressure, temperature, and solvent compositions. Brownian dynamics simulations show that coarse-grained nanoparticles can be designed to assemble into rectangular three-dimensional network structures which have various pore sizes. It was also found that, while maintaining three-dimensional network structures, the size and shape of pores can be varied depending on the external pressure due to the balance between surface graft's free volume (entropic effect) and nanoparticle's aggregation (enthalpic effect). Also the three-dimensional network structure can be transformed into two-dimensional nets or one-dimensional columns when solvent composition is varied. Self-assembly mechanisms as well as characteristics of structural changes are presented.

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Time-Gated Pre-Resonant Femtosecond Stimulated Raman Spectroscopy of DTTC Iodide

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한국화학연구원 나노기술융합연구단 [1]국민대학교 생명나노화학과 [2]대구경북과학기술원 (DGIST) 나노바이오연구부

We present time-gated femtosecond stimulated Raman spectroscopy (fSRS) in the pre-resonance Raman condition; a “pseudo emission-free” condition was achieved when we delivered the probe beam ahead of the pump beam. Regeneratively amplified pulse trains were employed to create an angle-geometry (non-collimated) mixing between the pump and probe beams, leading to the highly sensitive measurement of the stimulated Raman gain of 3,3′-diethylthiatricarbocyanine (DTTC) iodide molecules. Time-integration spectroscopy allowed for increased quantitative distinction of the contribution of the stimulated Raman scattering from the stimulated emission (STE). We successfully obtained a highly sensitive (S/N > 100) stimulated Raman spectrum under the optimized conditions, which was critically reviewed by two-dimensional correlation spectroscopy (2DCOS) methods. Given the optical pre-resonance of ~0.1 eV, the background signals that mostly originated from the stimulated emissions of excited electrons were significantly reduced by mismatching the pump-probe overlap, resulting in the acquisition of a genuine fSRS spectral profile when the temporal distance between two beams corresponded to ~0.2 ps.

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Modeling study of Human Smoothened Homolog SMOH using GALAXY

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서울대학교 화학부

G protein-coupled receptors (GPCRs) constitute a large membrane protein family related to various cellular signaling processes. Therefore, structures of GPCRs provide crucial information for understanding and regulating those cellular processes. However, only a limited number of GPCR structures of unique sequences have been determined by experimental methods, and all of them belong to class A. In this presentation, we report our recent trial to predict the structure of human smoothened homolog (SMOH), a GPCR Dock 2013 target. SMOH belongs to class F and shows a large sequence difference from class A GPCR proteins in transmembrane helices 6 and 7. Transmembrane helices 1~5 were modeled based on class A GPCR structures by homology modeling, and transmembrane helices 6 and 7 and loops connecting the helices were modeled by ab initio prediction methods based on our own structure refinement method. Loop modeling and structure refinement by repeated perturbation and relaxation were tried. Two antagonist ligands provided in the GPCR Dock 2013 experiment were docked to the predicted GPCR structures to provide information on important molecular interactions for ligand binding.

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Kinetic Analysis of 4-(Methylthio)benzoyl Chloride in Usual Solvolytic Conditions

박경호 경진범* **Dennis N. Kevill[1]**

한양대학교 과학기술대학 응용화학과 [1]Northern Illinois University, U. S. A.

The solvolysis study of 4-(methylthio)benzoyl chloride was performed in usual conditions, 25.0 oC, pure and hydroxylic binary solvents, and the conductivity method. Rate constants were analyzed by Grunwald-Winstein equations and compared with other benzoyl chlorides. Like 4-methoxybenzoyl chloride, the reaction of 4-(methylthio)benzoyl chloride was showed similar aspects, unimolecular characters, because para-substituent, 4-methylthio group has a resonance effect, then the results were compared with previous study of 4-methoxybenzoyl chloride primarily. There were supported by additional results of kinetic solvent isotope effect and thermodynamic parameters.

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Amyloid fibril structure를 형성하는 활성 peptide oligomer와 비활성 peptide oligomer의 질량분석실험을 통한 구조 연구

이은숙 김수아 김영주[1] 김호태

금오공과대학교 응용화학과 [1]금오공과대학교 응용화학

당뇨병, 알츠하이머병들을 유발하는 활성 peptide oligomer 들은 amyloid fibril structure 을 형성한다고 알려져 있다. 본 연구는 non-fibril 형태인 YGGFL 과 amyloid fibril 을 형성하는 것으로 알려진 6 개의 아미노산으로 구성된 oligomer 들을 질량분석실험으로 fragment pattern 을 분석하였다. 분석을 통해 6 개의 아미노산으로 구성된 oligomer 의 초기 stacking structure 을 알아보는 시도를 하였다. ESI Mass Spectrometer 을 이용하여 6 개의 아미노산으로 구성된 oligomer 의 MS 실험과 MS/MS 실험을 진행하였다. Gaussian program 을 이용하여 각 oligomer 의 optimize 된 structure 를 만들고, 각 구조의 energy 를 계산하였다. 계산결과와 실험결과를 비교하여 적합한 초기구조를 찾는 시도를 하였다.

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Modeling of loops in G-protein-coupled receptors using geometric constraints

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서울대학교 화학부

Protein loops are often involved in biological functions. Therefore, understanding their structures and relevance to function has been a critical issue. Especially, studies to unveil the role of intra- and extracellular loops in G-protein-coupled receptors (GPCR) have been ongoing with deep interest. The GPCR loops are currently known to be important for ligand recognition, receptor activation and furthermore to interaction with G-proteins. Therefore, the full knowledge regarding the structures of these loops is necessary since they can provide information not only to the whole three-dimensional structure of the receptor but also to the mechanism of signal transduction. However, accurate loop modeling to predict loop conformations has always been challenging since the loop regions are highly variable. Even for a family like GPCR within which the sequences are highly conserved, the loops, unlike the trans-membrane helices, show low sequence similarity yielding diverse conformations. This makes an ab initio loop modeling method compulsory since the widely used homology modeling method can't be applied to loop regions when they lack homologous sequences.In this work, we present recent results of applying our ab initio loop modeling method to reconstruct intra- and extracellular loops in GPCRs with known 3D structure. For some targets, while reconstructing the intracellular loop, we checked whether our method is capable of discriminating different receptor states: whether modeling the same sequence in receptor environments with different activity gives different conformations. In addition, we introduce a new loop modeling method for modeling the second extracellular loops and show its promising results.

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Synthesis and Characterization of coated Iron Oxide for cancer cell separation

김초롱 김성준 **Badrul Alam Bony Xu Wenlong tirusew tegafaw** 이강호* **Md. Wasi Ahmad**

경북대학교 화학과

암에 대해 관심이 깊어져 오면서 암세포를 tageting 하는 기술에 대한 연구가 활발히 진행되고 있다. 이 포스터는 Folate receptor 를 가진 암세포를 tageting 하기 위해 Iron Oxide 를 합성하고, 표면에 펩타이드를 코팅하는 방법을 나타낸다. Iron Oxide 는 크기에 따라 magnetism 이 다르기 때문에 3nm, 40nm, 200nm 크기로 합성하여 결과를 확인하였다. 코팅을 하기 위해 사용된 Iron Oxide 나노입자의 크기는 200nm 이고, 그 표면을 folic acid, D-glucuronic acid 로 코팅하였다. 이를 확인하기 위해 HRTEM, XRD, FT-IR 과 SQUID magnetometer 을 사용하였다. 세포분리실험을 위해서는 샘플의 농도를 ICP 로 측정하였다.

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APTES-modified Porphyrin-bound ZnO nanowires toward phototheragnosis : Optical properties

최선영 윤민중*

충남대학교 화학과

To develop phototheragnosis agent for cancer cell, protoporphyrin ix-bound ZnO nanowires(NWs) were synthesized by hydrothermal method, their surfaces were modified with APTES(3-Aminopropyltriethoxysilane), followed by characterization with measurements of XRD patterns, SEM and TEM images. Their diffuse-reflectance UV-Visible absorption spectra were observed to exhibit a porphyrin absoption bands at 410nm(soret band) and 550~580nm(Q-band) which are red-shifted from those of free porphyrin, indicating that porphyrin is bound with ZnO NWs. The photoluminescence(PL) spectra of porphyrin-bound ZnO NWs were measured upon excitation with 405nm and observed to exhibit red emission(580~630nm) from porphyrin as well as green emission(464nm) from ZnO NWs. The porphyrin red emission was observed to be quenched upon additional binding with APTES, while the ZnO NWs green emission was unaffected. The fluorescence decay time of the APTES-porphyrin-ZnO NWs was exhibited 1.2ns which is two times longer than that of porphyrin-bound ZnO NWs. These results indicate that the APTES-porphyrin- ZnO NWs could generate more $^1O_2$ and they can be promising phototheragnosis agent for the cancer cell.

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Synthesis of Regular and Size Regulated Ultrasmall Lanthanide Oxide Nanoparticles for MRI Contrast Agent

김성준 김초롱 이강호* **Xu Wenlong Badrul Alam Bony tirusew tegafaw Md. Wasi Ahmad**

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The synthesis of Lanthanide nanoparticles regulated size has long been an interest of scientific and technological. In case of MRI contrast agent, Particle size affects contrast improvement due to different magnetization(?) of nanoparticles. This reports an easy and simple synthesis of Lanthanide nanoparticles under the presence of stabilizing surfactant, oleylamine and oleylalcohol. They were coated and characterized them with MPXRD, HRTEM, FT-IR, TGA and MRI instrument.

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Spectroscopic Study on Size-dependent Ring-symmetry Manifestation in Acetylene Bridged Macrocyclic Oligothiophene Oligomers

박규형 김동호*

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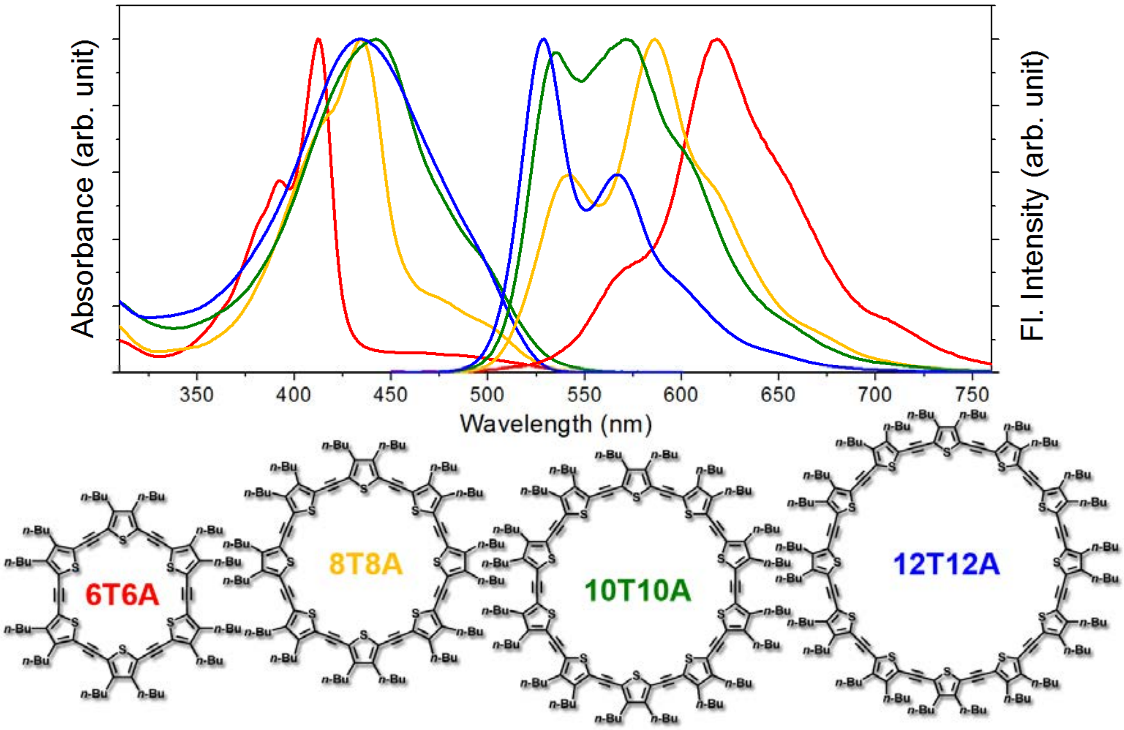
Functional oligothiophenes have attracted great interest in the field of material science as active components in organic electronic devices and molecular electronics. However, linear oligothiophenes synthesized so far have undesired perturbing end effects which downgrade their functionalities. To circumvent this problem, size- and shape-persistent macrocyclic oligothiophenes have been developed recently. These macrocycles, in comparison to linear oligomers and polymers, are benefited from their well-defined structures and infinite defect free π-conjugated chains free of unwanted end effects.Herein, we present photophysical properties of a series of macrocyclic oligothiophenes, *nTnA* (*n* = 6, 8, 10, and 12), in which 2,5-thienylenes are linked by acetylene spacers. Absorption spectra of *nTnA* show a broad peak centered around 500 nm which is gradually intensified with increasing ring size, in conjunction with vibronic peak ratio change of the emission peaks. This spectral behavior can successfully be described by breakage of ideal ring-symmetrized system and concomitant oscillator strength redistribution. Size-dependent excited state dynamics of nTnA were also confirmed using femtosecond transient absorption spectroscopy and DFT calculations.


Absorbance (arb. unit)
Fl. Intensity (arb. unit)
350
400
450
500
550
600
650
700
750
Wavelength (nm)
6T6A
8T8A
10T10A
12T12A
n-Bu
S

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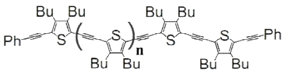
Relationship Between Exciton Delocalization and Excited-State Conformational Dynamics in Linear and Cyclic π-Conjugated Oligothiophenes

김표상 김동호*

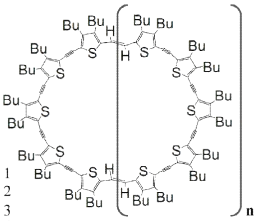
연세대학교 화학과

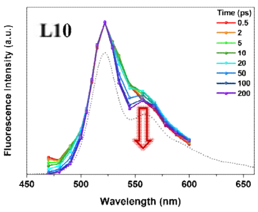
Understanding the complex nature of charge and energy transfer is an essential component in designing and optimizing the rich array of organic electronic devices. However, organic semiconductors fundamentally differ from their inorganic counterparts by having a significantly stronger electron-phonon coupling. In this regard, we have investigated the influence of nuclear geometric relaxation on the extent of the excited-state electronic delocalization in π-conjugated linear and cyclic oligothiophenes using methods of femtosecond time-resolved fluorescence upconversion. Anisotropy measurements show that light absorption generates an excited state is initially strongly delocalized along the oligothiophene but contracts rapidly following vibrational relaxation of the nuclei along C-C stretch coordinates on the subpicosecond time scales. We also demonstrate that interporphyrin torsional relaxation leads to a subsequent increase in the excited-state electronic delocalization on a relatively longer time scale (~30ps). These results therefore indicate that, following excitation, the initially highly delocalized excited-state first contracts and then expand again along the conjugated backbone in accordance with the time periods for the vibrational modes coupled to the electronic transition.

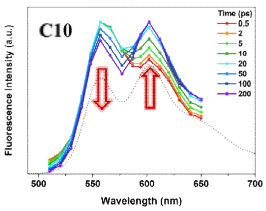


L4 : n = 1
L6 : n = 3
L10 : n = 7

C10 : n = 1
C15 : n = 2
C20 : n = 3
C25 : n = 4
C30 : n = 5







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Mn^{2+} doped Gd$_2$O$_3$ nanoparticles: MRI contrast agent.

<u>Badrul Alam Bony</u> Xu Wenlong tirusew tegafaw 김초롱 김성준 Md. Wasi Ahmad 이강호[*]

경북대학교 화학과

Gd_2O_3 nanoparticle is a well known candidate for magnetic resonance imaging (MRI) contrast agents which shows significant r_1 value. However, doped or mixed Gd_2O_3 nanoparticles show better contrast than individual one. In this work, we synthesized Mn^{2+} doped Gd_2O_3 nanoparticles which can be worked for both T_1 and T_2 MRI contrast agent. Moreover, to minimize the toxicity, biocompatible and hydrophilic D-glucuronic acid is used to coat the Mn^{2+}- Gd_2O_3 nanoparticles. The nanoparticles were characterized by XRD, HRTEM, FTIR, MPMS, TGA and MRI instruments. D-glucuronic acid coated Mn^{2+} doped Gd_2O_3 nanoparticles exhibit a relaxivity value of r_1 = 13.40 mM^{-1}s^{-1} and r_2 = 70.31 mM^{-1}s^{-1}; respectively.

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Synthesis of PEI Coated Iron Nanoparticles

tirusew tegafaw Xu Wenlong Badrul Alam Bony 김초롱 김성준 **Md. Wasi Ahmad** 이강호*

경북대학교 화학과

Iron is one of the most abundant and widely used elements on earth. Iron nanoparticles have a huge potential for different applications including magnetic fluids, catalysts for carbon nanotube formation, magnetic resonance imaging (MRI) contrast agents, and nickel-iron batteries. In this work, iron nanoparticles were synthesized by a chemical reduction method from iron chloride hydrate. Sodium borohydride was used as the reducing agent. Water-soluble iron nanoparticles with average diameters that range from 20-30 nm were synthesized and coated with PEI. They were characterized with XRD, HRTEM, FT-IR, PL spectrometer, TGA, confocal laser scanning microscope and SQUID magnetometer.

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Ultrasmall mixed dysprosium-europium oxide nanoparticles and holmium-europium oxide nanoparticles for dual imaging agent

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A multiple imaging is a seductive subject in molecular imaging. D-glucuronic acid coated ultrasmall mixed dysprosium-europium oxide (DyxEuyO3, x:y = 4:1) nanoparticles and holmium-europium oxide(HoxEuyO3, x:y = 4:1) nanoparticles were synthesized. They are water-soluble and biocompatible with an average hydrodynamic diameter of 5.18 nm and 4.69 nm respectively. We applied them for T2 MRI-FI in vitro and in vivo for the first time. They are non-toxic up to 500 μM Dy and 500 μM Ho as proved in cellular toxicity tests. They showed r2 of 82.5 and 81.8 s-1mM-1, respectively, and clear dose-dependent contrast changes in R2 map images. They showed negative contrast enhancements in 3 tesla T2 MR images of a mouse, and fluorescent confocal images in DU145 cells. These results clearly prove the T2 MRI-FI multi-functionality of D-glucuronic acid coated ultrasmall mixed dysprosium- europium oxide nanoparticles and holmium-europium oxide nanoparticles.

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Molecular Dynamics Simulations of the pH-induced Conformational Conversion of Human Prion Protein

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숙명여자대학교 화학과

Prion diseases are neurodegenerative disorders caused by misfolding of the cellular prion protein, PrPc, into the pathological scrapie form, PrPsc, which self-assembles and forms sporadic fibrils accumulating between neurons. Yet, the mechanism of this conversion towards the infectious misfolded conformation still remains unveiled. Acidic pH is known to trigger the conformational change that ultimately results in this conversion. Here, we carried out explicit-water molecular dynamics simulations of PrPc to investigate its conformational conversion at low pH. By further performing solvation thermodynamic analysis, we discuss thermodynamic consequences of such conformational transition.

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Using chemical shift information to improve protein homology models

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서울대학교 화학부

Homology modeling is a widely used method for predicting protein structures from amino acid sequences when homologous proteins of known structures are available. However, information from known structures may not be sufficient to provide models of atomic-level accuracy. In that case, additional use of available experimental data can assist improving the homology models. In this work, NMR chemical shifts are used to refine protein homology models. This approach can also accelerate the experimental structure determination processes because chemical shifts can be assigned relatively easily at the early stage. Difference between the chemical shifts assigned by experiments and those predicted from protein model structures were used as a restraint function which can drive relaxation of the model structures towards the native structures during molecular dynamics simulations. I will present meaningful results of this strategy in refining homology models covering a broad range of model quality. For starting models of relatively low accuracy, local parts with large errors can be detected using the chemical shift information and the detected regions can be sampled more diversely. In benchmark tests, the refined models showed comparable global structure accuracy and superior local structure accuracy compared to previous studies.

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Thiophene 유도체들의 기하학적 구조 및 안정성 연구

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경상대학교 화학교육과

염소원자로 치환된 terthiophene 과 bithiophene 유도체의 기하학적 구조를 HF 및 MP2 (6-31G**)수준에서 최적화하였다. 여러 가지 이성질체들의 상대적 에너지를 비교하여, 이들 유도체들의 안정성을 비교 분석하였다. Tetrachloro-terthiophene 유도체 중 cis-tetrachloro-2,3,7,12-terthiophene 이 가장 안정한 기하구조로 최적화 되었고, tetrachloro-bithiophene 유도체 중 tetracholoro-1,3,8,9-bithiophene 이 가장 안정하였다. Cis-tetrachloro-2,3,7,12-terthiophen 의 $R_{C4\text{-}C6}$ 는 1.450 Å 이고, $R_{C9\text{-}C11}$ 사이의 거리는 1.454 Å 이었다. 두 thiophene 사이의 이면각 $ø_{\angle S5CCS10}$ 는 79.3 °, 이면각 $ø_{\angle S5CCS10}$ 는 68.6 °로 나타나고, HOMO-LUMO 에너지 차이 10.3 eV 로 나타났다. Tetracholoro-1,3,8,9-bithiophene 의 $R_{C4\text{-}C6}$ 는 1.452 Å 이고, thiophene 사이의 이면각 $ø_{\angle S5CCS10}$ 는 131.9 °이었으며, HOMO-LUMO 에너지 차이 9.6 eV 로 나타났다.

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The Reaction of Pt/CNT Catalytic Oxidation for Removing VOCs

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원광대학교 생명나노화학부 [1]원광대학교 생명나노화학과 [2](주)바이오니아 분자생물적용팀 [3](주)바이오니아 [4]원광대학교 화학과

Catalytic oxidation of volatile organic compound such as benzene, toluene, ethylbenzene, and o-xylene (BTEX) over novel Pt/carbon nanotube (CNT) catalyst, fabricated by a molecular-level mixing method, was investigated at temperatures ranging from 40 to 150 °C. The surface composition of Pt/CNT catalyst were analyzed by EDS, XPS, SEM, TEM, and XRD. The breakthrough curves for multi-component mixtures show displacement effects, in which adsorbates with strong interaction force to displace weakly bounded substances in the course of competing adsorption. The catalytic oxidation was conducted with a BTEX concentration ranging from 100 to 500 ppmv in air at volume hour space velocity (VHSV) of approximately 7.5 ? 104 h^{-1} - 3.4 ? 105 h^{-1}. The complete oxidation was realized at temperatures as low as 115 ℃ with a 30 wt% Pt/CNT and the light-off curves were very steep. The catalyst was characterized by its unique hydrophobic property which facilitates the conversion of volatile organic compounds (VOCs) with high activity at relatively low temperatures unaffected by water vapor concentrations in the system.

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Characterization of S-nitrosyl hemoglobin in mid-IR.

이태곤 임만호

부산대학교 화학과

Nitrogen monoxide (NO) has been found to function as a physiological messenger regulating local responses of the cardiovascular, immune and neural systems. NO can bind to the hemes and cystein residues of hemoglobin (Hb), forming HbNO and HbSNO, respectively. It has been suggested that Hb functions as a NO transporter in addition to its function as an oxygen transporter. Recently we have observed two weak vibrational bands near 1770 cm^{-1}, which exhibits a ^{15}NO isotopic shift. They can be modeled with two Gaussian functions: one is centered at 1781 cm-1 with 11 cm^{-1} full width at half maximum (FWHM) and the other at 1755 cm^{-1} with 15 cm^{-1} FWHM. They likely arise from NO stretching modes of two geometrical isomers (syn and anti) of HbSNO. Using FT-IR spectroscopy of SD and NO stretching modes of the samples prepared by mixing various ratios of Hb and $NaNO_2$, a series of experiments are under progress to assign the bands and elucidate the mechanism of HbSNO formation. We will present the result and the implication of the assignment to the physiological role of Hb as

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PM3 and *Ab initio* Molecular Orbital Study on the Activity of Physiology for the Anthraquinones

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To investigate the activity of physiology for anthraquinones, we analyzed the quantum chemical indices for the R-anthraquinones(R=H, CH_3, C_2H_5, OCH_3, Cl) by calculation using the semiempirical PM3 methods. It was found that the electron is transferred from HOMO energy of guanine among DNA bases to LUMO enengy of capsaicinoids. It is appear that anthraquinones compound plays an important role in the formation of complex with guanine of DNA bases.

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Plasmon-Enhanced Fluorescence and Raman Spectroscopy with an optical nano-antenna tip functionalized by a single nanoparticle.

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고려대학교 화학과 [1]포항공과대학교 화학과

A single gold nanoparticle was attached at the tip apex through a mechanical pick-up and chemically grown using a single silver enhancing solution. The resulting tip is a Ag nanoparticle (diameter of 30-60 nm) attached at the apex of a Si-tip. The enhancement by this plasmon-resonant tip for the Raman scattering and fluorescence was investigated. The influence of the diameter of the tip on the enhancement was examined and compared with the classical electrodynamics simulation.

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Laser-induced nanoparticle rearrangements

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When nanoparticles such as fluorescent nanodiamonds, gold nanoparticles, and fluorescent silica beads were irradiated with a visible laser light at high power (> 1 mW), they were found to undergo remarkable geometrical rearrangements, often forming a doughnut shape in the lateral plane of the cover glass holding these nanoparticles. Various parameters affect the phenomenon, including laser power, irradiation time, mounting medium, etc. In particular, the absorbance of mounting medium plays a key role to initiate this process. Moreover, uncommon events were also observed, such as trapping, half sphere formation, and dual doughnut-formation, depending on the irradiation conditions.

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Intense near-infrared absorption of new tetrapyrrole derivatives: A DFT Study

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성균관대학교 화학과

The porphyrins and tetrapyrrole systems display characteristic Near-IR absorption bands with absorption peaks in the vicinity of 1000 nm in terms of monomer, leading to potential applications in dye-sensitized solar cells and organic solar antenna collector systems, but the infrared (NIR) light absorptive capacity is limited. Here, in order to achieve higher efficiency in solar energy absorption (from 300 nm to 2500 nm region), we performed structure-based molecular design of new materials ((tetrapyreneylporphyrin (TpyP)) based on porphyrins studied by DFT (B3LYP) and TD-DFT methods. In addition, the attractive feature of TpyP is the tunability of their electronic properties and steric effects by substituting of the electron-withdrawing groups (such as -F) and electron-donating groups (such as -NH2) at the peripheral positions (R1, R2, R3) of the four pyrene rings. In particular, the molecules having electron-donating substituents at R1 and R3 positions have large red/blue-shift effects on NIR-2 (region-III) due to the interplay between the peripheral π-electron aromatic conjugation system and 18π-electron porphyrin core conjugation system. Furthermore, we also investigated the effect of the metal insertion into the center of the porphyrins. In this work, we found that these new materials can absorb light in the range from UV to NIR region (300 to 2400 nm) with high molar extinction coefficient and the light harvesting efficiency of new material can be up to 100% for light in the region of 300 to 2400 nm.

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The Study of Magnetized Water using Infrared Absorption Spectrum

이성현 전상일*

강릉원주대학교 화학과

자화수(magnetized water)는 원래 물분자가 자화 되어서 자기장의 특성을 갖는다는 의미가 아니라, 자기장에 의하여 물분자 배열이 바뀌어져서 특이한 물의 특성을 보이는 상태를 의미한다. 자화수는 물 분자가 더 조밀하게 구조화되어 작은 cluster 들을 많이 형성함으로써 반응성 및 용해도가 증가됨을 보인다. 액체나 기체상태의 물질은 각각의 물질에 특유한 파장의 적외선을 강하게 흡수한다. 이 흡수스펙트럼을 조사하여 물질의 화학적 조성·반응과정·분자구조를 정밀히 추정하는 수단으로 쓰는데, 이것을 적외선분광법이라 한다. 본 연구에서는 적외선분광법을 사용하여 물 분자의 신축진동(stretching)과 굽힘진동(bending) 및 결합진동(combination)등을 측정하고, 이것을 자화수에 적용하여, 자기장에 의해 만들어진 자화수의 물 구조 변화를 확인하고자 한다. 자기장의 노출 시간에 따른 물 구조 변화 역시 적외선 분광법을 사용하여 살펴보아, 전에 우리 실험실에서 행해진 다른 실험 결과와 비교 분석한다.

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Semi-empirical simulation of rotational absorption spectra of isotopic formaldehyde molecules

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In nature, carbon (C) has two kinds of stable isotopes, ^{12}C and ^{13}C, with abundances of 98.85% and 1.11%, respectively. And oxygen (O) has three kinds of stable isotopes, ^{16}O, ^{17}O, and ^{18}O with 99.759%, 0.037%, and 0.204%, respectively. Among these carbon and oxygen isotopes, ^{12}C, ^{13}C, ^{17}O, and ^{18}O isotopes are very useful in semiconductor and medical industries.Stable isotope separation (SIS) is a process of enriching these useful isotopes out of isotopic mixtures. There are several methods to enrich a specific isotope. The MLIS (Molecular Laser Isotope Separation) is one of the promising isotope separation method. When a target molecule (useful isotope) absorbs a photon, the molecule gets ionized or dissociates to some fragments. Each isotopic molecule has its specific absorption lines, so information about absorption lines of useful isotopic molecule is extremely important in MLIS process.In general, absorption lines of isotopic molecule are complicated and obtained by absorption experiment. But in the case of low abundant isotopic molecule, semi-empirical simulation plays an important role because it is not easy to get such an absorption spectrum by experiment in a wide spectral range.In this paper, simulation of rotational absorption spectra of isotopic formaldehydes was implemented by employing scaling factors. A, B, and C values of $H^{12}CH^{16}O$, $H^{13}CH^{16}O$ and $D^{12}CH^{16}O$ were calculated by using TURBOMOLE package and its values were compared to the previous reference values. And then scaling factors were employed to simulate absorption spectra of other isotopic formaldehyde, for example, $H^{12}CH^{18}O$.Accuracy and usefulness of this semi-empirical simulation will be confirmed by the comparative study with experimentally observed absorption spectra.

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Correlation of the rates of solvolysis 2-adamantyl fluorothioformate under solvolytic conditions

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한양대학교 응용화학과 [1]한양대학교 과학기술대학 응용화학과

A solvolytic study of 2-adamantyl fluorothioformate (2-AdSCOF, 1) was performed as a extended research of 2-adamantyl chlorothioformate (2-AdSCOCl, 2). The specific rates of solvolysis of 2-adamantyl fluorothioformate (2-AdSCOF, 1) have been measured at 25.0^{o}C in pure and binary solvents. The results gave the satisfactory correlation over the full range of solvents when the analysis was calculated by the extended Grunwald-Winstein equation, $\log (k/k_o) = lN_T + mY_{Cl} + c$, with incorporation of the solvent nucleophilicity and the solvent ionizing power. Additional supplements were conducted, solvent isotope effect for methanolysis and activation parameter for five representative solvents. The results are compared with those reported previously of 2-adamantyl chloroformate (2-AdOCOCl), 2-adamantyl fluoroformate (2-AdOCOF), and alkyl chlorothioformate esters.

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Quantitative reproducibility of mass spectra in matrix-assisted laser desorption ionization and unravelling of the mechanism for gas-phase peptide ion formation

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In a previous study on matrix-assisted laser desorption ionization (MALDI) of peptides using α-cyano-4-hydroxycinnamic acid (CHCA) as matrix, we found that the patterns of single-shot spectra obtained under different experimental conditions became similar upon temperature selection. In this paper, we report that absolute ion abundances are also similar in temperature-selected MALDI spectra, even when laser fluence is varied. The result that has been obtained using CHCA and 2,5-dihydroxybenzoic acid (DHB) as matrices is in disagreement with the hypothesis of laser-induced ionization of matrix as the mechanism for primary ion formation in MALDI. We also report that the total number of ions in such a spectrum is unaffected by the identity, concentration, and number of analytes, i.e. it is the same as that in the spectrum of pure matrix. We propose that the generation of gas-phase ions in MALDI can be explained in terms of two thermal reactions, i.e. the autoprotolysis of matrix molecules and the matrix-to-analyte proton transfer, both of which are in quasi-equilibrium in the early matrix plume.

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A Simple Method for Quantification of Peptides and Proteins by Matrix-Assisted Laser Desorption Ionization Mass Spectrometry

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Even though matrix-assisted laser desorption ionization (MALDI) is a powerful technique for mass spectrometry of peptides and proteins, it is not quite useful for their quantification that is one of the outstanding problems in quantitative proteomics. The main difficulty lies in the poor reproducibility of MALDI spectra. In this work, a simple method to circumvent this problem has been developed. Themethod is based on a previous observation that the reaction quotient for the matrix-to-peptide proton transfer evaluated in temperature-selected MALDI was nearly constant regardless of the peptide concentration in the solid sample. This implied a direct proportionality between the relative abundance of an analyte ion in a temperature-selected MALDI spectrum and the concentration of the corresponding neutral in the solid sample. This relation has been confirmed by calibration curves obtained for some peptides. Another characteristic of the relation is that it holds even when other analytes are present. This has been demonstrated for mixtures containing peptides and proteins. This and the fact that the method does not require the addition of internal standards allow rapid and inexpensive quantification of any analyte amenable to MALDI.

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Iodine Coated Gadolinium Oxide Nanoparticles as T1 and T2 Magnetic Resonance Imaging (MRI)

Md. Wasi Ahmad **Badrul Alam Bony Xu Wenlong** 김초롱 **tirusew tegafaw** 김성준 이강호*

경북대학교 화학과

Magnetic resonance imaging (MRI) is widely used in modern clinical medicine as a diagnostic tool, and provides noninvasive and three-dimensional visualization of biological phenomena in living organisms with high spatial and temporal resolution. The surface modified Gd_2O_3 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. Therefore, considerable attention has been paid to magnetic nanoparticles as MRI contrast agents with efficient targeting ability and cellular internalization ability, which make it possible to offer higher contrast and information-rich images for detection of disease.In this study, the coating of iodine compound on the surface of Gd_2O_3 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 Gd_2O_3, forming a protective layer on the nanoparticles. The relaxometric properties, cytotoxicity and the MRI signal of iodine coated Gd_2O_3 nanoparticles were examined.

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Reproducibility of temperature-selected mass spectra in matrix-assisted laser desorption ionization of peptides

배용진 박경만[1] 안성희[2] 김명수

서울대학교 화학부 [1]서울대학교 화학과 [2]서울대학교 자연과학대학 화학부

Matrix-assisted laser desorption ionization of peptides was investigated using α-cyano-4-hydroxycinnamic acid as the matrix. In each experiment, a set of mass spectra was collected by repetitive irradiation of a spot on a sample. Even though shot-to-shot variation in spectral pattern was significant, it was reproducible for different spots and samples. Each spectrum was tagged with the temperature in the early plume (T_{early}) estimated through a kinetic analysis of the peptide ion survival probability. T_{early} decreased as the shot continued because the thermal conduction got more efficient as the sample got thinner. From each spectral set collected under various experimental conditions, a spectrum tagged with a particular T_{early} was selected. Then, patterns of the spectra thus selected were the same. The reaction quotient for the matrix-to-peptide proton transfer determined at a specified T_{early} was independent of the sample composition, indicating quasi-thermal equilibrium for this reaction. Furthermore, the van't Hoff plots were linear, also indicating quasi-thermal equilibrium. This, together with the thermal kinetics for the fragmentation of peptide and matrix ions, is responsible for the reproducibility of the mass spectral pattern at a specified T_{early}.

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Direct visualization of the conformation of dendronized polymers by STED nanoscopy

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서울대학교 화학부

We demonstrate direct visualization of the conformation of dendronized polymers by stimulated emission depletion (STED) nanoscopy at sub-diffraction-limit optical resolution. The dendronized polymers synthesized by the ring-opening metathesis polymerization method were covalently cross-linked with fluorescent probes for fluorescence imaging, which were developed to satisfy stringent experimental conditions such as depletion efficiency and affordable cost. The highly linear structure of rigid-rod polymers and the dependence of structural linearity on the polymer chain length were investigated using STED nanoscopy.

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Development of NIR dyes using Vanadium and Copper Phthalocyanines

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부산대학교 첨단정보및디스플레이소재협동과정 [1]부산대학교 화학교육과

Metal phthalocyanines (MPcs) absorb visible and near infra-red (NIR) light and have good physical and optical properties. But low solubility of MPcs causes processing difficulty for a homogeneous film and low transparency limits applications ,in the visible ray. To overcome these problems, substituents were introduced to prevent lamination by providing a long distance between numerators of phthalocyanines. The improved solubility was achieved from dwindling of the mutual attraction. The optical property of MPcs in NIR area changed depending on substituents and metals. Several MPcs were prepared and compared to enhance NIR absorbance.

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Formation and Properties of Alkylphosphonic Acid Self-Assembled Monolayers on Indium Tin Oxide Surface: Thermal Annealing Effect

김영우 황선민 **Eisuke ito[1] Masahiko Hara[2]** 노재근

한양대학교 화학과 [1]RIKEN, Japan [2]TITech, Japan

Surface modification of indium tin oxide (ITO) by various phosphonic acids have recently been developed for the application of crystal displays, solar cell, and organic light emitting diode device. In particular, a quality of self-assembled monolayerss (SAMs) formed by alkylphosphonic acids (APA) on ITO surfaces significantly affects the device performance. However, there have been few reports concerning the formation and property of APA SAMs depending on surface morphology of ITO due to thermal annealing. In this study, we examine thermal annealing effect and alkyl chain length effect on the formation and property of APA SAMs. Contact angle (CA) measurements showed that CA values of APS SAMs on ITO were measured to be ~115º, suggesting that the formation of closely packed SAMs. Surface morphology, adsorption condition, electrochemical behavior and electronic property of APA SAMs were examined by means of scanning tunneling microscopy, atomic force microscopy, X-ray photoelectron spectroscopy, cyclic voltammetry, and Kelvin probe measurements, and the results will be discussed in more detail.

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Substituent Position Effect on the Formation of 2,4- and 3,4-Difluorobenzenethiol Self-Assembled Monolayers on Au(111) Surface

강훈구 Eisuke Ito[1] Masahiko Hara[2] 노재근

한양대학교 화학과 [1]RIKEN, Japan [2]RIKEN, TITech, Japan

Self-assembled monolayers (SAMs) with strong electron-withdrawing groups such as fluorinated aromatic SAMs are found to decrease the barrier for electron or hole injection into the organic semiconductor. For this application, it is important to understand SAM structure of fluorinated aromatic thiols on metal surface. On the other hand, it is reported that surface structure of fluorinated aromatic thiol SAMs is changed depending on the position of the F atom relative to the SH group on the aromatic ring of fluorinated molecules because of the different dipole-dipole interaction. In this study, we observed the totally different surface structures of 2,4- and 3,4- difluorobenzenethiol (DFBT) SAMs on Au(111) surface using scanning tunneling microscopy, which result from different dipole-dipole interactions. 3,4-DFBT SAMs have usually disordered phases, while 2,4-DFBT SAMs contain the highly ordered surface structure. From this result, we can find that dipole-dipole interactions are very important factor for formation of fluorinated aromatic SAMs.

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Two-Dimensional Structural Control of Aromatic Thiol Self-Assmebled Monoalayers Guided by Displacement of Cyclohexanethiol on Au(111) Surface

성태현 강훈구 **Eisuke Ito**[1] **Masahiko Hara**[2] 노재근

한양대학교 화학과 [1]RIKEN, Japan [2]TITech, Japan

Self-assembled monolayers (SAMs) of aromatic thiols have drawn much attention due to their interesting electrical and optical properties that may be applicable in molecular electronics. However, to improve device performance and obtain reliable data, the ability to fabricate two-dimensional ordered SAMs of aromatic thiols is needed. Especially, it is known that the SAMs of simple aromatic thiols such as benzenthiol and p-substituted benzenethiols have usually disordered phases. In this study, to obtain long-range ordered aromatic thiol SAMs, cyclohexanethiol (CHT) SAMs were used as transient layers because of a weak lateral interaction and a lower adsorption density instead of alkanethiolate SAMs. By scanning tunneling microscopy observation, we found that well-ordered aromatic thiol SAMs can be obtained via the displacement of preadsorbed CHT SAMs on Au(111) by aromatic thiol molecules. Therefore, it can be concluded that CHT SAMs on Au(111) can be used as an effective transient monolayer for guiding well-ordered SAMs.

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Comparative Study of Propanethiol and Trifluoropropanethiol Self-Assembled Monolayers on Au(111) : Formation and Structure

임동원 강훈구 **Eisuke Ito[1] Masahiko Hara[2]** 노재근

한양대학교 화학과 [1]RIKEN, Japan [2]TITech, Japan

Fluorine-terminated thiols are of great interest since fluorine atoms have inherent properties such as inertness to most chemical reagents, low friction coefficient and excellent repellency. In this study, the formation and structures of self-assembly monolayers(SAMs) prepared by propanethiol (PT) and trifluoropropanethiol (TFPT) on Au(111) were examined and compared using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV) to explore the structure and electronic interface properties of differently substituted alkanethiol SAMs on Au(111). STM observation showed that the PT and TFPT SAMs formed at 70 0C for 10 min and 20 min, have very uniform surface structure and ordered domains compared to those formed at other immersion temperature and time. The TFPT SAMs formed after 20 min have unique ordered domains containing well-ordered structures. XPS measurements for PT and TFPT SAMs show that sulfur atoms are chemically bond to the gold surface. Therefore, we can find that the surface structure of short-chain alkanethiol SAMs is quite changed according to whether or not the terminal group of short-chain alkanethiol SAMs is functionalized with fluorine atom.

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Solvent-dependent switching of the rate determining step in thestepwise enzymatic reaction of 10-23 deoxyribozyme and RNA

배소현 김성근*

서울대학교 화학부

We investigated the real-time dynamics of the enzymatic reaction of 10-23 deoxyribozyme and RNA substrate by total internal reflection fluorescence spectroscopy. The reaction sequence consists of a series of distinct stepwise processes: enzyme-substrate binding, substrate cleavage, half-substrate dissociation, and full-substrate dissociation. We measured the lifetimes of individual steps at the single-molecule level and found that they depend strongly on the solvent. The cleavage step is sometimes so much accelerated that it no longer acts as the rate determining step of the overall reaction. We propose a mechanistic model for the solvent dependence of individual reaction steps.

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Effect of photobleaching on the detection of a kinetic event in single-molecule measurement

연규진 정지원 배소현 김선영[1] 김성근[*]

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학

In the single-molecule measurement of a kinetic event such as enzyme kinetics, one measures the time it takes for a specific event assuming that the fluorescent dyes persist during the measurement. In reality, however, fluorescent dye molecules are photobleached with a finite lifetime, which is often shorter than the detection time of the event of interest itself. In this study, we addressed how the finite lifetime of fluorescent dyes affects the results of a kinetic measurement in our real-time study of enzyme kinetics of 10-23 deoxyribozyme and RNA substrate by total internal reflection fluorescence spectroscopy.

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Composite Methods including relativistic effects at the molecular level

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In order to obtain the accurate thermo-chemical data while maintaining low computational, various types of composite methods are developed for each target system such as organic compound and transition-metal containing molecules. One type of composite methods uses one or more semi-empirical parameter. Gn1), CBS-n2), and MCCM3) theories belongs to this type of composite methods. Another type uses coupled cluster methods. Wn4), HEAT5), and ccCA6) theories utilize extrapolated basis set limits or full CI limits. Among them Gn theories are implemented in Gaussian program and ccCA theories for organic molecules are implemented in NWChem program. One of the deficiencies of prevailing composite methods is that heavy elements of 5th series and beyond are not included in the molecular systems, and usually relativistic effect correction at the molecular level is omitted. Using couple cluster method with relativistic effects with proper pseudo-potentials and basis sets, we suggest new types of composite method. New methods are tested for hydrides of group 13 elements, oxides, and dimers.[1] L. A. Curtiss, K. Raghavachari, G. W. Trucks, J. A. Pople, J. Chem. Phys. 94, 7221 (1991)[2] G. P. F. Wood, L. Radom, G. A. Petersson, E. C. Barnes, M. J. Frisch, J. A. Montgomery, J. Chem. Phys. 125, 094106 (2006)[3] P. L. Fast, D. G. Truhlar, J. Phys. Chem. A 104, 6111 (2000) [4] A. Karton, E. Rabinovich, J. M. L. Martin, B. Ruscic, J. Chem. Phys. 125, 144108 (2006) [5] M. E. Harding, J. Vazquez, B. Ruscic, A. K. Wilson, J. Gauss, J. F. Stanton, J. Chem. Phys. 128 (2008) [6] N. J. DeYonker, T. R. Cundari, and A. K. Wilson, J. Chem. Phys. 124, 114104 (2006)

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Characterization of optical property of photo-luminescent Graphene Oxide(GO) and its reduced rGO in water and various polymer matrix

김창호* 정세채[1]

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Single-layered graphene oxide sheets with a few nanometers in lateral offer interesting electronic, thermal, optical, and mechanical properties, which could be very potential for low-cost opto-electronics, biological applications, membranes, and transport barrier composites. Recently, tunning of PL from 400 nm 800 nm could be realized by gradual reduction of the GO suspension. Herein, we have characterized transient optical properties of prepared GO composites in water and polymer matrix. Transient PL spectroscopy was performed with TCSPC by utilizing 200 kHz tunable ultrashort pulses generated from Orpheus and Pharos combinations. Extensive studies on transient PL with a systematic changes in photoexcitation energy could allow us to have deeper understandings on inherent optical properties of GO and its derivatives affected by water and a given polymer matrix.

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Vibrational Predissociation of Ternary Clusters, AnWB+, AnWPy+, and AnWMe+:Molecular Structure and Time Resolved Analysis

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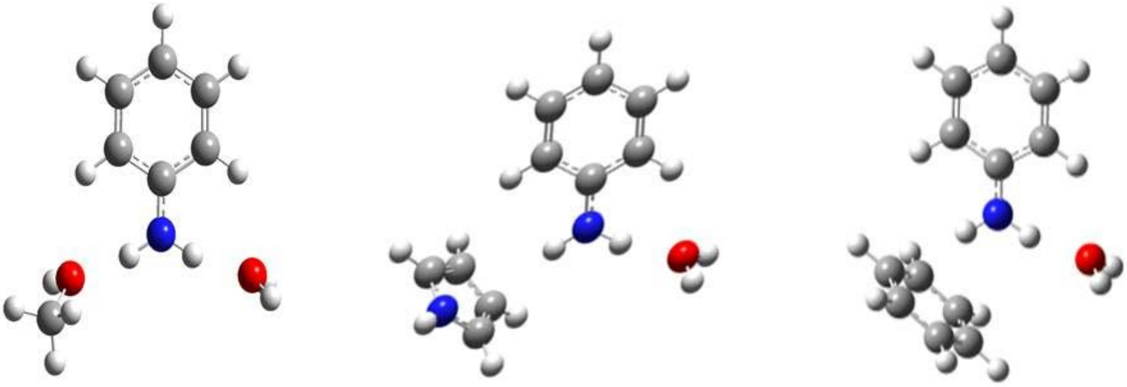
Cluster ions are generated by R2PI of 266 nm, photodissociated with IR light. Intensity of the major fragment is monitored as a function of IR wavenumber in the range of 2800-4000 cm-1. All vibration modes observed are assigned comparing with Gaussian calculation using DFT method and B3LYP/cc-pVDZ basis set. For all cases two ligands are bounded by H-bond with each N-H of Aniline, to give 1,1 most stable structure. Comparing Zero Point Vibrational Energy corrected value also confirms 1,1 structure is the minimum energy structure, which reflects our experimental results are perfect.For time resolved vibrational Predissociation analysis all the cluster ions are photodissociated exciting all vibration modes observed in the structure analysis applying some potential difference in the photodissociation region. All cases NH mode exciting gives slower rate of dissociation compared to OH mode excitation and most of the cases dissociation constant is about 107S-1 scale.



AnWMe$^+$ AnWPy$^+$ AnWB$^+$

Figure: Most Probable Structure

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The effect of ions in solution on the surface chemistry of Au NPs prepared by laser ablation in liquid

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Gold nanoparticles were synthesized by laser (Nd: YAG λ = 1064 nm) ablation of a gold target immersed in various aqueous electrolyte solutions (7 mM of LiCl, NaCl, KCl, NaBr, and NaI) as well as in deionization water. To investigate the effect of ions in aqueous electrolyte solutions on the stability of nanoparticles, the surface plasmon absorption peak was measured depending on elapsed time by UV-Vis spectrophotometer. Transmission electron microscopy (TEM) also used to observe the size change of nanoparticles depending on elapsed time and ions in aqueous electrolyte solutions. Surface chemistry of Au nanoparticles prepared in various electrolyte solutions are analyzed by X-ray photoelectron spectroscopy (XPS) to find out the effect of surface chemistry on stability of nanoparticles.

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The stability of uncapped gold nanoparticles produced by laser ablation in deionized water : the effect of post-irradiation

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Gold nanoparticle (AuNP) solution prepared by laser ablation in liquid (LAL) was irradiated by ns laser pulses to investigate the wavelength dependence on the size distribution of AuNPs and stability of post-irradiated AuNP solutions. We have employed 266, 355, 532, and 1064 nm lasers for post-irradiation source and found considerable wavelength dependence in the size distribution and stability of AuNPs. We also confirmed by DLVO theory, the interaction energy between the AuNPs.

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Characteristics of the charge-transfer state of H2N-H--X (X=F, Cl, Br)

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The geometry and vibrational frequencies of the ground electronic states of anion and the low-lying electronic states of neutrals of H2N-H--X (X=F, Cl, Br) are investigated by using a variety of density-functional-theory (DFT) methods and the coupled-cluster singles and doubles (CCSD) method. Not only vertical excitation energies but also the geometry and vibrational frequencies of the charge-transfer excited state of the neutrals are calculated by using the ionization potential equation-of-motion coupled-cluster singles and doubles (IPEOM-CCSD) method. All of the calculations were carried out with the aug-cc-pVTZ basis set. Calculated results are compared with previous theoretical results and some available experimental values. The characteristics of the charge-transfer states disclosed from this study provides a few insights for future experimental studies.

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Mechanism of carbon dioxide chemisorption by substituted anilines

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The mechanism of the reaction of carbon dioxide with substituted aniline was studied using the density functional theory (DFT) method. Six substituents, OH, CH_3, F, Cl, $CH=CH_2$, were considered in the mechanism and some good correlations between the properties of substituted anilines and energy barriers were obtained. In addition, the results showed that water molecule is beneficial and important to the chemisorption. This work can give insight to the design of new polymer materials for carbon dioxide capture.

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Theoretical study on the binding of flavone derivatives as as Helicobacter Pyloriβ-hydroxyacyl-acyl carrier protein dehydratase Inhibitor.

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인하대학교 화학과

Flavones were known as potential inhibitors of Helicobacter pylori which is a major cause of peptic and gastric cancer. And there were reports about x-ray crystal structures of three flavonoids. In this work, the binding modes were investigated by using AUTODOCK4.2 version. The docking structures for some flavone derivatives on HpFabZ were compared with the x-ray structures. Flavone structures were fully optimized at HF/6-31G(d) and B3LYP/6-31G(d). For docking calculation, polar hydrogen atoms were added and water molecules were removed. Kollman United Atom Charges and atomic solvation parameters were adopted. Using optimized geometries at HF/6-31G(d), we prepared force-field parameters for molecular dynamics.

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ONIOM study on reaction mechanism of desymmetrization of meso anhydrides catalyzed by bifunctional Bronsted Acid/Base organocatalyst

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The reaction between anhydride and methanol catalyzed by bifunctional Bronsted acid/base organocatalyst was investigated theoretically by ONIOM method. Calculations indicate that the energy barrier is quite high without catalyst, i.e. 30.8 kcal/mol. In the presence of catalyst, the reaction proceeds through a 2-step mechanism with the energy barrier of 19.0 kcal/mol and 0.9 kcal/mol. The pyridine moiety works as a Bronsted base to activate methanol substrate, and the N atom attached to P atom works as a Bronsted acid to activate anhydride by hydrogen bonding.

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Theoretical Studies on the Mechanism of Pyridinolysis of Y-Substituted Phenoxy Carbonyl Isothiocyanate

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The kinetics and mechanism of the pyridinolysis (XC_5H_4N) of phenoxy carbonyl isothiocyanate in gas phase are investigated at room temperature 25.0℃. The Hammett and Br?nsted plots for substituent X variations in the nucleophiles exhibit expected slopes with excellent correlations. These are interpreted to indicate a mechanistic behavior for the reactions whether these are following concerted or a stepwise route during expulsion of the isothiocyanate (NCS) leaving group from the intermediate or TS. The positive and negative β_X values imply the characteristics of the nucleophilic attack. In addition the steric effects of the ligands play an important role in determining the pyridinolysis rates of isothiocyano phosphates.

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Observation of photoexitation dynamics of NO bound ferric myoglobin by femtosecond IR spectroscopy.

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Femtosecond vibrational spectroscopy was used to investigate the photoexcitation dynamics of NO bound ferric myoglobin (MbIIINO). The stretching mode of NO in MbIIINO consists of a major band at 1922 cm^{-1} (97.7%) and a minor band at 1902 cm^{-1} (2.3%), suggesting that MbIIINO in room temperature solution has two conformational substates. The time-resolved spectra show small but significant new absorption features at the lower energy side of the main band (1920~1800 cm^{-1}). One new absorption feature in the region of 1920~1880 cm^{-1} are revealed as the NO band in the ground electronic state of MbIIINO. This absorption shifts toward higher energy and narrows with a time constant of 2.4 ps, indicating that it evolves with rapid electronic and thermal relaxation of the photoexcited MbIIINO without photodeligation of the NO from the heme. The remaining absorption bands peaked near 1867, 1845, and 1815 cm^{-1} were assigned to the vibrational band of the photodeligated NO, the NO band of MbIIINO in an intermediate electronic state with low-spin Fe(III)-NO(radical) character (denoted as the R state), and the NO band of the vibrationally excited NO in the R state, respectively. A kinetics model successfully reproducing the time-dependent intensity changes of the transient bands suggests that every rebound NO forms the R state that eventually relaxes into the ground electronic state nonexponentially. Most of the photodissociated NO undergoes fast geminate recombination (GR) and the rebinding kinetics depends on the conformation of the protein. GR of NO to MbIII in the major conformation shows highly nonexponential kinetics described by a stretched exponential function, exp $(-(t/290\ ps)^{0.44}$. The NO rebinding to MbIII in the minor conformation is exponential, exp (-t/1.8 ns), suggesting that the distal histidine, the interaction of which dictates the conformation of MbIIINO, participates in mediating the binding of NO to MbIII. In MbIIINO, the elusive low-spin Fe(III)-NO(radical) state, proposed in electronic structure calculations, indeed exists at >12 kJ/mol above the ground state and takes part in the

bond formation of Fe(III)-NO, suggesting that it plays a significant role in the function of NO bound ferric protein.

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Investigation of magnetic properties of $NaNiF_3$ and $K_3NaOs_2O_9$on the basis of spin dimer analysis

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The spin exchange interactions of the perovskite-type magnetic solids,$K_3NaOs_2O_9$(Os^{+7},S= 1/2) and $NaNiF_3$ (Ni^{+2}, S = 1), were examined by performing the spin dimer analysis based on the extended Huckel tight binding method. $K_3NaOs_2O_9$ contains isolated Os_2O_9units made up of face-sharing of Os_2O_9octahedra, so spin exchange interactions in $K_3NaOs_2O_9$occur through both super exchange and super-super change paths. Our spin dimer analysis shows that there are four strongly interacting spin exchange paths, J_1, J_2, J_4 and J_5. In addition, we found spin frustration takes place between triangular spin exchange paths. Although both perovskite and post-perovskite-type $NaNiF_3$ consist of $NaNiF_6$ octahedron, their $NaNiF_6$networks are different, i.e. the perovskite-type $NaNiF_6$ forms a three-dimensional network while the post-perovskite-type $NaNiF_6$ forms a two-dimensional network. Therefore, spin lattices made up of the super exchange paths form 3D and 2D structures for the perovskite-type $NaNiF_3$ and the post-perovskite-type $NaNiF_3$, respectively. Our spin dimer analysis indicates that super exchange interactions are much stronger than super-super exchange interactions and the spin exchange interaction in the perovskite-type $NaNiF_3$ is much stronger than in post-perovskite-type $NaNiF_3$. This finding is consistent with the experimental observation.

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Orientation dependence of electronic coupling in the cofacially juxtaposed donor-acceptor systems

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New π-stacked donor-acceptor (D-A) systems, 2-(8-(anthracen-2-yl)naphthalen-1-yl)cyclohexa-2,5-diene-1,4-dione (2-Q-An1) and its rotational isomer (2-Q-An2), and 2-(8-(anthracen-9-yl)naphthalen-1-yl)cyclohexa-2,5-diene-1,4-dione (9-Q-An) have been synthesized and characterized to interrogate electronic interactions between cofacially aligned donor (An) and acceptor (Q). Due to a 1,8-naphthyl pillaring motif, the closest distance between An and Q moieties are held fixed at sub van der Waals contact distances (3.00, 3.10, and 2.95 A for 2_Q_An1, 2_Q_An2, and 9_Q_An, respectively). The electronic coupling (HDA) between the ground and the charge transfer (CT) excited states have been analyzed by steady state absorption spectroscopy as well as the ultrafast visible-pump/IR probe transient absorption spectroscopy (TrIR). The low-energy electronic absorptions spectra manifest broad band that covers the whole visible region, which are mainly charge transfer in nature. TD-DFT calculation suggests that this spectral envelope is consists of approximately 10 electronic transitions and thus the magnitude of the HDA between ground and CT states cannot be analyzed by a conventional Mulliken-Hush analysis. For these systems, HDA values were successfully evaluated from the relative difference (ξ) of the carbonyl stretching frequency between the neutral Q and its one-electron radical anion, which was determined by an ultrafast TrIR spectroscopic method. TrIR results showed that the partial charge localized on the Q moiety in the lowest CT state was ca. 0.93e, and the corresponding HDA was ～2500 cm^{-1}. This value was in good agreement with that estimated by the Mulliken population analysis of the ground-state geometry.

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Synthesis of various surfactants-capped ZnO quantum dots and its deactivation of characteristic photocatalyst

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단국대학교 화학과

Various surfactants-capped ZnO quantum dots were synthesised via one-pot process. Particles of various surfactants-capped ZnO quantum dots were synthesised by sol-gel process. Various surfactants-capped ZnO quantum dots were prepared with Zinc acetate dihydrate, ethanol, tetramethylammonium hydroxide and various sufactants. For example, oleic acid, stearic acid and triethanolamine. Photocatalytic degradation of Rhodamine B was carried out with synthesized various surfactants-capped ZnO quantum dots powder. The crystal structure, optical properties and the characteristic photocatalyst of the surfactants-capped ZnO quantum dots were characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD) and UV-Vis spectrophotometer.

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Observation of SACI phenomenon in an acetaminophen-water cluster using LIF

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Acetaminophen (AAP) is the major component of Tylenol, and widely used as a fever and pain reducer. It is known from previous studies (Phys. Chem. Chem. Phys. 2011, 13, 16537; Phys. Chem. Chem. Phys. 2013, 15, 957) that two conformers of AAP exist in gas phase. SACI (solvent-assisted conformational isomerization) is a phenomenon where a less stable conformer of a molecule isomerizes to a more stable one using the binding energy with a solvent. We tried REMPI technique in order to observe SACI in an AAP-water cluster. However, it was hard to compare AAP-water with AAP because AAP sample absorbs water too easily under ambient condition. In addition, an AAP-water cluster dissociates upon ionization so that the absorption of a cluster is detected at the monomer mass channel together with that of monomer. In order to solve this problem, we used laser-induced fluorescence (LIF) that detects fluorescence instead of ion. Using LIF, we compared the fluorescence excitation spectrum of dry AAP and that of AAP expanded with water, and confirmed that the absorption of the trans conformer was reduced. We were also able to differentiate the conformers using the UV-UV hole-burning technique.

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Spectroscopic and quantum chemical study of 2-Methylpyridine(2MP), 3-hydroxypyridine(3HP), and 3-(Hydroxymethyl)pyridine(3HMP)

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Pyridoxine [4,5-Bis(hydroxymethyl)-2-methylpyridin-3-ol, PN] is a member of vitamin B_6 family together with pyridoxal (PL) and pyridoxamine (PM). All vitamin B_6 compounds are converted in vivo to the active form of pyridoxal 5-phosphate (PLP), which is a coenzyme that is involved in metabolism of more than hundred amino acids. Even though PN has such a central role in body metabolism, there has been no spectroscopic study of PN in gas phase to reveal its intrinsic nature. In order to understand the properties of substituents that PN has, we spectroscopically and quamtum chemically studied 2-Methylpyridine(2MP), 3-hydroxypyridine(3HP), and 3-(Hydroxymethyl)pyridine(3HMP).

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1+1’ REMPI Spectrum of Laser-Desorbed Proline-Acedan

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Two-photon microscopy (TPM) is a strong tool for study of biology and medicine due to its ability to take images within cells and tissues. To use TPM as a molecular imaging technique for a certain molecule, we need a two-photon (TP) probe that selectively binds to that molecule. ANO1 is one of the TP probes, which has dramatic increase of its fluorescence when it binds nitric oxide. Before we study the reason of fluorescence change of ANO1, first we study proline-acedan (PA), the precursor of ANO1. Despite small structural difference between PA and acedan, their fluorescence efficiency is very different. If we study how this big difference in fluorescence comes from small difference in structure, we can improve our understanding of fluorescence probes. As a start of this study, we obtained the 1+1’ REMPI spectrum of PA.

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Torsional Barrier of Glycine in Water Solution: The Importance of Hydrogen Bond

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경북대학교 화학과

Because of the central role in metabolism as building blocks of proteins, amino acids have been the subject of a variety of experimental and theoretical studies. Glycine has three internal rotational degrees of freedom are the rotation of hydroxyl group around the C?O bond (θ), the rotation around the C?C bond (Φ), and the rotation of the amino group around the C?N bond (ψ). The structures of all conformers of glycine and inter-conversion pathways between several conformers were determined by MP2/6-31++G(d) in gas phase and the conductor-like polarizable continuum model (C-PCM) were performed with the same basis sets. In addition to the ab-initio calculation, we performed molecular dynamic simulations to predict the local structures of glycine molecule in aqueous solution and characterize them. The molecular dynamic simulation shows that nine conformes are exist in aqueous solution and the solvent effects play an important role for the stabilities of glycine conformers as well as their torsional barriers. This MD simulations also show that the specific interactions between solute and solvent. It can explain the hydrogen bond interaction between glycine and sorrounding water molecules also.

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A theoretical study on the excimer formation of carbazole

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Due to the potential for the next generation electronics, organic semiconducting materials have widely been studied for last two decades. In particular for blue OLEDs, for example, host materials must have both good charge transport properties and higher triplet energy than light emitting guests and many molecules have been successful synthesized. Because of both good hole accepting/transporting properties and high triplet energy, carbazole has been considered as one of the most important building blocks for those organic semiconductors. Recently, however, researchers reported that carbazole may form excimer, leading to reduced triplet energy and hence lower device efficiency. Therefore, in order to prevent such excimer formation and keep device performance as high as possible, better understanding of excimer formation of carbazole is demanding.In this poster, we detail recent calculation results on the carbazole excimer both in the singlet and triplet states. We investigated various dimer configurations for which geometric and energetic features are presented. Covalent and ionic contributions to the wavefunction for excited-state carbazole dimers will also be discussed.

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Direct absolute pK_a predictions and proton transfer mechanisms of small molecules in aqueous solution by QM/MM-MD

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The pK_a values of HF, HCOOH, CH_3COOH, CH_3CH_2COOH, H_2CO_3, HOCl, NH_4^+, $CH_3NH_3^+$, H_2O_2 and CH_3CH_2OH in aqueous solution were predicted by QM/MM-MD in combination with umbrella samplings adopting the flexible asymmetric coordinate (FAC). This unique combination yielded remarkably accurate values with the maximum and root mean square errors of 0.45 and 0.22 in pK_a unit, respectively, without any numerical or experimental adjustments. The stability of initially formed Coulomb pair (CP) rather than the proton transfer stage (EB) turned out to be the rate-determining step, implying that the stabilizations of the created ions require a large free energy increase. A remarkable correlation between DWR(degree of water rearrangements) and pK_a was observed. As such, the large pK_a of ethanol can be in part attributed to the large water rearrangement, strongly suggesting that proper samplings of water dynamics at dissociated regions are critical for the accurate predictions of pK_a. Current results exhibit a promising protocol for the direct and accurate predictions of pK_a. The success of our protocol can be attributed to the balanced descriptions for both solute and solvents in such a way that quantum mechanics properly describe the proton transfer reactions between acid and quantum water, while the classical solvent parameter allows sufficient samplings of water dynamics during the event.

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Hydrogel-based Polymer Pen Lithography for Large-area Patterning of Biomolecules

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한양대학교 화학과

Dip-pen nanolithography (DPN) and polymer pen lithography (PPL) are popular methods for fabricating biomolecule patterns because those are relatively simple and cost-effective techniques. DPN can fabricate patterns with nanoscale resolution but is limited in throughput . PPL was developed to solve limitation of throughput . PPL technique using polydimthylsiloxane (PDMS) as a tip material needs surface modification and adding additives such as polyethyleneglycol and glycerol to fabricate biomolecules pattern due to their hydrophobic surface. Hydrogels, especially Agarose gel (AG), can fabricate large area patterns rapidly without additional modification and additives due to their hydrophilic, biocompatible, and water absorbable properties. In this study, we utilize the AG as a tip material for fabricating large area biomolecule patterns. We fabricated fluorescein isothiocyanate-labeled streptavidin (FITC-SA) patterns with one stamping on a silicon substrate. Fluorescence intensity and AFM topography were used to confirm uniformity of patterned FITC-SA dots and to measure size of dots, respectively. We present a simple and reproducible technique to fabricate biomolecule pattern without any surface modification methods and additives. This hydrogel?based PPL is suitable for fabrication of biomolecule pattern and it is potentially useful in biological fields.

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Conjugated Polymer Coated Three Dimensional Structure for the Ultra-Sensitive Biosensor Application

이수범 박미경 Chen Rui 조용덕[1] 조석진 서정은 김종만[2] 이해원[*] 이주섭[3]

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The importance of the signal amplification is arising in the biosensor field for the accurate and instant disease analysis and diagnosis. For example, the gold nanoparticles are used to increase the binding sites for antibodies and ultimately this leads to signal amplification. A PDA vesicle has double bond chain in the middle of the vesicle and when a signal is applied on the conjugated polymer, the back bone chain's energy band gap is changed and the chain emits intensive red fluorescence light. Many attempt has been tried to combine PDA with host matrices to fabricate ultrasensitive biosensors, however, the binding PDA on the three dimensional structure is rarely attempted. We coat PDA uniformly on the three dimensional structure which has larger surface area than the two dimensional substrate. The fluorescence intensity increased twelve times for the maximum than the fluorescence intensity from the two dimensional substrate. This result will contribute to the development of highly sensitive biosensors with excellent accuracy.

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Hierarchical Three-dimensional Network of Carbon Nanotubes for High-Sensitive Biosensor

박미경 오은결 조석진 조용덕[1] 서정은 **Chen Rui** 이해원[*] 이수범

한양대학교 화학과 [1]한양대학교 나노융합과학과

Early detection of the cancer biomarker in patients can reduce the risk of death from cancer. Traditionally, cancer researchers have used blood serum and urine to detect cancer. Saliva contains the same biomarkers as those found in blood. The saliva-based test meets the need for a quick, cheap, safe and convenient diagnosis.1 High-sensitive sensor would allow early diagnosis of cancer with the saliva. Recently, three-dimensional (3D) hierarchical structures have been introduced a wide attention as effective structures for high sensitive detection.2 These systems enable considerable increases in the contact area between substrates and biomolecules, thus enhancing the capture efficiency of cancer biomarker. In this research, hierarchical three-dimensional network of carbon nanotubes was demonstrated for high sensitive biosensor. The hierarchical three-dimensional carbon nanotubes was synthesized on Si pillar substrate by chemical vapor deposition (CVD). As the suspended carbon nanotubes were weakly adhered to Si pillars, the carbon nanotube networks were coaxially coated with Al2O3 layer using atomic layer deposition (ALD) techniques.3 High densities of biotin on the surfaces of the carbon nanotubes lead to greater binding of the FITC- Tagged streptavidin, which significantly enhances detection sensitivities. Furthermore, and application aspects of these new functional structures also will be discussed.

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Adsorptions of formic and acetic acids on ice surface: Surface binding configurations and a possibility of interfacial proton transfer

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Adsorptions of formic (FA) and acetic acids (AA) on Ih ice surface were studied using our quantum mechanical/effective fragment potential (QM/EFP) scheme. Unlike earlier studies in which trans-conformers were found as major surface configurations, our QM/EFP models found various cis-and trans-conformers on ice surfaces with the cis-conformers being more stable. The favorable surface-parallel configurations of cis-conformers comparatively enhance the binding strength. The surface binding energies and configurations were largely dependent on the surface heterogeneity, showings the importance of surface dangling hydrogens. In addition, overall the binding energies of acetic acid are slightly higher as compared to formic acid, implying that the additional methyl group of acetic acid enhances the surface bindings. Our study also found a feasible deprotonation route of adsorbed trans-formic acid. On the other hand, acetic acid prefers to stay as molecular form, due to the unfavorable hydrophobic methyl group. Therefore it is interesting to note that the additional methyl group of acetic acid enhances surface binding energies. But at the same time it reduces the possibility of its deprotonation. Our ice model clearly demonstrated the importance of intrinsic structural heterogeneity of ice on the distributions of surface binding energies and configurations, which cannot be represented by small water clusters.

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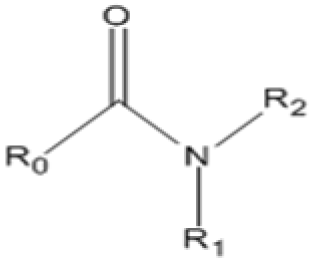
여러가지 Amide 화합물의 sc-CO_2 용해도에 관한 이론적 연구

신서은 김학원 김용호*

경희대학교 응용화학과

최근 sc-CO_2 를 사용하여 방사능 핵 폐기물을 처리하기 위한 시도가 활발히 이루어지고 있다. 그 중, Amide 결합을 가지는 화합물이 sc-CO_2 에 잘 용해될 수 있는 킬레이팅 화합물로 사용될 수 있다는 것이 제시되었다. Amide 분자의 sc-CO_2 용해도를 알아보기 위하여 여러가지 Amide 화합물과 CO_2 간의 binding energy 를 계산하였다. Amide 분자 간의 이합체 형성은 sc-CO_2 용해도를 저해하는 요인이다. 따라서 Amide 이합체 형성의 수소 결합 에너지를 계산하여 CO_2 binding energy 와 비교하였다. 본 연구의 결과 수소 결합 이합체 형성이 불가능한 tertiary Amide 의 용해도가 secondary Amide 보다 크게 예측되었다. 그리고 킬레이팅 화합물의 conformation 에 따른 binding energy 에 대하여도 연구하였다.



$R_0 = CH_3$ / CF_3

$R_1 = H$ / CH_3

$R_2 = C_5H_{10}N$ / $C_3H_5O_2$

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The Effect of Obstacle Size Distribution on the Diffusion of Tracers in Two Dimensional Porous Media

조현우 성봉준*

서강대학교 화학과

Diffusion of molecules in two-dimensional (2D) porous media has drawn a great deal of attention because 2D porous media might serve as an excellent system to study the protein dynamics in heterogeneous and crowded cell membranes. Recent experiments and theoretical studies revealed that protein diffusion in cell membranes were anomalous: diffusion coefficients were time-dependent and protein dynamics were sub-diffusive, resulting in interesting non-classical kinetics of biochemical reactions in cell membranes. Extensive studies suggested that such anomalous dynamic behaviors should arise because (1) immobile proteins in cell membranes would becomes obstacles and hinder the protein diffusion, (2) attractive intermolecular interactions between proteins would slow down the protein diffusion, or (3) there would be a slow-decaying distribution of hopping times of proteins. In this work, we illustrate that the anomalous sub-diffusion may also occur due to the obstacle (immobile protein) size distribution, which is inherent all cells. We show that the diffusion behavior of the tracers changes drastically from normal diffusion to anomalous and confined dynamics as the size distribution of obstacles becomes narrow, even for fixed average obstacle size and obstacle area fraction. We also find that diffusion coefficient D follows the scaling relation $D \sim (\varphi-\varphi_c)^\gamma$ regardless of the size distribution of the obstacles, where φ and φ_c are the area fraction of the obstacles and its value at the percolation threshold, respectively and γ is the scaling constant.

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High yield expression and structural characterization of human transmembrane proteins

박유근 김용애*

한국외국어대학교 화학과

Human transmembrane proteins (hTMP) are known to play an essential role in a variety of biological function. These proteins are closely related to major disease of human and are the target of over 50% of recent medicinal drugs. In order to study the structure and function of these hTMP, it is important to prepare reasonable amounts of proteins. However their preparation is seriously difficult and time-consuming. We tried to produce large amounts of human amyloid-b (hAb) and human melanocortin-4 receptor (hMC4R) in membrane protein. Human transmembrane proteins (hTMP) like hAb protein that is related to the dementia and hMC4R protein that is related to the obesity. The hAb transmembrane protein shows membrane-bound oligomeric state, and the Ca2+ permeable ion channel formation of non-fibrillar in the cell membrane. To determine the three dimensional structures of the intact hAb-TM, the isotopically labeled protein must be expressed and purified in sufficient quantity. We succeed to produce large amounts of the hAb-TM. Structural characterizations of the hAb-TM in the membrane-like environments were obtained by solution and solid-state NMR spectroscopy. The hMC4R has a critical role in part of energy homeostasis. Heterozygous mutations in second transmembrane domain of hMC4R relate in genetic cause of severe human obesity. We succeed to produce the second trans-membrane domain from the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). But, the purified protein contains considerable amounts of KSI fragment somehow. Therefore, we spend a lot of time to optimize the purification schemes. Circular Dichroism and MALDI-TOF MS spectroscopy were used to identify the initial secondary structures and purity. We also obtained high resolution solution NMR spectra of hMC4R TM2.

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Fullerene 표면의 흡착위치에 따른 Palladium의 Binding Energy 변화에 관한 이론적 연구

현은재 김용호*

경희대학교 응용화학과

플러렌을 비롯한 그라펜, 탄소나노수소 등의 수소 저장능력에 대한 연구가 많이 실행되고 있다. 이러한 탄소골격구조 물질들에 팔라듐, 칼슘 등의 금속물질을 dopping 시키면 수소 흡착 시 그 흡착 양이 증가한다는 보고 또한 있다. 따라서 이러한 탄소골격구조 물질에 금속을 dopping 시키는 데 있어서 그 결합에너지를 예측하고 효율성을 높이는 것 또한 중요한 과제로 떠오르고 있다. 본 실험에서는 플러렌의 dopping 위치에 따른 팔라듐의 binding energy 를 계산하여 플러렌의 hollow site, bridge site, top site 중 선호성이 강한 site를 알아내었다. 또한 다양한 곡률을 가지는 플러렌을 가지고 팔라듐과 플러렌의 binding energy 를 계산함으로서 곡률에 따른 플러렌-팔라듐의 binding energy 변화의 경향을 알아보았다.

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Au-R6G@SiO_2 core-shell nanoparticles as SERS tag for immunoassay

사영조 정영미 **Lei Chen[1] Bing Zhao[1]**

강원대학교 화학과 [1]Jilin University

Surface enhanced Raman scattering (SERS)-based immunoassay has been developed by using SERS tags which are combining Raman active dyes with metallic nanoparticles. In this study, we present a rapid and straightforward procedure for the preparation of SERS tags. The SERS tags are functionalized with anti-Immunoglobulin G (anti-IgG) for immunoassay exhibited a potential application of the core-shell particles in biosensing. Characterization of Au-R6G@SiO_2 core-shell nanoparticles and application in SERS-based biosensing will be discussed in details.

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Detection of the Thrombin with SERS

신민화 정영미*

강원대학교 화학과

As an ultrasensitive technique, surface-enhanced Raman scattering (SERS) has been developed into protocol for biosystem detection. Introduction of thrombin into the gold nanoparticles solutions in the presence of fibrinogen generates reaction of blood coagulation, and thus, fibrinogen modified gold nanoparticles can potentially be employed as effective SERS sensors for label-free protein detection. Addition of fibrinogen to a solution of gold nanoparticles led to ready conjugation through electrostatic and hydrophobic interactions. The products were investigated by means of UV-vis, SEM, and TEM. In this presentation, the detection of thrombin by using label-free SERS will be discussed in details.

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Temperature and pH-induced denaturation of ovalbumin studied by 2D correlation spectroscopy

강대훈 유수련 정영미*

강원대학교 화학과

The folding or denaturation process of proteins is a key issue to understanding the molecular structure changes that are responsible for various conformational diseasessuch as Alzheimer disease. Two-dimensional correlation spectroscopy (2DCOS) has attracted a high level of interest of analytical science community, as it provides considerable utility and benefit in many fields of spectroscopic studies. In the present study, we investigated temperature and pH-dependent unfolding or folding of ovalbumin by using 2D FTIR correlation spectra in order to monitor the secondary structure of ovalbumin. The details of 2D correlation spectra of temperature and pH-induced denaturation will be discussed.

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A study of thermal effects of biodegradable polymer blends by 2D correlation spectroscopy

박준후 정영미[1,*] Isao Noda[2]

강원대학교 화하과 [1]강원대학교 화학과 [2]The Procter & Gamble Company

Poly(3-hdroxybutyrate)(PHB)-based copolymers, such as poly(3-hydroxybutyrate-*co*-3-hydrohexanoate)(P(HB-*co*-HHx)) has been studied as environment-friendly polymer. Physical properties of P(HB-*co*-HHx) can be improved by using blend with other biopolymers.To study the thermal dynamics of P(HB-*co*-HHx)/PEG blend according to the content of the PEG, 2D correlation spectroscopy are applied to the temperature-dependent infrared-reflection absorption spectra of P(HB-*co*-HHx)/PEG blend. The details of thermal effects of P(HB-*co*-HHx)/PEG blend will be discussed.

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SERS-based Immunoassay for Disease-related Proteins

이영주 Lei Chen[1] 정영미[*]

강원대학교 화학과 [1]Jilin University

As an ultrasensitive technique, surface-enhanced Raman scattering (SERS) has been developed into protocol for the detection of immunocomplex system. Especially, SERS immunoassays based on antigen-antibody bonding have been studied for biomarkers for early diagnosis of related diseases. In this study, we applied microcontact printing method to prepare a patterned substrate of a sandwich type SERS immunoassay in which antigens on the substrate selectively capture antibodies on a Raman reporter, which can be successfully applied biosensors for cancer detection. This SERS immunoassay method can be applied successfully for biosensors. Details of the SERS immunoassay and SERS images will be discussed.

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Characterization of solid-electrolyte interface film on the cathode materials by using VC and FEC

박연주 신수현 최현철[1] 정영미*

강원대학교 화학과 [1]전남대학교 화학과

Solid-electrolyte interface (SEI) film plays a key role in the performances of Li-ion-battery. An understanding of components and structure of SEI is important to enhance the battery performance and the safety. We have recently investigated the composition and formation mechanism of SEI on cathode surface under high voltage condition by using XPS, XAS, FTIR, Raman and 2D correlation spectroscopy. Based on this work, chemical additive such as vinylene carbonate (VC) and fluoroethylene carbonate (FEC) were used in Li-ion battery to enhance the safety problem. We investigated the characterization and formation mechanism of SEI on the cathode surface with and without additive system by using electrochemical and spectroscopic techniques. In this presentation, the effect of electrolyte additives on cathode surface under high voltage condition will be discussed in more detail.

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Study of magnetic properties of magnetite ferrofluid by measuring magnetic weight change

진대성 김학진[1]

대전고등학교 수리과학부 [1]충남대학교 화학과

Magnetite nanoparticles of 11 nm diameter are synthesized via a coprecipitation method and dispersed in aqueous solution. Weight changes of this ferrofluid under different magnetic fields are observed with a conventional electronic balance. Magnetic weight of the superparamagnetic ferrofluid reveals hysteresis as the nanoparticles agglomerate at high magnetic fields. Morphological changes of the ferrofluid after Neel and Brown relaxation appear as the slow change of magnetic weight, which follows the stretched exponential relaxation. Interparticle interactions in the ferrofluid at high magnetic fields play an important role in the change of magnetic properties of the ferrofluid. The superparamagnetic ferrofluid is considered to convert into superspin glass or superferromagnetic state.

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System Size Effect in Lattice-Based Monte Carlo Simulation

김태준 김효준*

동아대학교 화학과

Generally, lattice based Monte Carlo simulations using boundary conditions because simulations are fast and exactly. It has some error from determination system size and lattice constant. We find new equation from how much this error in lattice based Monte Carlo simulations. We compared simulation data to general exact data of general movement, geminate reaction, and pseudo-first reaction.

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Quantitative model of the gene expression network under negative feedback regulation

박성준 성재영*

중앙대학교 화학과

We present a new mathematical model of stochastic gene expression under the negative feedback regulation. In previously reported models, mostly based on Pauli master equation, the reactivity or the productivity of the gene expression network has been assumed to be homogeneous among cells with the same genetic information, which, however, is not the case for living cells with dynamic and heterogeneous reaction environment. In the present model, we first takes into account the general influence of the complex cell environment on the reactivity of the gene expression network under the negative feedback regulation. For the model, we obtain the exact analytic expressions for the mean and the relative variance or the noise of the copy number distribution of the mRNA and protein. Our results show that the effects of negative feedback on the noise in mRNA and protein levels can be various and dependent on the stochastic nature of gene network fluctuation, in contradiction to the previous literature in this field.

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Effect of Alkyl Chain Length at the 9,9-position of Fluorene-based Organic Chromophores for Dye-Sensitized Solar Cells

김동희* **Mannix Balanay** 이상희

군산대학교 화학과

Two dipolar dyes containing 9,9-dialkyl-N,N-diphenyl-9H-fluoren-2-amine as electron donor moieities with thiophene and 2-cyanoacrylic acid as linker and acceptor group, respectively, were designed, synthesized, and used as sensitizers for dye-sensitized solar cells (DSSCs). The comparison between methyl or octyl groups at the 9,9-position of the fluorenyl moiety were analyzed based on theoretical and experimental results. Density functional theory was used to gain insight on their geometries and electronic properties. The results revealed, under standard global AM 1.5 solar condition, that increasing the length of the alkyl group attached to the fluorenyl moiety (KS-F2) increases the solar-to-electric conversion efficiency by up to 19 % compared to the methyl group (KS-F1). In comparison with N719 with the same electrolyte, KS-F1 and KS-F2 achieved 73 and 87 % of its efficiency, respectively.

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Vibronic Spectra of Jet-cooled 3-cyanoindole and Its Solvent Clusters Studied by UV-UV Hole-burning and IR Dip Spectroscopy in the Gas Phase

민아름 문철주 안아름 최명룡[*] 김성근[1]

경상대학교 화학과 [1]서울대학교 화학부

3-cyanoindole (3-CI) as a derivative of indole has an important intrinsic properties for its enormous biological activities in biological systems. In a previous study, we have identified one 3-CI conformer via the REMPI and UV-UV double resonance spectroscopic studies in the gas phase experiments. In this study, we have further investigated (3-CI)-solvent (water, methanol, and ethanol) clusters. For the (3-CI)-water (3-CIw) clusters, their REMPI spectra having a red-shifted origin band compared to that of monomer showed a clear identification of the two conformers of 3-CIw. Further investigation on the structures of the two conformers of 3-CIw with other alcohol clusters will be investigated and discussed by IR dip spectroscopic studies in this poster.

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Matrix isolation infrared spectroscopy and theoretical study of 2-acetylfuran

이지훈 이슬기 안아름 문철주 민아름 고은미[1] 조수경[2] 최명룡[*]

경상대학교 화학과 [1]국방과학연구소 국방신기술본부 [2]국방과학연구소 국방신기술센터 융복합부

Matrix isolation infrared spectroscopy has been combined with theoretical calculations for the characterization of 2-acetylfuran(2-AF)The matrix isolation technique was employed for the isolation, stabilization, and spectroscopic characterization of reaction species in inert cryogenic matrices(~6K) combined with the MIS experiments, theoretical calculations have also been conducted on the monomers and cluster of 2-AF. In this poster the structural, energetic, and spectral properties of th 2-AF compleats will be presented and discussed

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Excited state dynamics of DCM and ultrafast energy transfers near plasmonic metal nanoparticles

이재범 이인구 이세복 방윤수*

광주과학기술원(GIST) 물리화학부

We synthesize various silver nanoparticles and nanosurfaces which are optimal for metal-enhanced fluorescence by reducing silver ions. Fluorescence and absorbance enhancements of various chromophores including rhodamine 6G, rhodamine B, and 4-dicyanomethylene-2-methyl-6-p-dimethylaminostyryl-4H-pyran (DCM) in the existence of colloidal silver nanoparticles and silver island films have been investigated. Especially, silver island films (SIFs) are found to be most effective substrates for MEF of these chromophores with about 30-fold increases in emission intensity.The excited state dynamics of DCM near plasmonic metal nanoparticles (NP) and ultrafast energy transfers between them have been studied by a femtosecond transient absorption (TA) technique. Emission from the charge transfer singlet state (S1-CT) of DCM decays slower on the existence of SIFs, when the excitation of 400 and 500nm are used, and the energy transfer between DCM and metal NP might be the reason for the dynamics change. We will further investigate the interaction between these chromophores and plasmonic metal NP by femtosecond TA and Time correlated single photon counting techniques.

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Molecular Structure Modification of Fused π-bridge Dyes for Dye-Sensitized Solar Cells

김동희* **Enopia Camille Marie** 이상희 이경구

군산대학교 화학과

Four organic dyes with fused π-bridge structures tPx1, and tPx3, and Silicon-based fused π-bridge tPx2 and tPx4, patterned after the donor-π-acceptor system were investigated using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) to elucidate the effect of fused structure with Silicon in the photophysical property of the dye. Essential parameter such as optimized geometry structure, light harvesting efficiency (LHE), highest occupied molecular orbital and lowest unoccupied molecular orbital spatial orientation, different polarizabilities, ionization potential, electron affinity, and intramolecular reorganization energy were discussed in relation to the short circuit currect (JSC) and efficiency of the dye sensitizer. Theoretical results affirm that fused structures greatly affects the photophysical properties of the dye with the observed planarity of the π-conjugation and better electronic coupling between the donor and the acceptor. However the replacement of Carbon atom with Silicon does not heighten the potential of the dye structure. Among the dye structures, txP1 is the most promising with the most red-shifted absorption spectra, and favorable ionization potential, electron affinity, and electron intramolecular reorganization energy. The theoretical criteria for these dye structures reveals an improved properties than an non-fused dye structure.

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Dynamics of Br(^2P_j) Formation in the Photodissociation of oxalyl bromide near 234 nm and 265 nm

김현국 김태규

부산대학교 화학과

The photodissociation dynamics of oxalyl bromide have been investigated near 234 nm and 265nm using a velocity map ion imaging technique coupled with a state selective [2+1] resonance-enhanced multiphoton ionization [REMPI] scheme. The nascent Br atoms stem from the primary C-Br bond dissociation leading to the formation of C_2O_2Br and Br($^2P_{3/2}$) and Br*($^2P_{1/2}$). For more detail information, we analyze the translational energy distribution and recoil anisotropy from two dimensional images. In case of excited state, there translational energy distribution can be fitted by single Gaussian shape. However, in ground state translational energy distribution can be fitted by two Gaussian functions. From this result, we can find possibility about secondary dissociation of C_2O_2Br radical. The anisotropic parameter, β, is 0.79(0.73) and 1.11(1.38) for Br and Br* near 234nm(265nm). Finally, we measured quantum yield about each component.

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Design and construction of a high energy e-VMI for attosecond imaging

Paul Dababrata 김태규

부산대학교 화학과

The electron localization of atomic gas or dissociative molecules is the important arena of dynamics study. To obtain the detail of dynamics, the translational energy distribution and recoil anisotropy parameters of photoelectron are very essential and more challenging, especially in the presence of strong field, and these two parameters may extract simultaneously from the velocity map imaging (VMI) spectrometer. We constructed a high energy resolution electrostatic lens with multielectrode concept which offers to precisely control the field distribution along the whole spectrometer, for resolving photoelectron energies up to 1KeV. SIMION simulation of electron trajectories in an electric field has been performed. The larger number of electrodes can give a better control over the field distribution along the spectrometer, has smoother field gradients and thus better energy resolution. The test of this system will be presented in terms of the kinetic energy and angular distribution of photoelectron.

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Synthesis of luminescence Silica Nano-particles by Eu(III) Complexes-Incorporated on Silica Nano-Ball.

정용광 강준길*

충남대학교 화학과

Highly luminescent Eu(III) complexes, Cs[Eu(dbm)4] (1) and [Eu(dbm)3phen] (2) (dbm = dibenzoylmethanido, phen = 1,10-phenanthroline) were synthesized and their luminescence properties were investigated. Exciting the Eu(III) complexes with near-UV light resulted in sensitized red luminescence by a transfer of energy from the triplet excited state of dbm to the Eu(III) ion. Although phen has been used as a sensitizer in rare earth complexes, the phen excitation route was forbidden in 2. The Eu(III) complexes were incorporated into the silica nanoparticles as outer-shell or core-shell by a modified St?ber synthesis. For 2, the capsulation increased the luminescence intensity by more than twice. The incorporations of 1 and 2 into the core-shell of silica nanoparticles reduced the luminescence. However, the thermal stabilities of the complexes were significantly enhanced by the encapsulation into silica nanoparticles. To increase thermal stabilities, silica as thermal protector was capsulated on Eu(III) complexes-incorporated silica nano-ball. As a results, thermal stabilities and photo-luminescence were increased more than encapsulated Eu(III) complexes by silica as outer-shell.

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Assessment of DFT Functionals for Al clusters

PARANTHAMANSELVARENGAN 김중한[1] 김태규

부산대학교 화학과 [1]가톨릭대학교 화학과

Aluminum clusters are one of the important metal clusters in superatom chemistry. These clusters with exceptional stability exhibit some of the properties of elemental atoms. In the present investigation, we have performed a benchmarking study on hybrid, hybrid-meta, and meta-generalized gradient approximation (GGA) density functional methods for Aluminum (Al) clusters. The molecular structures and vibrational frequencies of Al clusters have been obtained using Density functional methods. Further, the performance of the functionals have also been assessed by calculating vertical ionization energy for neutral Al clusters, and vertical electron detachment energy for anionic Al clusters along with cohesive energy and dissociation energy. The calculated structural parameters, vibrational frequencies and energetical parameters were compared with available experimental and high-level ab initio calculated results. Our calculations indicate that M06-2X functional provide better results in comparison with other studied functionals, whereas PBE0, mPW1PW91, and TPSSh functionals give reasonable trend while studying structural and energetical parameters. Similarly, B3LYP and M06-L functionals were in poor agreement with available experimental and high level theoretical results. These results indicate that mixing of some exact exchange energy improves the calculated results.

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Reduction potential of heavy metal complexes using relativistic effective core potentials

김형준 이윤섭*

한국과학기술원(KAIST) 화학과

Reduction potential of metal complexes is an important research field of the redox flow battery. Theoretical prediction using density functional theory (DFT) is a popular and widely used method. Nonrelativistic approach using DFT and all electron basis sets shows comparable results with the experimental findings for fourth-row metal, iron, complexes.1) For the heavier metal complexes, such as 5th- and 6th-row metal, nonrelativistic calculation with all electron basis sets is no longer valid due to their large relativistic effects. One way to include the relativistic effect is to use relativistic effective core potentials. (RECPs) Ruthenium and osmium atom which have the same number of valence electron with iron atom are tested. Bipyridine, water and ammonia ligands are complexed to the metal atom. Hybrid functional, B3LYP and PBE0, are tested. A geometry optimization is done with stuttgart small core RECPs for metal atoms and 6-31G* for other light atoms. Single point energy is calculated using larger basis sets, 6-31+G* for light atoms and solvent environment is considered through the implicit solvation model. The inclusion of the cavity creation energy and the addition of basis sets describing d-orbital is carried out to improve the theoretical accuracy. 1) H. Kim, J. Park, Y. S. Lee, manuscript in progress

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The Inner-Sphere Electron Transfer Single Iodide Mechanism for Dye-Regeneration in Dye-Sensitized Solar Cells

전지원 **William A. Goddard III[1,*]** 김형준[2,*]

한국과학기술원(KAIST) EEWS [1]California Insitute of Technology [2]한국과학기술원(KAIST) EEWS대학원

During the regeneration of the oxidized dye in dye sensitized solar cells (DSSC), the redox couple of I-/I3- reduces the photo-oxidized dye. The simplest mechanism would be a direct charge transfer mechanism from I- to D+ [D+ + I- -> D0 + I], called the Single Iodide Process, SIP. How-ever this is an unfavorable equilibrium because the redox potential of I?/I- is 1.224 V vs. SHE, which is 0.13 V higher than that of the dye. This led to the postulating of the Two Iodides Process (TIP) [(D+…I-) + I- -> (D…I2-) -> D0 +I2-)] for a sufficiently high reducing power, but TIP is not consistent with either the recent experimental data suggesting the first-order kinetics or recent time-resolved spectroscopic meas-urements. To resolve this conundrum, we used quantum mechanics including Poisson Boltzmann solvation to exam-ine the electron transfer process between I- and D+ for the Ru(dcb)2NCS2 or N3 dye. We find that I- is attracted to the oxidized dye positioning I- next to the NCS. At this equilibri-um position, the I- electron is already 40% transferred to the NCS, showing that the redox potential of I- is well matched with the dye. This matching of the redox potential occurs because I- is partially desolvated as it positions itself for the Inner-Sphere Electron Transfer (ISET). The previous analyses all assumed an outer-sphere electron transfer process. Thus our ISET-SIP model is consistent with the known redox po-tentials and with recent experimental reports. With the ISET-SIP mechanism, one can start to consider how to enhance the dye regeneration kinetics by redesigning ligands to maximize the interaction with iodide.

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Wavepacket dynamics of diazirine in the S1 state

박영춘 안희선[1] 백경구[1,*] 이윤섭[*]

한국과학기술원(KAIST) 화학과 [1]강릉원주대학교 화학과

In this poster, we present quantum mechanical dynamics of diazirine in the S1 state. As reported in the previous experiment, Fano resonance in S1 state dissociation is obserbed. This is due to the resonance of potentials in two symmetric and asymmetric C-N vibration coordinates. Following the experimental results, two restricted dimensions describing C-N vibration were set in the theoretical study. The potential energy surfaces (PESs) of the S0, S1 states were obtained from CASSCF(10,12)/6-311++G(d,p) and fitted analytically. The spectrums obtained from the wavepacket propagation agreed well with the experiment and the characteristics of dissociation dynamics were discussed as well.

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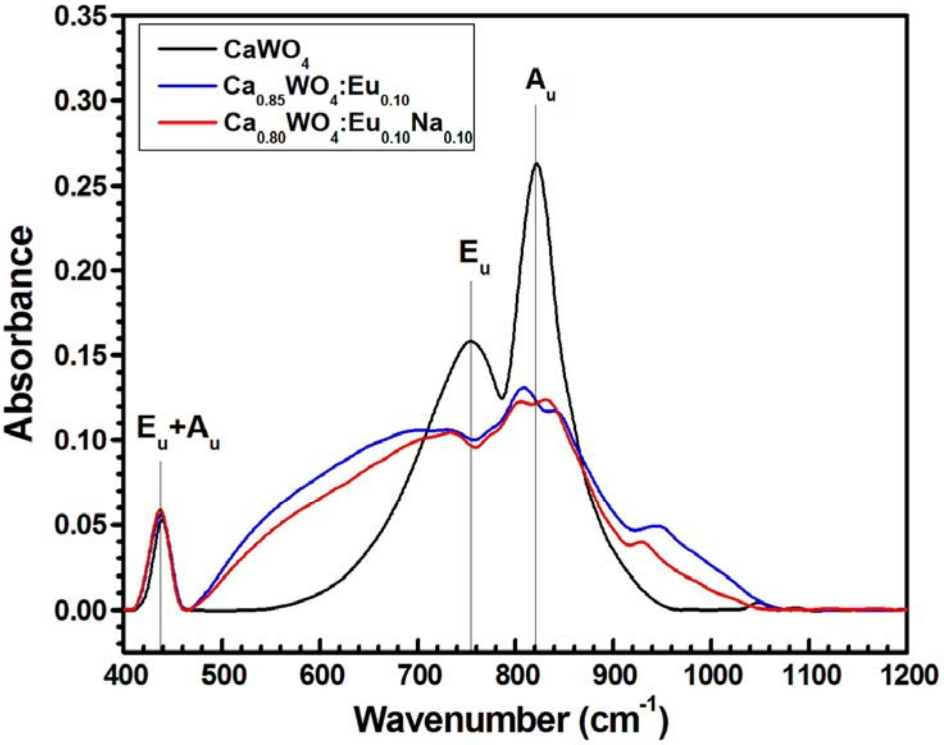
Raman and FT-IR Spectroscopic Studies of Red Phosphors $Ca_{(1-1.5x)}WO_4:Eu_x$ and $Ca_{(1-2x)}WO_4:Eu_x,Na_x$

조선욱

신라대학교 신소재공학과

Red phosphors $Ca_{(1-1.5x)}WO_4:Eu_x$ and $Ca_{(1-2x)}WO_4:Eu_x,Na_x$ were synthesized with different concentrations of Eu^{3+} ions by using a solid-state reaction method. The crystal structure of the red phosphors were found to be a tetragonal system. X-ray diffraction (XRD) results showed the (112) main diffraction peak centered at 2 theta=28.71°, and indicated that there is no structural difference with or without the Na^+ ions in the crystals. Clearly, both Na^+ and Eu^{3+} ions replace the Ca^{2+} ions in the host material $CaWO_4$. Also, the photoluminescencce spectra show the same optical properties caused by the same crystal structue. Raman spectra show that all the gerade normal modes occur at the same frequencies with same shapes. However, the FT-IR spectra show that the ungerade normal modes have shifted positions and different shapes, caused by differnt masss of Eu^{3+} and Na^+ ions. * Correponding E-mail: swcho@silla.ac.kr (S.-W. Cho)


CaWO$_4$
Ca$_{0.85}$WO$_4$:Eu$_{0.10}$
Ca$_{0.80}$WO$_4$:Eu$_{0.10}$Na$_{0.10}$
A$_u$
E$_u$
E$_u$+A$_u$
Absorbance
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
400
500
600
700
800
900
1000
1100
1200
Wavenumber (cm^{-1})

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High-Yield thermal decomposition Synthesis of Metal Nanocrystals

김창현 명윤 임형순[1] 조용재 정찬수 임영록 백승혁 이강호[2] 박정희

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자공학 [2]경북대학교 화학과

We have developed a method which can produce nanometer size metal particles in a large scale. This method combines a thermal decomposition of metal carbonyls with a collision induced clustering. Metal carbonyls are thermally decomposed with a hot filament and resultant bare metal atoms undergo collisions to produce nanometer size metal particles. This method requires a very simple experimental setup even though it is a high efficiency production method. Using this method, we have produced, high purity Fe, Mo, W, Co nanoparticles.

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Effect of solvent viscosity on the kinetics of 10-23 deoxyribozyme

김선영 정지원[1] 배소현[1] 연규진[1] 김성근[1]

서울대학교 생물물리 및 화학생물학 [1]서울대학교 화학부

10-23 deoxyribozyme is a DNA enzyme which cleaves specific RNA sequence through a series of distinct reaction steps involving enzyme-substrate binding, substrate cleavage, half-substrate dissociation, full-substrate dissociation, and an erratic process called looping. The reaction rate can be strongly dependent on the viscosity of solvent, especially in a diffusion-controlled reaction step. At high viscosity, for example, Kramers' theory predicts that the reaction rate is inversely proportional to viscosity. We studied the effect of solvent viscosity on the reaction rate of each enzymatic step for 10-23 deoxyribozyme by single molecule total internal reflection fluorescence measurement.

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Field Emission properties of a three-dimensional network of single-walled carbon nanotubes inside porous silicon

박태희 이종택 이휘건*

한양대학교 화학과

We synthesize well-distributed single-walled carbon nanotubes (SWCNTs) on the top surface and inside the pores of a PS layer three-dimensional (3D) SWCNTs inside PS using thermal chemical vapor deposition (CVD).We measured field emission (FE) properties of SWCNTs synthesized on the inside pores of a porous silicon (PS) substrate, as well as on the top surface of a PS substrate. Their turn-on fields and emission current densities are measured and compared with those of other types of SWCNTs in similar environments. Investigation of field emission properties of SWCNTs synthesized on the inside pores of a porous silicon (PS) substrate reveals a low turn-on field of about 2.25 V μm?1 at 10 μA/cm2 and a high field-enhancement factor (6182) compared with other samples.

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Resonance Enhanced Multi-Photon Ionization and UV-UV hole-burning Spectroscopic Studies of Jet-cooled acetanilide derivatives

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경상대학교 화학과 [1]서울대학교 화학부

In this work, we present the conformational investigations and photochemistry of jet-cooled methacetine (MA) and phenacetine (PA) using one color resonant two-photon ionization (REMPI), UV-UV hole-burning and IR-dip spectroscopy. MA and PA are derivatives of acetanilide, substituted by methoxyl, ethoxyl group in the para position of acetanilide, respectively. Moreover, we have investigated conformational information of the acetanilide derivatives (AAP, MA and PA)-water. In this poster, we will present and discuss the solvent effects of the hydroxyl group of acetanilide derivatives in the excited state.

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Theoretical Study for The Mechanism of DDQ Mediated Oxadiazole Formation.

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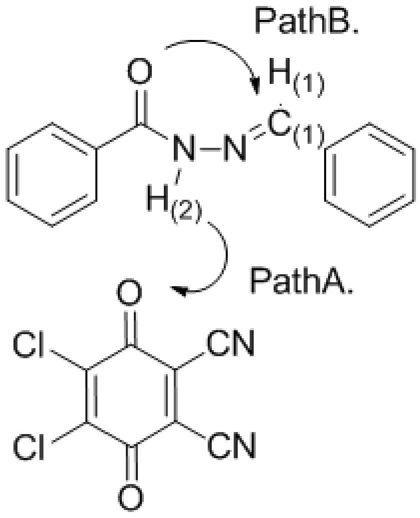
DDQ(2,3-dichloro-5,6-dicyano-1,4-benzoquinore)는 benzoquinone 중의 하나로 산화제로써 여러 유기반응에 쓰인다. DDQ 를 이용한 대표적인 유기반응에는 알코올의 탈수소반응과 산화반응, 벤질기의 oxidative deprotection 가 있다. DDQ 반응 메커니즘의 중요한 중간체로써 charge-transfer complex 가 형성되는 것으로 알려져 있다. 본 연구는 DDQ 을 이용한 2,5-diphenyl-1,3,4-oxadiazole 생성반응의 메커니즘을 알아보기 위해 이론적 계산을 수행하였다. 반응물, 생성물, 중간체에 대한 모든 전자 구조와 에너지는 M062X/6-31+G(D,P) 수준에서 계산되었다. 반응메커니즘으로써 DDQ 에 의해 반응물의 수소 ($H_{(2)}$) 가 떨어져 나가는 과정에서 charge-transfer complex 를 형성하는 경로 (PathA) 와 반응물의 Carbonyl 의 산소가 탄소 ($C_{(1)}$) 를 공격하면서 링이 형성되는 과정에서 charge-transfer complex 가 되는 경로 (PathB) 를 고려할 수 있다. 위의 두 가지 반응 경로의 에너지 프로파일을 계산하여 어떤 메커니즘에 의하여 반응이 진행되는지 알아보았다.


PathB.
O
H(1)
N
N
C(1)
H(2)
PathA.
O
Cl
CN
Cl
CN
O

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Effective screening strategy for CO2 electro-catalysis

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Electro-catalytic reduction of carbon dioxide (CO2) has been in the spotlight since the global warming issue has been one of scientist’s biggest concerns. Carbon monoxide (CO) is the most attractive species among various types of products from CO2 reduction because it has a variety of uses. However, no electro-catalysts that accelerate the electro-reduction of CO2 with a low overpotential at reasonable current densities have been developed, and what aspects of and which materials play the important role in the improved catalytic efficiency for CO2 electro-reduction are not fully understood yet. Here, we focus on elucidating fundamental reaction steps for CO2 reduction to CO and suggest a new fundamental guideline for efficient electro-catalyst to convert CO2 to CO based on quantum mechanics (QM).

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Sensitized and luminescence properties of Eu(III) complex with Schiff base, o-N2O4, and phen

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Europium(III) complexes with homoleptic Schiff-base, o-N2O4, and mixed o-N2O4 and phen (phen = 1,10-phenanthroline) were synthesized and their photophysical properties were investigated. The schiff base, o-N2O4H2 (o-N2O4H2 = 2,2'-(1E,1'E)-(1,2-phenylenebis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)dibenzoic acid) , used in this work as chelating ligand was synthesised using 2-carboxybenzaldehyde and o-phenylenediamine. The synthesized Eu(III) complexes were confirmed with EA, ICP and TGA. The Eu(III) complexes excited at UV produced sensitized red-luminescence. The excitation spectra measured by monitoring the red emission proved that the energy transfer took place effectively via the o-N2O4 ligand, no matter whether phen was included or not in the complex. In this presentation, the energy transfer between the o-N2O4 and the europium(III) ion will be precisely discussed.

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Synthesis and Characterization of Luminescent Polymer Nanoballs Incorporated with Eu(III) Complexes with Application to Detection of Some Cations in Water

강명현 강준길*

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Luminescent polymer nanoballs were synthesized by self-organization process via two steps. First, a solution of a mixture of Eu(III) complex and polymer dissolved in THF solvent was gradually diluted with water and then the volatile THF solvent was gradually evaporated from the mixture. The polymers used in this work were poly(methylmethacrylate) (PMMA). The size of Eu(III)-encapsulated polymer nanoball was controllable by adjusting the concentration of the complex and the volume ratio of water to THF. The morphology of the fabricated polymer nanoball was confirmed by FE-SEM. The photophysical properties of polymer nanoballs were investigated by excitation and luminescence spectra. Also we observed cation can give rise to emission quenching. The cation quencher used in this work were Cu2+,Cd2+and Cr3+.The emission quenching of Eu-(III)-encapsulated polymer nanoball were investigated by UV, luminescence spectra.

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Synthesis of three dimensional (3D) nickel nanostructure and its application to supercapacitor.

류일환 주은리 김형민 임상규*

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Supercapacitor is an important candidate for a next generation energy storage device because of its extraordinary electrical properties. Three-dimensionally nanostructured electrode is widely studied as ideal electrode architecture for the supercapacitor since it can provide direct paths for efficient charge transport along the three-dimensional (3D) network. Nickel is one of the widely developed and commercially available conductive materials due to its great stability and low price. In this work, we fabricated nickel electrodes with 3D nanostructures using polystyrene nano-opal substrate. We also electrodeposited several other transition metals onto these 3D nanostructures and investigated their morphological and electrochemical properties.

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Synthesis and phosphorescence properties of bright green emitting oxynitride phosphor

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Eu2+, Nd3+-doped SrAl2Sb0.5ON green phosphors were synthesized ammonia nitridation method. First, SrAl2Nx was prepared in liquid ammonia, following by thermal treatment. Second, the initial materials SrSi2Nx and BN, Sb2O3, Nd2O3, Eu2O3 were taken in stoichiometric properties. The mixture was fired at 1450 ?C for 6 h under NH3 gas. Then it was treated at mixed with Eu2O3 and some metal nitrides. Photophysical properties of SrAl2Sb0.5ON:Eu2+,Nd3+,B3+ were characterized luminescence spectroscopy. It was found that Eu2+, Nd3+ doped SrAl2Sb0.5ON phosphor excited at blue light produced strong green emission and long-term phosphorescence. Furthermore, the prepared phosphors were casted on blue LEDs and their luminescence properties were investigated.

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Enhancement of photo-current conversion efficiency in quantum-dot-sensitized solar cell by using carbon nanotubes

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Cadmium sulfide (CdS) and cadmium selenide (CdSe) are sequentially assembled onto a nanocrystalline TiO2 film to make a CdS/CdSe co-sensitized photo-electrode for QD-sensitized solar cell application by successive ionic layer adsorption and reaction (SILAR) method. The results show that CdS and CdSe QDs have a complementary effect in the light harvest and the performance of QDs solar cell is strongly dependent on the number of deposition layer of each CdS and CdSe. Single-walled nanotubes (SWNTs) are incorporated with our CdS/CdSe QD solar cell by mixing them with TiO2 film to enhance electron transfer. Absorbance at low wavelength is increased. So photo-current conversion efficiency of cell is increased.

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$C_{20}Li_y$(y=1,2,8,20)의 원자구조와 IR 스펙트라 계산: 혼성 범밀도 함수법

이설 이기학[1,*]

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$C_{20}Li_y$(y=1,2,8,20) 분자에 대하여 원자구조의 특성과 IR 스펙트라를 범밀도 함수 법으로 계산하였다. 각 분자의 원자 구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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Excited-State Dynamics of Carotenoids and Dye Molecules Attached to TiO2 Nanoparticles

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광주과학기술원(GIST) 물리화학부

TiO2 nanoparticles which have a high density of state are eager to trap electrons and carotenoids which are susceptible to oxidation can inject electrons into TiO2 nanoparticles. Thus, carotenoids and TiO2 nanoparticles can be an ideal model system for electron transfer. It is known that polar carotenoid, all-trans-8’-apo-β-caroten-8’-oic acid injects electrons from its S2 state into the conduction band of TiO2 nanoparticle and the electrons recombine with longer time scales into the carotenoid. The photoinduced electron injection and recombination dynamics between all-trans-8’-apo-β-caroten-8’-oic acid and TiO2 nanoparticles will be shown by transient absorption measurements in ultrafast time scales by exciting the S2 state of the carotenoid.Organic and inorganic dyes which have functional groups such as hydroxyl and carboxyl group, Coumarin 343, [Ru(bpy)3]2+, alizarin, (NH4)2[Ti(cat)3]?2H2O, and catechol can also be utilized in the electron transfer study with TiO2 nanoparticles. We will investigate the excited state dynamics of these dyes and electron transfer to TiO2 by femtosecond transient absorption measurements.All-trans-8’-apo-β-caroten-8’-oic acid has been synthesized from oxidation of 8’-apo-β-carotenal with Ag2O for an efficient attachment to the TiO2 surface. TiO2 nanoparticle has been synthesized from TiCl4 in a colloidal solution. All-trans-8’-apo-β-caroten-8’-oic acid will then be added to the TiO2 colloidal solution.

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$C_{20}H_{20}Li_y$(y=1,2,20)의 원자구조와 IR 스펙트라 계산 :혼성 범밀도 함수법

이설 이기학[1,*]

원광대학교 생명나노화학부 [1]원광대학교 화학과

$C_{20}H_{20}Li_y$(y=1,2,20) 분자에 대하여 원자구조의 특성과 IR 스펙트라를 범밀도 함수 법으로 계산하였다. 각 분자의 원자 구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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Excitation-dependent excited-state dynamics of carotenoids by femtosecond transient absorption spectroscopy

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광주과학기술원(GIST) 물리화학부

Carotenoids play very important roles in photosynthesis such as light harvesting and photo-protection. The carotenoid 8'-apo-β-carotenal contains carbonyl group on one terminal and belongs to Cs symmetry slightly off from the C2h symmetry of most carotenoids. This carotenoid shows very complex excited-state dynamics between three singlet states ; the bright S2 and the dark S1 excited state and the ground S0 state. In this research, we will investigate excitation dependent excited state dynamics of 8'-apo-β-carotenal by using 400nm and 500nm excitation pulses in femtosecond transient absorption measurements.To measure transient absorption signal, two femtosecond laser pulses, pump and probe pulses, are required. Pump pulses which excites carotenoids' S2 excited state are generated by the second harmonic generation of fundamental pulses in a BBO crystal and by a noncollinear optically parametric amplifier (tunable between 450nm and 650nm). Probe pulses generated by white light generation in a sapphire window covers a broad range of wavelengths between 450 nm and 750nm. By changing time delay between two pulses, we can measure time-dependent transient absorption intensities and excited-state dynamics of the carotenoid down to 50fs time resolution can be obtained by analyzing the transient absorption results.

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Calculation of potential energy curves of excited states of molecular hydrogen by multi-reference configuration-interaction method

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아주대학교 화학과

For all the excited states of a hydrogen molecule up to n = 3 active spaces, potential energy curves (PECs) are obtained for values of the internuclear distance R in the interval [0.5, 10] a.u. within an accuracy of 1 × 10-4 a.u. (Hartree) compared to the accurate PECs of Kolos, Wolniewicz, and their collaborators by using the multi-reference configuration-interaction method and Kaufmann's Rydberg basis functions. It is found that the accuracy of the PECs can be further improved beyond 1 × 10-4 a.u. for that R interval by including the Rydberg basis functions with angular momentum quantum numbers higher than ℓ = 4.

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$H_2@C_{20}H_{20}$(charge=1,-1)의 원자구조와 IR 스펙트라 계산 : 혼성 범밀도 함수법

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$H_2@C_{20}H_{20}$(charge=1,-1)분자에 대하여 원자구조의 특성과 IR 스펙트라를 범밀도 함수 법으로 계산하였다. 각 분자의 원자 구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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Prediction of oxidation potentials of TEMPO and its derivatives using density functional theory calculations.

이상연

경북대학교 응용화학과

Density functional theory calculations have been performed to calculate the redox potentials of TEMP and its derivatives in acetonitrile. The geometries have been optimized with the M062X/6-31+G** level, the single point energy calculations have been performed with the M062X/6-311+G** level at the optimized geometries, and the solvation energies have been calculated with the SMD/M062X/6-31+G** level. The calculated absolute redox potentials have been converted to the standard redox potentials using the experimental redox of TEMPO. The calculated redox potentials gives the mean absolute error of 0.1 V for the test set. This procedure has been applied to predict the standard redox potentials of some TEMPO derivatives. The calculated standard potentials have been used to screen TEMPO derivatives for redox flow battery.

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Electroporational detection of a cancer cell by AFM and fluorescence microscopy

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We demonstrate the feasibility of discriminating a cancer cell from a normal cell using AFM (atomic force microscopy) and fluorescence microscopy. When the cell is subject to an electric field (of ~1 kV), pores are produced on the cell membrane. We found that the pore size and the voltage to create the pore on the cancer cell membrane are significantly different from those for the normal cell membrane. This phenomenon is believed to be due to the differences in the membrane elasticity and intracellular structure between the two types of cell.

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Fluorescent probes with anti-carcinogenic effect

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서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과 [2]한국화학연구원 나노기술융합연구단 [3]서울대학교 자연과학부/생물물리 및 화학생물학과 [4]동국대학교 약학대학 약학과

A set of naturally-occurring compounds with a known anti-carcinogenic effect were turned into highly fluorescent compounds by a simple photochemical reaction. The new compounds, which may become promising fluorescent probes, were found to share similar photophysical characteristics (such as a high fluorescence quantum yield and large two-photon absorption cross section) as well as similar chemical properties with each other. Among their notable chemical traits are their strong cytotoxicity toward cancer cells at the same time with minimal cytotoxicity toward normal cells, which have been verified in a series of cytotoxicity tests involving various cell lines. The selective nature of anti-carcinogenic effect of these highly fluorescent probes raises the prospect of using these compounds as a highly efficient imaging agent with a potent therapeutic effect against cancer.

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$H_3@C_{20}H_{20}$의 원자구조와 IR스펙트라 계산 : 혼성범밀도 함수법

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$H_3@C_{20}H_{20}$ 분자에 대하여 원자구조의 특성과 IR 스펙트라를 범밀도 함수 법으로 계산하였다. 각 분자의 원자 구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합 특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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$C_{20}H_{17}br_3$의 원자구조와 IR스펙트라 계산 : 혼성 범밀도 함수법

이설 이기학[1,*]

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$C_{20}H_{17}br_3$ 분자에 대하여 원자구조의 특성과 IR 스펙트라를 범밀도 함수 법으로 계산하였다. 각 분자의 원자 구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합 특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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$CH_y(3-y)H@C_{24}(y=1,2)$의 원자구조와 IR스펙트라 계산 : 혼성 범밀도 함수법

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$CH_y(3-y)H@C_{24}(y=1,2)$분자에 대하여 원자구조의 특성과 IR 스펙트라를 범 밀도 함수법으로 계산하였다. 원자구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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$H_y@C_{24}$(y=1,2)의 원자구조와 IR스펙트라 계산 : 혼성 범밀도 함수법

이설 이기학[1,*]

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$H_y@C_{24}$(y=1,2)분자에 대하여 원자구조의 특성과 IR 스펙트라를 범 밀도 함수법으로 계산하였다. 원자구조와 IR 스펙트라의 진동수 특성을 분석하였다. 또한 분자의 원자 결합특성에 미치는 Basis set superposition error 를 분석하였다. 모든 분자들은 B3LYP/6-31g(d,p)의 수준에서 최적화 하였다.

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Multireference configuration interaction (MRCI) 방법에 의한 질소 분자의 dipole allowed state 들인 b', c', e' $^1\Sigma_u^+$와 b, c, o $^1\Pi_u$에 대한 퍼텐셜 곡선 계산

이천우* 김영록

아주대학교 화학과

질소 분자의 광이온화 스펙트럼의 계산에 필요한 dipole allowed state 들인 b', c', e' $^1\Sigma_u^+$와 b, c, o $^1\Pi_u$ 에 대한 퍼텐셜 에너지 곡선 (PEC)을 Multireference configuration interaction (MRCI) 방법에 의해 계산을 하였다. 질소분자의 이들 state 들에 대한 PEC 의 계산은 매우 까다로운 것으로 정평이 나 있는데, Gilmore 가 1965 년에 RKR 방법에 의해 일부 퍼텐셜에너지 곡선을 얻었고, Stahel 등은 Lefevbre-Brion 의 deperturbation 방법을 개량시켜 이들 state 들의 diabatic PEC 와 coupling matrix element 들의 값을 얻었다. 이들의 연구에 기반하여 Spelsberg 와 Meyer 는 이들 state 들의 이론적인 계산의 획기적인 전기를 마련하였다. 본 발표에서는 Spelsberg 와 Meyer 의 일을 재현하여 이들 state 들의 PEC 를 얻은 후 이들 PEC 를 통해 photionization spectrum 의 multichannel quantum defect theory (MQDT) 방법에 의한 계산에 필요한 quantum defect parameter 들의 계산에 대해 시도한 것을 발표할 예정이다.

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Nanodiamond-nanocrystal FRET pair for long-term FRET measurement

임영빈 강주연[1] 김성근[1]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Recently, single-molecule fluorescence resonance energy transfer (smFRET) is widely used to investigate structures, motions, and kinetics of biomolecules. Despite the remarkable success of the smFRET technique, a notable shortcoming of smFRET becomes increasingly evident. That is, the window of detectable time in smFRET is very severely limited due to the photobleaching of organic dyes. Although there have been attempts to circumvent this problem, the most direct way to address it is to develop a FRET pair that does not exhibit photobleaching for a long time. In this study, we developed and demonstrated a long-term FRET pair for smFRET using a biotinylated fluorescent nanodiamond (FND) and a streptavidin-conjugated nanocrystal linked together by the biotin-streptavidin interaction.

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Carbon-13 solid-state NMR study of some arylboronic acids

오세웅

목포대학교 화학과

Boronic acids are used extensively in organic chemistry as chemical building blocks and intermediates and the most widely used example is the Suzuki-Miyaura coupling, which is useful synthetic route to biaryl compounds. The diverse number of applications of boronic acids means that an understanding of the structural and electronic properties of these compounds is imperative. Carbon-13 chemical shifts of the ipso carbon which is attached to boron of arylboronic acids have not been reported with high precision. Although they have been reported, they were not determined accurately. This is due to residual dipolar coupling and J coupling due to the quadrupolar nuclei ($^{10/11}B$) attached to the carbon. The ^{13}C NMR peak therefore exhibits fine structure due to directly bonded quadrupolar nuclei. The fine structure may or may not be clearly resolved from other peaks in the ^{13}C MAS NMR spectrum, depending on the compound. If the fine structure overlaps with other peaks, it is very difficult to determine the chemical shift of the ipso carbon. In the present work, we report accurate chemical shifts of the ipso carbons of arylboronic acids and one bond spin-spin coupling constants between ^{13}C and ^{11}B in the same compounds.

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Theoretical study of three Guanine-Cytosine pairs in water by combining quantum mechanics and statistical mechanics

임슬기 함시현*

숙명여자대학교 화학과

Molecular interactions between the DNA bases and water molecules are critical in nature. Yet, the effect of water on the stability of DNA bases is not fully understood. Here, we report our theoretical study on three Guanine-Cytosine pairs of DNA bases solvated in water based on the combined method of quantum mechanics and statistical mechanical theory of liquids. B3LYP/6-31+G(d,p) level of theory was used to calculate the direct base-pair interaction energies, and the effect of solvent is quantified by the electronic reorganization energy and the solvation free energy using statistical mechanical theory of liquids. We discuss whether Guanine-Cytosine Watson-Crick pair is most stable combination in aqueous environments.

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카바졸 기반 물질의 비정질 박막에서 원자가 전자상태의 에너지 분포에 의한 분자들 간의 상호작용 효과

조양진 위경량 강상욱*

고려대학교 소재화학과

카바졸 기반 물질에서 비정질 고체의 occupied 전자 구조에 대한 분자간 상호작용 효과에 관한 계산은 유기 고체의 이합체들이 무질서한 방향으로 구성되어 있는 가정하에 조사되었다. 전자적 에너지 상태는 많은 수의 이합체들이 무질서하게 분포된 상태에서 계산되었으며 이러한 분포은 semiempirical van der Waals density functional theory 를 이용하여 계산하였다. 에너지레벨 분할과 같은 분자들간의 상호작용은 분자들의 무질서한 분포에 의해 일어난다. 결과적으로, frontier occupied energy 상태는 Gaussian distributions 에 의해 다음을 묘사하고 있다. 1) 주된 분포의 전체 너피를 half maximum 80?110 meV 에서 relaxation 하였고 2) 중심으로부터 150 meV 의 를 벗어나는 부분을 shoulder 로 분리하였다. 이러한 shoulder 들이 나타나는 이유는 더 많은 단단한 구조의 이합체들의 집합에 기인한 것이다.

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Investigation of S_1 Vibrational Structures of DMS and DMS-d_6 and Mode-specific Dynamics of DMS-d_3

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한국과학기술원(KAIST) 화학 [1]한국과학기술원(KAIST) 화학과

We observed the S_1 ($^1B_1$) vibrational structures of DMS, CH_3SCH_3 and DMS-d_6, CD_3SCD_3 for the first time by CH_3 (CD_3) photofragment excitation (PHOFEX) spectroscopy and velocity map ion imaging (VMI). Due to strong electronic coupling with repulsive S_2 ($^1A_2$) state, every vibrational peak shows broad line width (~100cm^{-1}) and distinct perpendicular character of anisotropy (~-0.65). Fitting each peak into Lorenz function determines the S_1 life time about ~50fs. Such a short life time makes the mode-specific reaction dynamics overcome intramolecular vibrational energy redistribution (IVR) despite several vibrational degrees of freedom of polyatomic molecules. Herein, we investigated mode-specific photodissociation dynamics of both CH_3 and CD_3 fragments for CH_3SCD_3. Strikingly, C-S-C symmetric stretching mode enhances the CD_3 dissociation yield 2.1 times as CH_3. Angular distribution is also searched, but it shows no difference between CH_3 and CD_3. Now, we believe the vibrational wavefunction for the symmetric stretching mode is extended to S-CD_3 reaction coordinate more than S-CH_3, and theoretical investigation to prove this is going on.

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Stability of G-quadruplex containing metal ion

김연주 함시현*

숙명여자대학교 화학과

G-quadruplexes are guanine-rich sequences in telomere DNA that are capable of forming a four-stranded structure. G-quadruplex is of biological interest for new anticancer drug target in recent years. Metal ions have been demonstrated to significantly impact the stability and structural polymorphism of G-quadruplexes. Here, using the ab initio quantum chemistry method, we investigate G-quadruplexes containing a metal ion (Na+, K+, Rb+) in a central channel between each pair of tetrad. We perform geometry optimization and frequency analysis to evaluate equilibrium conformation of metal-ion-containing G-quadruplexes, and discuss which of those G-quadruplexs is more energetically stable.

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Ab-initio Calculation Study on the Mechanism of Nitric Oxide Sensor using Rhodium(II) Acetate Complexes with Dansyl-piperazine and Nitric Oxide

양난희 구은희[1,*]

고려대학교 바이오마이크로시스템 [1]한국세라믹기술원 기초소재융합본부/나노IT소재팀

In our exhaled breath includes about 1000 molecular compounds and it’s important to diagnosis of a variety of illness. Especially nitric oxide (NO) called magic molecule because it is related cardiovascular, nervous and immune systems and tumor progression. But it can't be stored in organ cells and quickly reacts with oxygen within a few seconds. Therefore methods of detecting nitric oxide (NO) are diverse such as electrochemical, EPR, chemiluminescent, and fluorescence signaling. We developed the nitric oxide sensors based on the fluorescence-quenching strategy by bonding with NO with transition metal complexes with partially filled d-shells. For various composition contacting different numbers of ligands of fluorophore dansyl-piperazine(Ds-pip) and nitric oxide(NO) with Rh complex; $[Rh_2(AcO^-)_4(Ds\text{-}pip)_x(NO)_y]$, we performed the structures by ab-initio calculation. In results, the molecular structures of Rh-complex are bonded with nitric oxide(NO) shorter and stronger than dansyl-piperazine(Ds-pip). Also we compare the HOMO/LUMO energy level of electronic structures depending on the ligands to explain the “turn on” and “turn-off” state as a mechanism of nitric oxide(NO) detecting sensor.

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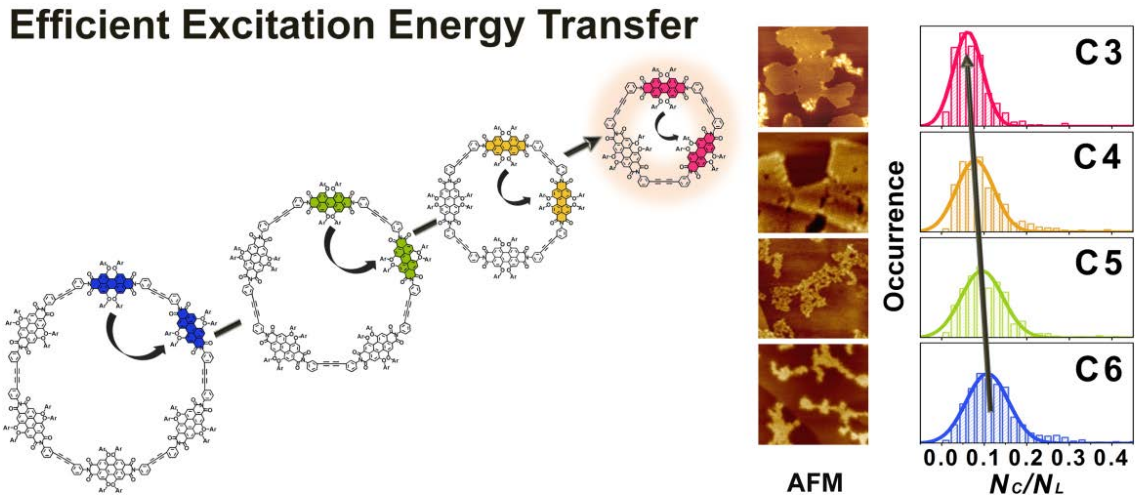
Structure-Property Relationship of Perylene Bisimide Macrocycles Probed by Atomic Force Microscopy and Single-Molecule Fluorescence Spectroscopy

이지은 양재성 유혜진 김동호*

연세대학교 화학과

Properties of a series of acetylene-linked perylene bisimide (PBI) macrocyclic arrays with different ring size composed of three to six PBI dyes were investigated by atomic force microscopy and single-molecule fluorescence spectroscopy. It was demonstrated that the structures of PBI cyclic arrays (CNs, N = 3, 4, 5, and 6) become distorted with increasing the ring size through the atomic force microscopy height images of CNs on highly ordered pyrolytic graphite surface. Moreover, we showed that the fluorescence properties of single CN molecules are affected by the structural changes. The fluorescence lifetimes of CNs became shorter and the fluorescence lifetime distributions became broader due to the structural distortions with increasing the ring size. The polarization trajectories of the single-molecule revealed that CNs show intermolecular Forster-type energy transfer. We have evaluated the excitation energy transfer efficiency of CNs via coincidence measurements; the efficiency of C3 was the highest due to the more defined planar structure compared to the other systems. Consequently, these observations provide evidence that not only PBI macrocycles are promising candidates for artificial light-harvesting complexes due to the efficient excitation energy transfer processes, but also the photophysical properties of CNs are strongly related to the structural rigidity of CNs.


Efficient Excitation Energy Transfer
AFM
Occurrence
C3
C4
C5
C6
0.0 0.1 0.2 0.3 0.4
N_C/N_L

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DNA base pair-Water Interactions: a theoretical study

이진경 함시현*

숙명여자대학교 화학과

The interaction between the nucleic acid bases and water molecules has an important effect in organism. While adenine-thymine Watson-Crick pair has been demonstrated to be most stable in a gas phase, the stability in an aqueous phase remains elusive. Here, we have calculated electronic energy and solvation free energy of four adenine-thymine pairs in water by combining the quantum mechanical method with the 3D-RISM theory, the statistical mechanical theory of liquids. First, we have optimized adenine-thymine Hoogsteen pair, reverse Hoogsteen pair, Watson-Crick pair, and reverse Watson-Crick pair in a gas phase at the B3LYP/6-31+G(d,p) level. We then studied four adenine-thymine pairs solvated in water by combining density functional theory and 3D-RISM theory. Thereby, we discuss the effect of water on the stability of adenine-thymine pairs, and argue whether adenine-thymine Watson-Crick pair is most stable in aqueous environments.

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Theoretical investigation of electronic structure and thermoelectric properties of new quaternary chalcogenides, $Tl_{18}Pb_2M_7Q_{25}$ (M=Ti, Zr and Hf; Q=S and Se)

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포항공과대학교 화학과

Recently, it was reported that C. Sankar *et al*. synthesized new semiconducting quaternary chalcogenides of the general formula $Tl_{18}Pb_2M_7Q_{25}$(M=Ti, Zr and Hf; Q=S and Se). They studied the crystal and electronic structures of the compounds. The heavier group 4 element causes an decrease of the band gap as calculated for $Tl_{18}Pb_2Ti_7Se_{25}$ (0.18eV) and $Tl_{18}Pb_2Zr_7Se_{25}$(0.10eV), and incease of the Seebeck coefficient. These trends in the size of band gap can readily be understood based on electronegativity differences, because a more electronegative anion (S compared to Se) causes a lower lying valence band, and a more electronegative cation (Zr vs Ti) a higher lying conduction band, and thus a larger gap between valence and conduction band.All of these compounds exhibit semiconducting behavior, with band gaps tunable between 0.10 to 1.0eV by changing the metal and/or chalcogen atoms: all selenides and the Ti sulfide exhibit gaps below 0.5eV and may thus be of interest for thermoelectric energy conversion, in combination with their complex crystal and the large (positive) Seebeck coefficient of the undoped materials.[1]In this study, we have investigated the bandstructures by using density functional theory and also calculated thermoelectric properties of these compounds, and predict the properties of the corresponding Tellurides.[1] Sankar, C.; Becker, A.;Assoud, A.; Kleinke, H. *Inorg. Chem.* 2013, *52*, 1895.

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Infrared Probing of Hydrogen-Bond Structures and Dynamics in Aqueous $NaPF_6$ Solutions

손혜원 박성남*

고려대학교 화학과

Hydrogen-bond structure and dynamics in aqueous $NaPF_6$ solution were studied by using FTIR, IR pump-probe, and 2DIR spectroscopy. FTIR spectroscopy had revealed two spectrally distinct peaks in the region of OD stretch. The broad low frequency peak was corresponding to the OD stretch mode of HOD molecules forming hydrogen-bond with other water molecules (denoted OD_w) and the high frequency peak at 2670 cm^{-1} was assigned to the HOD molecule directly interacting with the anion (denoted OD_A). Hydrogen-bond dynamics in aqueous 6 M $NaPF_6$ solution were studied by using IR pump-probe and 2DIR experiments. The vibrational relaxation of OD_A was found to be much slower than that of OD_w. Orientational anisotropy decay was analyzed using the wobbling-in-a-cone model. The results suggest that OD_w should have more restricted and slower wobbling motion than OD_A and the full orientation diffusion motion of OD_w and OD_A should be similar. Hydrogen-bond exchange, which is accompanied by the full orientational diffusion of water molecules, was found to occur with a time constant of about 8 ps. 2DIR experiments were performed to directly measure the hydrogen-bond exchange rate constants in aqueous 6 M $NaPF_6$ solution

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Rotational Dynamics of Metal Azide Ion Pairs in Dimethylsulfoxide Solutions

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Azide ion is an excellent vibrational probe for studying ion-ion and ion-dipole interactions in solutions because its frequency is sensitively dependent on its local environments. When azide ion forms contact ion pairs with cations in dimethylsulfoxide (DMSO), free azide ion and contact ion pairs are spectrally well distinguished in FTIR spectra. Here, we investigated vibrational population relaxation, $P(t)$, and orientational relaxation dynamics, $r(t)$, of free azide ion and contact ion pairs (LiN_3, NaN_3, NH_4N_3, MgN_3^+ and CaN_3^+) in DMSO by IR pump-probe spectroscopy. For metal azide ion pairs, the metal ion slowed down the vibrational relaxation of azide ion by acting like a thermal insulator. Bi-exponential behavior of $r(t)$ was analyzed in the wobbling-in-a-cone model. The long time component of $r(t)$ of free azide ion was found to be viscosity-dependent. The wobbling motion of azide ion within the frame of metal azide ion pairs was weakly dependent on the countercation. When the overall orientational relaxation of metal azide ion pairs was analyzed by the extended Debye-Stokes-Einstein equation, it was well described under stick or super-stick boundary conditions due to a strong interaction between the metal ion and DMSO molecules. Our experimental results provide important insight in understanding the rotational dynamics of small ionic species in polar solvents when the size of the ionic species is smaller than or comparable to that of the solvent molecule.

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Reactions of Iron atoms with molecular nitrogen, Infrared spectra of Fe(N2H), Fe(NN)x, (x=1-5), and Fe(NN)3-

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The experiments for laser ablation and matrix isolation infrared spectroscopy was employed for making the iron dinitrogen complexes Fe(N2), $Fe(NN)_x$ (x=1-5). A SHI Cryogenics Model SPR-082B-F70L refrigerator was operated at 6±l K as measured by a Lake shore Cryotronics diode sensor mounted on the copper block. The Nd:YAG laser fundamental (1064 nm, 10 Hz repetition rate with 10 ns pulse width) was focused on the rotating Fe target. The laser-ablated iron atoms were codeposited with N2 in excess neon onto a ZnSe window cooled to 6 K. IR spectra were recorded on a Bruker VERTEX 80 FT-IR spectrometer at 0.5 ㎝$^{-1}$ resolution using a liquid nitrogen cooled HgCdTe(MCT) detector for the spectral range of 4000-400 ㎝$^{-1}$.

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Ejection process of photofragment ions from a quadrupole ion trap

백지영 김남준*

충북대학교 화학과

We investigate the ejection process of photofragment ions from a quadrupole ion trap (QIT) that occurs immediately after irradiation of dibenzo-18-crown-6 complexes with alkali metal cations (M^+-DB18C6, M = K, Rb, and Cs) in the QIT by an ultraviolet (UV) laser pulse. The first detection of those fragment ions escaping from the QIT using a reflectron time-of-flight (reTOF) mass spectrometer attached next to the QIT provides a basis for our recent development of a new UV?UV hole burning (HB) spectroscopic technique applicable to ions in a QIT. To understand the ejection process, we measure the dependences of the ejection time of the M^+ ions on the rf amplitude, time delay between the laser and the extraction direct current (DC) pulse, and buffer gas pressure inside the QIT. We suggest that the photofragment ions undergo unstable oscillatory motion upon their generation in the QIT due to their larger values of the Mathieu parameter q_z than that of the stability boundary. The fragment ions increase their oscillation amplitudes by taking up energy from the rf field and are eventually ejected out of the QIT. The lower limits of the q_z values necessary for the escape of K^+, Rb^+, and Cs^+ ions from the QIT are determined to be ～1.7.

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Correlated environmental effect on Hamiltonian describing light harvesting complex in photosynthetic system: beyond a Markov process

이원규 이영민

포항공과대학교 화학과

Light harvesting complexes in photosynthetic systems transform light energy to electronic excitation and transfer it to the reaction center. These complexes consist of pigments and protein environment, and the environment has influence on the energy transfer path through the pigments. Much theoretical research has been focused on finding the detailed mechanism of the involved energy transfer phenomena, such as transfer rates and degrees of coherence. Environmental effect causes fluctuations of both transition energies and the couplings between pigments, and the widely adopted Haken-Strobl-Reineker (HSR) model describes it as a stochastic process. This model is good at describing correlations between different fluctuations when the correlations themselves originate from the same source as those different fluctuations. Usually, a simple Gaussian Markov process is adopted for this purpose, but it cannot account for reorganization energy by the environment. We propose a new model that modifies the discrete Markov process by accumulating continuously decaying random numbers at previous time points with the purpose of generating a non-Markov process. Modifying the decay rate can adjust fluctuations toward a given spectral density. We can confirm that the effects of the correlations with the Markov process can be reproduced with our non-Markov model. We also discuss more sophisticated issues regarding how correlations and spectral densities affect the energy transfer.

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Autofluorescence generation and elimination: a lesson from Glutaraldehyde

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서울대학교 화학교육과

Autofluorescence, either emerging in biological imaging or nanomaterials synthesis is usually one of the unwanted fluorescence sources in spite of valuable usage as a featured signal in diagnostic tissue imaging of specific organelles. This illudes the origin of target signal and significantly decrease the signal-to-noise ratio even at low concentration. The synthesis of luminescent nanomaterials also encounters the creation of unwanted emissive species in the presence of organic molecules. The unwanted emissive species might appear spectrally-pure but chemically-negligible when such organic molecules undergo extreme treatments such as oxidation, heating or microwaving. Spectral purity and Chemical-negligibility makes it difficult to assign the actual emissive species. Glutaraldehyde, widely used as fixative and cross-linking agents in bioimaging and biomedical engineering, causes especially high autofluorescence. We investigated the fluorogenic mechanism of glutaraldehyde. It reacted with proteins and synthetic peptides to generate visible to near?IR emitters. A model compound indicated that ethylenediamine and a secondary amine in the molecule are key components for the formation of emissive species. The proposed yellow emitter presented structural and photophyscial similarity to Cy3 dye. With current mechanism, the generation and elimination of autofluorescence can be controlled. Our results not only allow an explanation for the formation of unwanted emissive species during luminescent materials synthesis, but also a way to decrease autofluorescence in biological imaging.

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Proximity and tunneling in the hydride transfer of NAD$^+$ dependent enzyme models

박예은 김용호* 백지혜

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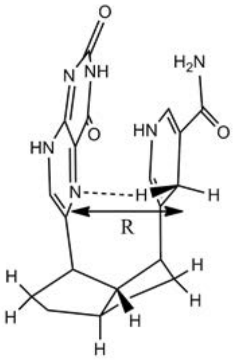
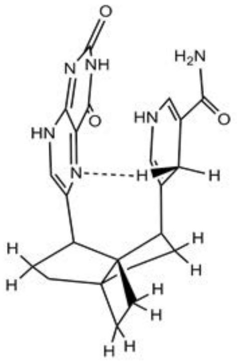
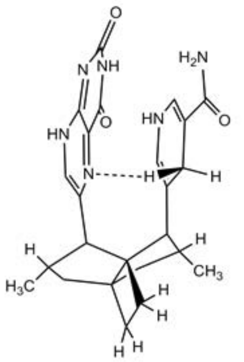
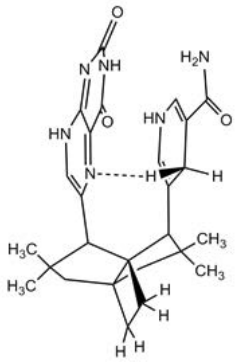
최근 효소 내의 수소원자이동 반응에 턴넬효과가 중요한 역할을 한다는 것이 알려졌다. 특히 단백질 내의 낮은 진동수를 갖는 운동이 수소전달 반응에 영향을 미쳐 매우 크고 온도와 무관한 KIE 값을 만든다고 알려져 있다. 본 연구에서는 단백질의 운동이 수소전달의 주개와 받개의 거리를 변화시키고, 결국 턴넬효과에 어떻게 영향을 미치는지 알아보기 위하여, 주개와 받개의 거리가 다른 여러 모델 시스템을 만들어 반응속도와 턴넬링 효과, KIE 값을 다차원 턴넬링 근사가 포함된 변분적 전이상태 이론을 사용하여 계산하였다.









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The influence of laser wavelength and fluence on the palladium nanoparticles produced by pulsed laser ablation in deionized water

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Palladium nanoparticles were synthesized by pulsed laser ablation in deionized water without the addition of surfactant agent. Nd:YAG laser and pure palladium metal were applied for the synthesis of nanoparticles. The formation was observed at the different laser fluence (8.92 and 12.74 J/cm2) and wavelength (355, 532 and 1064 nm). The products were characterized by transmission electron microscopy (TEM), energy dispersive x-ray spectroscopy (EDS) and UV-vis spectroscopy. Electron microscopy shows a typical mean diameter of single Pd nanoparticle is 3.5-7.3 nm and the average size grow with increase in the laser fluence and wavelength. Energy dispersive x-ray spectroscopy (EDS) data confirms that the produced nanoparticles clearly show homogeneous character. Also, UV-vis spectroscopy indicates the production rate of nanoparticles under different experimental conditions. In addition, selected area electron diffraction (SAED) pattern suggests that obtained Pd nanoparticle is face-centered cubic (FCC) structure.

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Comprehensive analysis of complex lipid mixtures by online two-dimensional strong anion exchange and reversed-phase nanoflow liquid chromatography/tandem mass spectrometry (SAX-nRPLC-ESI-MS-MS)

방대영 문명희*

연세대학교 화학과

In this study, a total of 22 different lipid standards were utilized to develop an analytical condition for simultaneous separation and characterization using 2D-SAX-nRPLC-ESI-MS-MS. Based on the lipid classification, major lipids have been divided into four categories such as glycerolipids, glycerophospholipids, sphingolipids, and sterol lipids. However, complexity in lipid mixtures still remains a barrier toward a complete identification even with sophisticated HPLC methods. The study demonstrates that different lipid classes were separated on a strong anion exchange (SAX) column in the first dimension and lipid molecular species were separated on a reversed-phase column in the second dimension, so that the ion suppression effects can be reduced and the number of identified lipids can be increased . In the 2D-SAX/RP nLC, the strong anion exchange eluate was divided into four different fractions by lipid classes based on their electrical propensities. Before the salt step elution began, a breakthrough run was carried out to resolve some materials that were not expected to be retained in the SAX column during the sample loading. The first solvent washing step began by delivering methanol solution from the autosampler to displace neutral lipids such as PC, TG, CE and SM from the SAX column to the RPLC-MS. When the concentration of ammonium acetate solution was increased to 10 mM, weak anionic lipids including PI, PE, PG began desorbing from the SAX column. The final salt step was made at 250mM in order to detach all remaining anionic lipids such as PA, PS, CL in the SAX column. As a result, online separation through this 2D-SAX/RPnLC was achieved with a good linearity, sensitivity, and recovery. This method was applied to the human plasma.

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Separation of Methanol-water Mixtures with Membranes

황보연 정용희*

한림대학교 화학과

Separation of methanol-water mixtures have been studied with various membranes. 65.0 weight percent methanol was used along pure methanol at temperatures ranging from 18 to 20 ℃. The membranes of the different pore size and porosity were employed in the work. The separation was performed at two peak pumping rates such as 200 and 400 ml/min. The preliminary result showed that the membrane of the higher porosity allowed less methanol to pass through it at both pumping rates, leading to a lower methanol concentration in the effluent solution. The membranes of the lower porosity appeared to show a similar tendency, but they have to be scrutinized further.

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Dependence of Membrane Separation on Concentration of Methanol-water Mixture

황보연 김연수 정용희*

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Membrane separation of methanol-water mixtures of various concentrations has been examined at two pumping rates and ambient temperature. The values of methanol weight percent range from 0 to 100. The peak pumping rates are 200 and 400 ml/min. The polyethylene membranes of the different pore size and porosity were used for the separation. Their porosities are 41 and 55%. Methanol-water mixtures with higher concentrations than 65 weight percent methanol were measured to pass through the membranes of interest, while it could not permeate them at the lower concentrations. The effluent volumes of methanol-water mixtures were observed to depend on the methanol concentration, duration of pumping, pumping rate and porosity.

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A study on the matrix interference of arsenic species in seaweed by ion chromatography coupled with inductively coupled plasma - atomic emission spectrometry

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Chemical speciation of an element involves quantitative determination of the different chemical forms. The chemical speciation of elements has been very critical because their bioactivity and toxicity depends on the different chemical forms of elements in various samples. The quantitation of the total arsenic in seaweeds has routinely been performed. But, it has been very well known that toxicity and biological effect depend not only on the total concentration of arsenic but also on the chemical species of arsenic in samples. Of the chemical species of arsenic, inorganic arsenic (As^{3+} and As^{5+}) are highly toxic. Therefore, the importance on research of arsenic species has greatly increased. It is necessary to develop the analytical method of arsenic species because the oxidation states of arsenic species should not be converted into each other during sample preparation. This study has been focused on the sample preparation (use nitric acid and Methanol as extraction liquid) of total arsenic and arsenic species in several seaweeds (laver, green laver, sea tangle and sea mustard). And the matrix of the seaweed was also investigated. Various methods were carried out by using IC (Ion Chromatography) coupled with ICP-AES (Inductively Coupled Plasma - Atomic Emission Spectrometer).

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Separation and Collection of Crude Oil Fractions by High Performance Liquid Chromatography

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경북대학교 화학과

Crude oil is a complex mixture composed of numerous compounds and hence it pose a difficulty in understanding the material at the molecular level. High resolution mass spectrometry has been successfully used to understand the detailed chemical compositions of crude oil but it has been shown that it is necessary to combine separation with high resolution mass spectrometry for more complete understanding of crude oil. Conventionally, saturates, aromatics, resins, and asphaltenes (SARA) separation technique has been widely used to separate crude oil into fractions. However, the conventional SARA fractionation procedure includes many manual steps and hence reproducibility of the method is critically dependent on the skill of the operator. In this study, fractionation of crude oil has been performed by High Performance Liquid Chromatography (HPLC) connected with a fraction collector. The optimum condition for the separation were investigated and the obtained fractions were characterized by GC/2D-GC and high resolution mass spectrometry.

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A study on proton source for positive mode LDI-TOF MS analysis with nanostructured gold surface

조은지 안미리[1] 김종원[1] 김영환[2] 김성환

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A proton source of (+) mode laser desorption ionization-time of flight mass spectrometry (LDI-TOF MS) analysis employing nanostructured gold surface was investigated. The analysis of a per-deuterated compound showed that solvent and compound itself did not played a role as a proton source. Therefore, it was concluded that residual water remaining in the nanostructured gold surface was the source of proton. When extra proton source such as thiolate compounds and/or citric acid was added to the nanostructured gold surface, the signal abundance was greatly improved up to ~15 times. It was also shown that adding extra proton source with thiolate compounds and citric acid improved (+) LDI-TOF MS analysis of a crude oil sample. The data provided in this study clearly shows that proton is one of the limiting components of the (+)LDI-TOF MS and more efforts has to be spent to find compounds providing protons but not generating peaks interfering mass spectral interpretation.

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Investigating photo-degradation of nitrogen containing aromatic compounds

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경북대학교 [1]경북대학교 화학과

In this study, photo-degradation of aromatic compounds containing basic and acidic nitrogen atoms were investigated. The degraded products were analyzed to investigate the effects of UV light irradiation. This investigation was conducted followed by our previous in-vitro photo-degradation experiment where oil samples were irradiated by UV light and fractionated into SARA (saturate, aromatic, resin, and asphaltene) prior to characterization by Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). In-vitro photo oxidation experiments showed that levels of N_1 and N_1O_1 class basic nitrogen compounds increased after degradation compared to non-basic nitrogen compounds. The same trend of change was also observed from samples acquired obtained from M/V Hebei Spirit oil spill site.

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End Point Detection by a Light Emitting Diode Based Reflectance Detector in Argentometric Titration

엄인용

대구가톨릭대학교 생명화학과

Hwang and Eom reported showed that the binary halogen mixture of I- and Br- were quantitatively analyzed by differential agentometric titration system equipped with a light emitting diode (LED) based reflectance detector.1 The light intensity reflected from the surface of precipitates was recorded while AgNO3 standard solution added into the titrant solution under a stopped-flow mode. The titration system was modified by replacing burette with a precise syringe pump (48000 steps) which can add AgNO3 standard solution into the titrant by both a stopped-flow and a continuous mode. This modification enabled us to study and understand precipitation titration (e.g. argenotmetry) process more clearly. For mono halide anion solution, both stopped-flow and continuous flow modes were applied successfully to find end points. However, the stopped-flow mode was more precise to find both 1st and 2nd end points for binary halogen anion mixtures.

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Investigation on the Restricted Rotational Dynamics around Coordinated Amide Bond

민지은 이소정 김민경 진경수 곽경원 안상두*

중앙대학교 화학과

The rotational barrier about the C-N bonds in the complex of 2-(bis(pyridin-2-ylmethyl) amino)-N,N-diethylacetamaide with metal ions were investigated by variable temperature (VT) NMR spectroscopy and computational calculations with the GAUSSIAN 09W. From the VT-NMR data, the rotation barriers about C-N bonds have been determined with Gibbs energy by the coalescence temperature (TC) analyses. In computational calculations with GAUSSIAN 09W, the Gibbs energy was calculated by using the Hartree-Fock method and DFT method with the charge of metallic ion, singlet spin, and 6-31G the basis set as the condition. When analytes form the metal complex, the electrons of nitrogens in pyridine rings and those of amide oxygen make coordinate bonds with metal ions. As a result, we could observe the changes in the chemical shift of N-CH_2CH_3 groups in 1H NMR spectra before and after the complexation with metal ion. It seems that if the electrons in the amide oxygen participate in the coordination of metal ion, the electrons of amide nitrogen is more donated to C-N bond, which means that double bond character of the C-N bond becomes strong. This can be verified from the NMR experiments and computational calculations.

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MALDI-TOF Analysis of Polyhexamethylene guanidine (PHMG) Oligomers used as a Commercial Antibacterial Humidifier Disinfectant

오한빈* 남정주

서강대학교 화학과

Polyhexamethylene guanidine (PHMG) polymers, which were used as an active ingredient of an antibacterial humidifier disinfectant, were reported to cause harm to the human health when these molecules are inhaled, although the physical contact to this material is known to present low toxicity to human. Due to this reason, it is necessary to develop an optimal analysis method which enables us to detect and analyze the PHMG polymers. MALDI-TOF investigations of PHMG were made with a variety of matrices, and it was found that CHCA and 2,5-DHB are excellent matrices which well reflects the polymer population even of high mass. For the provided PHMG sample, the number-average (Mn) and weight-average (Mw)molecular masses were determined to be 744.8 and 810.7, respectively, when the CHCA was used as a matrix. The rank of the matrices in the averaged molecular weights was CHCA ~ 2,5-DHB > 5-NSA > DHAP, THAP > ATT > IAA ~ super-DHB ~ HABA. In addition, PSD of the PHMG oligomer ions exhibited a few unique fragmentation characteristics. The formation of a- and c-type fragments was the major fragmentation pathway, and the 25-Da loss peaks generally accompanied a- and c-type fragments.

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Limited proteolysis using a trypsin-immobilized monolithic bioreactor

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Limited proteolysis is a method, with which conformational features of proteins can be probed and the flexible region along the sequence can be determined. In this study, limited proteolysis experiments were carried out using trypsin-immobilized reactor that is made of organic-inorganic hybrid silica monolith. The silica-based sol-gel method was used for preparing the silica monolithic support in a 100 µm i.d. capillary. Specifically, tetraethylorthosilicate (TEOS) and 3-aminopropyltriethoxysilane (APTES) mixture were used as precursor materials, and cetyltrimethyl ammonium bromide (CTAB) was used as a surfactant. The capillary surface and matrix was activated by glutaraldehyde, wherein trypsin was immobilized. Limited proteolysis experiments were made by flowing proteins such as ubiquitin and myoglobin through the trypsin-immobilized reactor at various flow rates (0.3~100µL/min). The eluted peptide fragments were analyzed by MALDI-TOF MS (matrix-assisted laser desorption ionization time of flight mass spectrometry). Analysis of limitedly cleaved peptide-fragments provides information about the structural flexibility or the unfolding features of the protein of interest.

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Spectroscopic studies of P-doped soft carbon

권영민 이영일*

울산대학교 화학과

Soft carbon material as an anode of lithium ion battery has been recently received much attention for large scaled energy storage systems. Generally, it has excellent high performance, but low discharge capacity and low crystallinity than that achieved with the conventional carbonaceous materials. Herein, the soft carbon anode materials treated with phosphoric acid to achieve improved electrochemical properties have been characterized by using ^{31}P solid-state NMR, small angle X-ray scattering (SAXS), and wide angle X-ray scattering (WAXS). ^{31}P MAS NMR spectra are shown that the two types of P are encapsulated and relative intensity ratio is changed depending on condition of preparation. Inter-domain distance and interlayer distance in the soft carbon have been calculated by using SAXS and WAXS profiles.

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Free Radical Initiated Peptide Sequencing for guanidinated peptide.

전애란 오한빈*

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TEMPO-FRIPS method is previously shown to be tandem mass spectrometry tool useful for peptide sequencing. But in TEMPO-FRIPS, a TEMPO-radical initiator can be attached to a lysine side chain as well as to a desired N-terminus, which makes the interpretation of peptide sequencing mass spectrometry results complicated. In order to overcome this problem, a lysine side chain is guanidinated to direct the conjugation of the TEMPO-derived radical initiator only to the N-terminal amino group. Then, TEMPO-radical initiator is attached to the desired N-terminus. Guanidination is done by reacting o-methylisourea with the peptide of interest. Peptides prepared in this way were subjected to the consecutive collision activations. The resulting FRIPS fragmentation pattern from guanidinated peptides differed much from that of unguanidinated peptides.

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TEMPO-FRIPS sequencing analysis using bromine

남정주 문봉진 오한빈*

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FRIPS (free-radical initiated peptide sequencing) approach is a recently developed peptide sequencing method that makes use of odd-electron radical-driven fragmentation chemistry. In this study, we incorporate the bromine atom in the N-terminal TEMPO-derived conjugated radical initiator, for example, at the ortho position of the benzyl group, in order to utilize the unique isotopic pattern of bromine for the purpose of distinguishing N-terminal fragments from C-terminal fragments. Indeed, the bromine-incorporated TEMPO-Bz- conjugated group gave rise to the unique isotopic pattern that facilitates the easy identification of N-terminal peptide fragments. We demonstrate in this study that by utilizing bromine of a unique isotopic pattern de novo sequencing of peptides can be easily accomplished without the aid of other fragment identification algorithm.

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MALDI-MS of a TEMPO-based FRIPS method

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Recently, we have shown that peptide sequencing can be made using the so-called free radical initiated peptide sequence (FRIPS) method, in which a radical initiator is attached to the N-terminus of the peptide and the consecutive collisional activations led to the radical-induced peptide fragmentations. This approach was made in the platform of the electrospray ionization (ESI) method. In this study, we attempt to apply the TEMPO-based FRIPS method to the platform of MALDI ionization method. As an effort towards this goal, we seek to find an adequate matrix and found that DHAP is superior to other matrices in ionizing the TEMPO-Bz-CO-peptides in an intact form. Further, we performed PSD using LIFT technique to generate the radical-peptide species. The subsequent collisional activation of the radical-peptide species will be soon implemented in other mass spectrometer, for example, MALDI-IT-TOF, in order to induce radical-based peptide sequencing even using the MALDI ionization platform.

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Development of an On-line Microbore Hollow Fiber Enzyme Reactor Combined with Nanoflow Liquid Chromatography-Tandem Mass Spectrometry for Global Shotgun Proteomics and Application to Enrichment of N-linked Glycopeptides

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연세대학교 화학과

Bottom-up proteomic approach is the well-established protocol for identifying proteolytic peptides and getting the information about their post-translation modifications in research field of Proteomics. The shotgun proteomic method is carried out by the digestion of proteins in advance, followed by the separation of proteolytic peptides and the analysis using tandem mass spectrometry. Even though there is no doubt that proteolytic preparation of proteins is essential step for shotgun proteomics, the conventional methods of proteolytic digestion (in gel or in-solution digestion) have some shortcomings, such as long incubation times (about 18-24 hours), manual operation, low efficiency, irreproducibility, and autodigestion of proteases. In this study, we developed of a microbore hollow fiber enzyme reactor (mHFER), which is a simple, highly reproducible, inexpensive to assemble, and user friendly device coupled to nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS-MS) as an alternative digestion method for global shotgun proteomics. First, we evaluated on-line mHFER-nLC-ESI-MS-MS system with bovine serum albumin (BSA) by varying the temperature of digestion, protein to enzyme ratio, and amount of proteins injected. In addition, we evaluated the ability of the mHFER system to enrich glycopeptides by injecting a mixture of lectin (concanavalin A) and digested peptides from glycoprotein into the mHFER, followed by delivery of PNGase F for endoglycosidic digestion. The developed method was applied to human urinary proteome sample with prostate cancer, resulting in the identification of a total 67 N-linked glycopeptides.

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Biomarker Profiling of Prostate Cancer in Urine by Multiple Reaction Monitoring of Ultra Performance Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry & Statistical Methods

임상수 방대영 문명희*

연세대학교 화학과

Prostate cancer is one of the most frequently occurring cancers among men worldwide. Though its diagnosis is widely processed by screening serum prostate-specific antigen (PSA) level, it remains imperfect due to the lack of strong correlation with actual existence of tumor in prostate. Lipidomics is a study of comprehensive analysis of lipids in biological fluids including structural and metabolic elucidation. Thanks to brisk development of mass spectrometry-related methods for lipidomic researches, its significance has expanded to biomarker discovery for various diseases such as mitochondrial dysfunction, breast cancer, and coronary artery disease. In addition, a couple of studies have introduced lipid biomarkers for prostate cancer by comparison of urinary and plasma lipidomes, but still remain to be studied. In this study, from urine samples of 22 controls and 45 prostate cancer patients, 52 phospholipid (PL) candidates including 10 lysophospholipids (LPLs) were selected and quantitatively analyzed by MRM utilizing UPLC-ESI-MS-MS. The results from UPLC-ESI-MS-MS were examined upon the different Gleason's scores of prostate cancer patients. Among the candidates, 20 LPLs and PLs (1 LPE, 7 PCs, 3 PEs, 1 PG, and 8 PIs) were assessed by varying defined thresholds for several statistical methods and its significance was compared with conventional markers.

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Plasma Lipids in Coronary Artery Disease : Potential Biomarkers by Flow Field-Flow Fractionation and Nanoflow LC-ESI-MS-MS

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Lipids play significant roles in biological system by controlling cell proliferation, signaling, apoptosis, and growth. Many types of human diseases are triggered and developed by changes in lipid metabolism and as lipid analysis has broadened its perspective from biological sciences to clinical fields for purposes of diagnostic and prognostic applications, studies on chemically complex lipids as sophisticated biomarkers of human diseases are conducted around the world for more detailed comprehension of the diseases. Coronary artery disease (CAD) is one of the most common types of heart diseases, caused by aberrantly accumulated plaques on coronary arteries. Limited amount of blood flow to the heart because of narrowed arteries and this can lead to sudden heart attack and death. The purpose of this study is to identify lipids from CAD patients and discover potential biomarkers from human plasma. Since high level of low-density lipoproteins (LDL) and low level of high-density lipoproteins (HDL) are reported risk factors of CAD, HDL and LDL from human plasma were successfully separated using flow field-flow fractionation (FlFFF), which is an elution method based on a size-separation. After fractionated particles of HDL and LDL were collected, plasma lipids were extracted using lipid extraction method. Comprehensive lipid profiling from HDL and LDL was conducted by nanoflow liquid chromatography electrospray ionization tandem mass spectrometry (nLC-ESI-MS-MS) and quantitative measures of identified lipid species were thoroughly searched in order to discover biomarkers of CAD. The species that exhibited greater than five-fold of difference in concentration between ten CAD patients and ten healthy controls were selected as biomarkers.

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Optimization in Analysis of Sodium Hyaluronate in Asymmetrical Flow Field-Flow Fractionation and Multiangle Light Scattering (AF4-MALS)

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연세대학교 화학과

Sodium hyaluronate (NaHA), which widely exists in nature, is aqueous polymer having very high molecular weight composed of disaccharide repeating units. Recently, NaHA evokes a lot of applications in various fields such as cosmetics, orthopedic operation, ophthalmic treatment due to its unique characteristics such as viscosity and elasticity. Since molecular weight of NaHA is an important parameter in controlling the role of NaHA in the industrial applications, it is a crucial step to measure accurate molecular weight of NaHA. To determine molecular weight of polymer, size exclusion chromatography (SEC) has been generally utilized, but it shows in some cases difficulties in the separation of ultrahigh MW polymers due to the limitation of proper pore sizes and the possible shear degradation. Flow field-flow fractionation (FlFFF) compensates for the drawbacks of SEC because separation in FlFFF is achieved in an empty channel without packing materials.In this study, we evaluated the efficiency of both asymmetrical FlFFF (AF4) channel and frit inlet AF4 channel on the separation of NaHA by comparing the molecular weight distribution. While AF4 channel utilizes a static relaxation procedure by using focusing/relaxation, frit inlet AF4 utilizes hydrodynamic relaxation which does not require stoppage of migration flow during relaxation, resulting in the smooth continuous relaxation and migration. The latter channel may improve the separation of ultrahigh MW NaHA materials due to the removal of focusing procedure. In order to examine the difference between the two channel systems, of the various experimental parameters including crossflow rate, out-flow rate and relaxation time were varied along with NaHA samples having diverse molecular weight distributions.

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Top-Down Analysis of Phospholipids from Human Plasma by Chip-type Asymmetrical Flow Field-Flow Fractionation and ESI-MS-MS

양이슬 문명희*

연세대학교 화학과

Chip-type Asymmetrical Flow Field-Flow Fractionation (Chip-type AF4) channel on-line coupled to electrospray ionization tandem mass spectrometry (cAF4-ESI-MS-MS) has been utilized for the quantitative analysis of lipid species contained in lipoprotein particles from human plasma samples of coronary artery disease(CAD). First, we optimized conditions adjusting flow rates to keep stable spray, splitting the flow stream in order to reduce the flow into the mass spectrometer and identified overall tendencies by comparing lipid distribution of cAF4-ESI-MS-MS and nanoflow liquid chromatography-tandem mass spectrometry (nLC-ESI-MS-MS). To reduce ionization suppression by proteins, albumin and immunoglobulin were removed in blood plasma by protein depletion kit and for the quantitative analysis of phospholipids, carbonic anhydrase which was relatively low abundant in plasma was utilized as an internal standard for the calculation of relative peak area ratio of phospholipids. And we performed experiments for evaluating reproducibility and ionization efficiency since carbonic anhydrase added in plasma may interfere with lipid ionization. Then, we monitor phospholipids as potential biomarkers in LDL and HDL of controls and patients and examined their patterns by utilizing tandem mass spectrometry(MS/MS) which based on collision-induced dissociation(CID)-selected reaction monitoring(SRM). Therefore, we propose possibility that Chip-type AF4 connected with ESI-MS-MS may be a convenient tool for quantitative analysis.

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Comparison of size analysis of TiO_2 nanoparticles by sedimentation field-flow fractionation, SP-ICPMS, DLS and SEM

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Sedimentation field-flow fractionation (SdFFF) provides effective mass-based separation of colloidal particles, and thus a size-based separation if the particles are of uniform density. The particle size can be measured from the retention time in SdFFF if the density of the particle is known. In the single-particle mode of inductively coupled plasma-mass spectrometer (SP-ICPMS), single colloidal particle is ionized in plasma, producing ions that are detected by a mass spectrometer. The signal intensity depends on the particle size, and the frequency is proportional to the particle concentration. In this study, SdFFF was employed for size-based separation of TiO_2 nanoparticles of rutile and anatase type. Results from SdFFF revealed that the rutile and anatase TiO_2 particles have the mean diameters of 78 and 98 nm, respectively, which agreed well with those obtained from dynamic light scattering (DLS). SdFFF fractions were collected and analyzed by SP-ICPMS. The SP-ICPMS data of the SdFFF fractions were processed to produce the size distributions of the TiO_2 nanoparticles. The size and concentration of TiO_2 fractions obtained from SP-ICPMS were well correlated with SdFFF results.

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Application of sedimentation field-flow fractionation for characterization of Fe_3O_4@MWCNTs composite

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한남대학교 화학과

Multi-walled carbon nanotubes decorated with Fe_3O_4 magnetic nanoparticles (Fe_3O_4@MWCNTs) were prepared by co-precipitation method with ultrasonic assistance. The Surface and structure properties of Fe_3O_4 particles and Fe_3O_4@MWCNTs were characterized by X-ray diffraction (XRD), field emission transmission electron microscopy (FE-TEM), X-ray photoelectron spectroscopy (XPS), and dynamic light scattering (DLS). Also the applicability of sedimentation field-flow fractionation (SdFFF) for size characterization of Fe_3O_4 particles was investigated. For SdFFF analysis of Fe_3O_4 nanoparticles, experimental parameters such as filed strength, channel flow rate, and the types of surfactant (added as a particle dispersing agent) were optimized. At the field strength (channel rotation rate) of 1600 rpm and the flow rate of 0.3 mL min^{-1}, a good resolution and sample recovery was achieved. Addition of Triton X-100, a nonionic surfactant, yielded a good resolution with slightly reduced sample recovery, due to attraction of the particles onto the channel wall. Results from SdFFF were compared with those from TEM and DLS. Results from SdFFF and TEM were in reasonable agreements, whereas the results from DLS tended to shift toward larger sizes. It was found that Fe_3O_4 particles have a relatively narrow size distribution. Then a screen printed electrode (SPE) modified by Fe_3O_4@MWCNTs was fabricated, and tested for analysis of dopamine. Results showed that: (1) SdFFF is a useful tool for the separation and characterization of Fe_3O_4 nanoparticles; (2) Proposed methods for preparation of Fe_3O_4 nanoparticles and Fe_3O_4@MWCNTs are mild and fast (about 30 min); (3) SPE modified with Fe_3O_4@MWCNTs shows potential applicability for biosensing.

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Flow field-flow fractionation with light scattering and fluorescence detection for monitoring of formation of PAMAM-DNA complex

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한남대학교 화학과

Polyamidoamine (PAMAM) dendrimers bear multiple primary amines on the surface and internal tertiary amines as branching sites. The peripheral amines allow formation of nano-scaled polyplexes of PAMAM with DNA through electrostatic interaction, thus promoting cellular uptake. PAMAM dendrimers have shown excellent properties as a gene-delivery vehicle as they are water-soluble, biocompatible, and nonimmunogenic. They have also demonstrated excellent efficiency for in vitro transfection of plasmid DNA. The online combination of flow field-flow fractionation (FlFFF) with a multi angle light scattering (MALS) detection (FlFFF-MALS) is useful for gentle (nondestructive) separation of various types of macromolecules including synthetic or natural polymers, nanoparticles, proteins and viruses. FlFFF-MALS provides absolute (requires no calibration) determination of molecular weight and size distributions of samples. Merits of FlFFF-MALS include: (1) enhanced separation capability in broader molecular weight range (from 10^3 to above 10^8 g/mol) than size-exclusion chromatography (SEC); (2) absence of stationary phase ensures separation of sample components with little (if not no) interaction (or adsorption); (3) possibility of investigating non-purified solution or mixtures of various components.In this study, asymmetrical FlFFF was combined online with MALS and fluorescence detector (AsFlFFF-MALS-FD) to monitor formation of PAMAM-DNA complexes formed at various molar ratios of the PAMAM to DNA. AsFlFFF provided good separation of dendrimers and DNA, and MALS yielded absolute size and molecular weight of DNA and PAMAM-DNA complexes. FD was employed as a concentration detector for enhanced sensitivity.

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Gold Nanocube-enhanced sandwich bioassays for brain natriuretic peptide

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경북대학교 화학과

In this poster, a highly sensitive detection method for brain natriuretic peptide (BNP), which is an important cardiac biomarker, is described using the combination of antibody functionalized gold nanocubes with a BNP specific aptamer chip. BNP has two different binding sites for a BNP-aptamer and an anti-BNP which allows us to form a surface sandwich detection platform; a covalently attached BNP-aptamer onto the chemically modified gold surface was exposed to BNP followed by the inetraction of anti-BNP coated Au nanocubes (NCs). The surface sandwich complex of BNP-aptamer/BNP/anti-BNP coated NCs was then detected using real-time surface plasmon resonance technique.

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Electrochemical enzyme linked sandwich assays with biofunctionalized gold silver core shell nanoparticles for phenol

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In this poster, we demonstrate a new electrochemical sandwich assay for the sensitive and selective detection of phenol based on the use of biofunctionalized gold/silver core shell nanoparticles in conjunction with surface enzyme reaction. An electrode surface was first modified with silver/gold core shell nanoparticles (Au@Ag NP) functionalized with phenol specific antibody (mouse). The Au@Ag NP modified electrode was then soaked into a solution of phenol followed by the sequential adsorption of the anti-phenol (rabbit) and the secondary anti-rabbit-IgG-HRP conjugate. This resulted in the formation of the surface Au@Ag NP-anti-phenol/phenol/anti-phenol/secondary anti-phenol-HPR conjugate complex which was then reacted with the substrate, peroxide. The electrochemical reaction of the surface bound HRP and peroxide was characterized using cyclic voltammetry and differential pulse voltammetry.

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Effects of biofunctionalized nanoparticle concentrations on SPR dynamic ranges

백승희 이혜진*

경북대학교 화학과

In this poster, we studied the effect of the nanoparticle concentration on the dynamic range for detecting biomolecules in a surface sandwich assay platform with surface plasmon resonance (SPR). As a model biomolecule, thrombin (Th) was chosen since this can form a robust surface sandwich complex with an anti-Th and a thrombin specific aptamer (Th-apatmer). The surface sandwich complex was first created via the adsorption of thrombin on Th-aptamer molecules immobilized on a chemically modified gold surface followed by the adsorption of anti-Th coated gold nanoparticles. The variation of linear concentration ranges for Th detection as a function of the concentration of anti-Th coated nanoparticles was then monitored and analyzed using a real-time SPR technique.

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Quantitative determination of Salinomycin in Ham using Laser Induced Fluorescence Microscope (LIFM).

박지현 김수민 고정아 임흥빈*

단국대학교 화학과

Salinomycin is an anticoccidial drugs used as feed additives for the prevention and treatment of coccidiosis in poultry farming. Their residue in livestocks could be absorbed to human. And the exposure of humans to salinomycin via inhalation or ingestion can cause severe toxicity. To protect consumers, maximum levels for their presence in food and feed have been set by the European Union (EU). In this work, we developed a sensitive and selective analytical method to determine salinomycin using dye doped silica nanoparticle. We synthesized two nanoparticles, Cy5 doped silica nanoparticle as a probe and Magnetic nanoparticle for sample collection. The nanoparticles with uniform shape are modified with amine functional group. For quantitative detection, we use a lab-built laser induced fluorescence microscope (LIFM) with Photomultiplier tube (PMT) and 632.8 nm He/Ne laser (with 692±25 nm interference filter). The pretreatment of ham sample was based on extraction with acetonitrile and defatting with hexane. As a result, the limit of detection (LOD) for Salinomycin was 0.0305 ng/mL, which was about 164 times lower than that of ELISA method.

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Application of photon initiated in-source atmospheric pressure hydrogen/deuterium exchange for structural interpretation of petroleum compounds

조윤주 AHMED ARIF[1] 김성환[*]

경북대학교 화학과 [1]경북대학교 Chemistry

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is one of the powerful techniques that can cope with the complexity of crude oils. However, even with FT-ICR MS, structural elucidation of compounds comprising crude oils is not currently available. Structural analysis is a very important field of petroleum research for a more complete understanding of heavy crude oils and oil shale extracts. Hence there has been research devoted for structural interpretation of crude oil such as planar limit by using FT-ICR MS. In this study, hydrogen/deuterium exchange in the process of atmospheric pressure photo ionization (APPI) was applied to structurally study heavy crude oils and oil shale extracts at the molecular level. Hydrogen/deuterium exchange is performed by dissolving oil samples in deuterated toluene(C_7D_8):deuterated methanol (CD_3OD) mixture at the one to one ratio and these oil samples were analyzed by APPI (+) FT-ICR MS. Saturates/Aromatics/Resins/Asphaltenes (SARA) fractions extracted from Qinhuangdao (QHD) and Anvil Points Mine (APM) shale oil extracted by Fischer assay pyrolysis were used in this study. Each SARA fractions were compared and it was shown that core structures of nitrogen contained compounds could be classified as pyridine, pyrrole, 1°, 2° and 3° amine-type in each fraction. Overall, the molecular structures of compounds existing in each oil fraction were predicted based on the hydrogen/deuterium exchange technique at the molecular level by using APPI (+) FT-ICR MS.

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Growth of carbon nanofibers on C-fiber textiles by thermal CVD using Fe nanoparticles as catalyst

이상원 남기목 이창섭

계명대학교 화학과

In this study, growth of carbon nanofibers on C-fiber textiles by thermal CVD. Prior to Iron deposition, the C-fiber substrate was oxidized by refluxing in concentrated nitric acid for 30 mins. The oxidation creates hydroxyl group containing surface groups on C-fiber which acts as anchoring sites on which the Iron precursor can nucleate and anchor. For deposition of Iron, we varied the concentration of Iron solution before heating and then Urea hydrolysis was carried out. Hydrolysis helps to deposit Fe(III) on C-fiber. In reduction process, H_2/N_2 mixture gas was used. In the last step, CNFs were prepared on C-fiber textiles by flowing ethylene gas. The resultant samples were characterized by Scanning Electron Microscopy(SEM), Energy Dispersive Spectroscopy(EDS), X-Ray Diffraction(XRD) and N_2-sorption(BET). AcknowledgementThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation.

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Carbon nanofibers grown on Fe and Cu catalysts by Chemical Vapor Deposition

현유라 이창섭

계명대학교 화학과

The carbon nanofibers (CNFs) in this study have been synthesized using iron and copper catalysts by CVD method. The fiber thickness and surface area have been studied from the influence of both iron and copper concentration. The catalysts were prepared by dissolving the calculated amounts of iron nitrate and copper nitrate in water. The precipitate of catalysts obtained through filtering after drying at 110℃. The CVD process in a high-temperature furnace by the following steps: 1) heating up to 700℃ at a rate of 10℃/min a N_2 for 1h and 10min to reduce the Fe^{3+} to Fe; 2) stabilized at 700℃ under the flow of H_2/N_2 for 30min; 3) CVD process in mixture of 20% ethylene and H_2/N_2 at 700℃ for 1h. Finally the resultant samples were analysed via SEM, EDS, TEM, Raman, XRD and BET. The CNFs have an average diameter of 25-35 nm and a specific surface area of 250-305 m^2/g.AcknowledgementThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation.

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Synthesis of Carbon nanofibers on Co and Cu catalysts by Chemical Vapor Deposition

박은실 이창섭

계명대학교 화학과

In this study, carbon nanofibers were synthesized by CVD method using Co and Cu-based catalyst. To evaluate activity of a catalyst suitable for the growth of carbon nanofibers, optimum concentration of catalyst was found by synthesizing nanofibers with various concentrations of Cobalt nitrate ($Co(NO_3)_3{\cdot}9H_2O$) and Copper nitrate ($Cu(NO_3)_3{\cdot}9H_2O$). This mixed solution of Cobalt nitrate ($Co(NO_3)_3{\cdot}9H_2O$) and Copper nitrate ($Cu(NO_3)_3{\cdot}9H_2O$) was reacted with Aluminum nitrate ($Al(NO_3)_3{\cdot}9H_2O$) and Ammonium Molybdate ($(NH_4)_6Mo_7{\cdot}O_{24}$) and filtered to get precipitates. The Obtained precipitates were then dried at 110℃, to get powder of catalyst. Carbon nanofibers then synthesized by deposition of this catalyst as thin layer on quartz by using chemical vapor deposition method. Then by selecting the most reactive substances of specific concentration, the synthesized Co and Cu-based carbon nanofiber was compared with Ni and Cu-based carbon nanofibers with the various synthesis conditions, such as synthesis temperature (600~900℃) and synthesis time. The structure of the carbon nanofibers was investigated by SEM, TEM measurements. Properties were analyzed using XRD and Raman. Carbon nanofibers are used as a structural material in a variety of industries. The results of this study are expected to make a significant contribution in the development and application in carbon fiber industries. Acknowledgement This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea(NRF) through the Human Resource Training Project for Regional Innovation.

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Monitoring Structural Changes of α-Synuclein in the Membrane Systems Using Ion Mobility Mass Spectrometry

이신정 김준곤*

포항공과대학교 화학과

α-Synuclein is one of amyloidogenic proteins involved in regulation of neural vesicles. Although α-synuclein is natively unfolded physiologically, it can be helically folded by interaction with lipid molecules. In this study, we generate the model membrane systems, which mimic the mammalian neural vesicles and investigate conformational changes of α-synuclein in the membrane systems using electrospray ionization traveling wave ion mobility mass spectrometry. To obtain further structural details, molecular dynamics simulation is also utilized. Of particular interests are the lipid-protein interaction and its effect on the structural properties of the protein. We observe that the solution phase properties originated from the phospholipid-protein interactions can be partially preserved in the gas phase. The correlation between gas phase structures and solution phase structures of intrinsically disordered proteins is also discussed.

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Investigation of Binding Properties of α,ω-alkyldiammonium Complexes with Cucurbituril Using Electrospray Ionization Ion Mobility Mass Spectrometry and Isothermal Titration Calorimetry

노동훈 이신정 김준곤*

포항공과대학교 화학과

Previously, our group has investigated the complex formation between the positively charged ammonium group of lysine side chain in peptides and cucurbit[6]uril[1]. In this study, we investigate host-guest chemistry between cucurbiturils (CB[6] and CB[7]) and a series of α,ω-alkyldiammonium ions (+NH3(CH2)nNH3+, n = 4, 6, 8, 10, and 12) in the gas phase and the liquid phase, using electrospray ionization ion mobility mass spectrometry (ESI-IM-MS) and isothermal titration calorimetry (ITC). Relative abundance of complex ions are measured by ESI-IM-MS and the gas phase stability of complex ions is also measured, using collision induced dissociation analysis. The gas phase complexation is compared to the solution phase binding affinity obtained by ITC. For the structural analysis of host-guest complexes, we additionally perform molecular dynamics simulations. Of particular interest is the complexation depending on the acyl chain length of the guest molecules and the size of cucurbituril cavities. Detailed enthalpic and entropic effects on the formation of diammonium-cucurbituril complexes related to the release of water molecules from the cucurbituril cavities for the observed host-guest chemistry are further discussed. 1. Heo, S. W. et al, Anal. Chem., 2011, 83, 7916.

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Analysis of NSAIDs in environmental sample using three phase hollow fiber based liquid phase microextraction (HF-LPME) and HPLC-UV

차용병 명승운*

경기대학교 화학과

The development of faster, simpler and more environmentally friendly sample-preparation technique is an important issue in chemical analysis. Liquid phase microextraction only needs to a little amount of organic solvent and simple preparation technique. Extraction efficiency in HF-LPME system depends upon a variety of factors which include extraction time, stirring rate, ionic strength of sample solution, temperature, donor phase and acceptor phase. In a three-phase mode, the analytes were extracted from the aqueous sample, through the organic solvent, and further into the aqueous acceptor solution present inside the lumen of the hollow fiber. Seven NSAIDs were extracted from 4 mL of aqueous solution with pH 3 (donor phase) into dihexyl ether immobilized in the wall pores of a porous hollow fiber, and then extracted into the acceptor phase with pH 13 located in the lumen of hollow fiber. After the extraction, the acceptor phase was directly injected into the HPLC system. The enrichment factors(EF) were obtained between 202 and 284. Limit of detection(LOD) and limit of quantitation (LOQ) in spiked urine matrix were in the range of 0.31~1.38 ng/mL and 1.02~4.60 ng/mL, respectively. The developed method showed low ng/mL levels of NSAIDs in the urine.

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Three phase hollow fiber liquid phase microextraction combined with HPLC-UV for determination of three tetracyline antibiotics

오웅교 명승운*

경기대학교 화학과

Tetracyclines(TCNs) are some of the most commonly used antibacterial compounds having broad spectrum of activity against gram-positive and gram-negative bacteria. In the present study, a simple and efficient preconcentration method was developed using three phase liquid phase microextraction prior to HPLC-UV for simultaneous extraction and determination of tetracycline antibiotics including tetracycline(TCN), oxytetracycline(OTCN), and Chlortetracycline(CTCN) in aqueous solution. For extraction, 1.5 mL of the aqueous sample containing TCNs and 0.1 M NaOH (pH 9.0) was filled into a 1.5mL vial. The organic solution of heptanal was immobilized in the pores of a polypropylene hollow fiber. Aqueous acceptor phase (AP, 11 µL of 0.1 M HCl with pH=1.0) was located inside the lumen of hollow fiber and the fiber was transferred into the aqueous sample. 700 rpm was selected as the optimum stirring speed for the rest of the experiments. Based on these observations, 60 min period was selected as the optimum extraction time. No salt was added in the experiments. Finally, the applicability of the proposed method was evaluated by extraction and determination of the antibiotics in aqueous sample. The results indicated that hollow fiber microextraction method has excellent clean-up and high-preconcentration factor and can be served as a simple and sensitive method for monitoring of antibiotics.

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Polystyrene coated partially sub-2micrometer silica particulate stationary phase of exceptional high separation efficiency

Faiz Ali

인하대학교 화학과

Uniform polystyrene layer of suitable thickness has been deposited on the surface of partially sub-2micrometer porous silica particles by RAFT polymerization. Sodium diethyldithiocarbamte was bonded to silica surface as initiator entity after attaching 3-Chloroprophyltrimethoxy silane as a spacer. Reversible addition-fragmentation chain transfer (RAFT) polymerization was carried out using styrene monomer under reflux. Micro-columns (1.0 mm ID and 300 mm length) were packed with the resultant phase and a mobile phase of 60/40 (v/v) acetonitrile/ water containing 0.1% TFA and a flow rate of 15microL/min were found to be the optimized conditions resulting in exceptionally high separation efficiency. Numbers of theoretical plates obtained were ca 50,000 (165,000/m).

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Cerium Doped Silica Nanoparticles for the Determination of Human Tumor Marker CEA in Serum

최혜원 조희경 장하나 임홍빈*

단국대학교 화학과

Nanoparticles show many unique properties, such as optical, electrical magnetic and chemical properties, which are not observed in the bulk material, therefore they have been used in various fields such as medicine, electronics, energy, cosmetic products and others. Especially, nanoparticle-based biotechnology has greatly developed for several decades. Our laboratory aims the development of the most sensitive method for tumor markers using optical and inorganic mass spectrometry because for the early detection of tumor marker in small amount of blood or urine requires an analytical method with good sensitivity. In this paper, for sandwich immunoassay using particle tagging, two types of nanoparticles, superparamagnetic nanoparticles for sample collection and CeO2 coated silica nanoparticles for detection are used. 140Ce coated nanoparticles tagged particle is a remarkable probe with ICP-MS measurement because of its low spectral interference compared to the fluorescence tagging and any other element. The developed analytical method using nanoparticle tagging is applied to the quantification of carcinoembryonic antigen (CEA), a widely used tumor marker that is overexpressed in many carcinomas.

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Development of the matrix array for the analysis of crude lipid extracts by MALDI mass spectrometry

이광빈 손정진 차상원*

한국외국어대학교 화학과

MALDI MS is a very useful tool for rapid lipid metabolite fingerprinting from crude extracts. However, since lipid ion signals are strongly dependent on matrix selection and chemical characteristics of lipid analytes, only preferentially ionized lipid species can be observed when using a single matrix. In order to overcome this issue, we surveyed ionization characteristics of various matrices including small organic acids, inorganic nanoparticles, and nanocomposites. In addition, we also investigated the effect of additives such as salts, acids & bases, and ion paring agents. From this extensive investigation, we finally generated a robust matrix array which can detect various lipid classes from crude lipid extracts with high sensitivities and also with high orthogonality.

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Development of capillary electrophoresis inductively coupled plasma mass spectrometry (CE-ICP-MS) for separation and quantitative analysis of phosphate

김진일 임용현[1] 이경석[1,*] 김태규[*]

부산대학교 화학과 [1]한국표준과학연구원(KRISS) 분석화학표준센터

Inorganic elements play key roles in biochemical field as constituents of biomolecules. Especially, phosphorylation is an important protein activity due to its participation in many cellular processes. In this paper, inductively coupled plasma mass spectrometry (ICP-MS) hyphenated to the capillary electrophoresis (CE) was performed for separation and quantitative analysis of phosphate biomolecules including phosphate group such as ATP, ADP and phosphorylated peptide. CE has been used to separate phosphate group whose separation is determined by the charge to size and electrical mobility of analyte. CE separation data shows that CE provides a narrow peak and a high resolution. After separation, quantitative information of phosphate biomolecules was analyzed by counting the number of phosphorus ions in ICP-MS using medium mass resolution with high sensitivity. The concentration of phosphate biomolecules could be obtained from the peak area in electropherogram by CE-ICP-MS. In addition, the limit of detection and dynamic range of phosphorus measurements by the developed CE-ICP-MS method have been also studied. Finally, it is considered as an excellent technique in analyzing biomolecules due to its good detection limits and selectivity with providing traceability to SI.

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The structural characterization of liquid wastes produced in PCB stripping process by photooxidation

김종부[*] 장다영[1,*] 서항복[2] 박종오[3] 최영하[4]

(주)해동테크놀로지 기업부설연구소 [1]해동테크놀로지 기업부설연구소 [2](주)해동테크놀로지 대표이사 [3](주)해동테크놀로지 상무 [4](주)해동테크놀로지 이사

This study was undertaken as a basic experiment to elucidate the structural change of stripping wastewater by photocatalytic oxidation and to develop more effective treatment system for water and wastewater. Photooxidation of stripping wastewater(at pH 7.0) were carried out in three system of UV only, UV/TiO_2 and UV/H_2O_2. The treated stripping wastewater at different reaction time were analyzed by ^{13}C-NMR spectroscopy to evaluate its structural changes. In untreated stripping wastewater, The aromatic carbons(δ : 110~160 ppm) account for 43.8% of all carbon and aliphatic(δ : 160~200 ppm) account for 18.0% and 23.4% respectively. The photooxidation of wastewater showed that the transformation ratio of aromatic carbons to aliphatic and carboxylic carbons was increased with UV irradiation time. The ratios of aromatic carbons of the treated wastewater for 200min. were reduced from 43.8% to 38.5%(UV only), 23.8%(UV/TiO_2) and 15.5%(UV/H_2O_2). On the other hand, carboxylic carbon contents were considerably increased from 23.4% in untreated wastewater to 25.7% in UV only, 30.8% in UV/TiO_2, 43.4% in UV//H_2O_2 system. From the analysis of the peak positions in the spectra, it, could be suggested that aromatic and aliphatic components including alcohol, amine, and carbohydrates were effectively transformed into various type of carboxylic acids ahead of their mineralization. Acknowledgement : This research was supported by the Program for the Construction of Eco Industrial Park(EIP) which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

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Trimethylamine analysis using SPME and INME

방예진 배선영*

서울여자대학교 화학과

Volatile Basic Nitrogen(VBN), such as trimethylamine(TMA) generated by proteins spoilage is common chemical indicator of seafood and meat freshness. To make a database for establishing meat's spoilage index and develop of VBN analysis method, this experiment was performed. There are few methods available on VBN such as conway micro-diffusion(CMD) method, DHS(Dynamic Headspace) method and SPME(Solid Phase Micro Extraction). Among the various method of analysis of VBN, SPME and INME(In needle microextraction) which both methods are solvent-free and rapid methodology for the analysis of various volatile compounds are used for analysis of TMA in this study. Recently developed INME method's principle is micro-bore tunnel of needle coated with adsorbent that is kept inside of the needle while SPME has the fiber exposed to headspace.SPME's absorbent were PDMS(Polydimethylsiloxane) and PDMS/DVB(Divinylbenzene) while INME's absorbent were PDMS and PDMS/PAA(Polyaceticacid). To optimize TMA analysis condition various parameters have been changed including adsorption time(5, 10, 15, 20, 25 min), adsorption temperature(30, 40, 50, 60 ℃), desorption time(1, 2, 3 min) and desorption temperature(200, 220, 240℃). TMA in methanol standard solution was used for TMA calibration curve and further analysis. TMA adsorbed via microextraction was analyzed by GC-FID (Hewlett-Packard, 5890 II) with a capillary column (DB-WAX, 30 m × 0.25 mm × 0.25 μm). Extraction efficiency of both methods was computed and presented. Keywords: VBN(Volatile Basic Nitrogen), TMA(Trimethylamine), SPME, INME.

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여러 흡착제를 이용한 수중의 다이아지논 흡착 특성에 관한 연구

유건상 홍용표 최종하[1] 정선영

안동대학교 응용화학과 [1]안동대학교 화학과

다이아지논은 광범위한 살충 작용을 나타내는 40 종 이상의 유기인계 살충제 중 대표적인 물질로 순수한 상태일 경우 무색무취의 액체이며 상업적으로는 방향족 유기용매에 용해된 상태로 유통 사용된다. 다이아지논은 농작물의 해충방제, 거주시설 내부와 애완동물의 벼룩과 진드기와 같은 해충 구제, 양, 염소와 같은 가축의 해충 구제, 정원과 골프장 등의 해충 피해 방지 등의 다양한 용도로 사용된다. 다이아지논의 인체 위해 가능성으오 인해 2001 년에서 2004 년에 걸쳐 미국, 유럽국가들에 의해서 비농업적 사용이 금지되고 잇는 추세이나, 농작물의 해충 피해를 방지하기 위한 목적으로 현재도 세계적으로 널리 사용되고 있다. 그러나 다이아지논은 다양한 경로를 거쳐 자연계에 노출됨을써 인체의 건강을 위해할 수 있으며 토양에 지속적으로 잔류하며 이는 지하수를 따라 하천으로 유입되거나 대기 중으로 기화되어 전체적인 오염을 일으키는 원인이 된다. 본 연구는 활성탄(activated carbon), 황토(yellow sand), 비산재(fly ash)와 같은 다양한 흡착제를 이용하여 수중에 있는 다이아지논을 흡착 제거할 수 있는 가능성을 탐구하고자 하였다. 이를 위해 온도, 접촉시간, 흡착제의 양 등 다양한 실험조건 별로 흡착 특성을 비교 분석하였다.

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단분산 나노입자의 표면 전하 조절 및 세포 독성평가

<u>이의연</u> 정덕호 송남웅[1] 권영은*

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나노 물질은 그 크기가 작고 (100 nm >), 크기에 비해 넓은 표면적을 가지므로 마이크로 입자에서는 볼 수 없었던 새로운 물성을 나타낸다. 이런 물성은 여러 분야에서 기존 기술의 한계를 뛰어넘을 수 있는 가능성을 제공함에 따라 다른 분야와의 융합을 통해 새로운 분야를 구축하는데 이용되고 있다. 나노기술에 대한 대규모 투자와 상업화에도 불구하고, 나노물질의 안전성 측면에 대한 이해는 여전히 불충분한 상태이다. 나노물질은 다른 위해성 화학 물질들과 달리 크기, 표면적, 결정 구조 등의 물리화학적 특성이 안정성을 결정하는 주요 인자가 된다. 기존의 나노물질의 독성을 보고한 연구 중에서 많은 경우 물리화학적 특성이 고려되지 않았으며, 체계적인 독성 평가 방법이 정립되지 않은 상태이다. 본 연구에서는 표면 전하가 조절되고 단분산된 나노입자를 대량으로 만들 수 있는 표면 개질 기술을 개발함으로써, 나노물질의 안전성 평가에 사용될 수 있는 Certified Reference Material(CRM)의 효과적인 제조 기술을 확보하였다. 계면활성제를 티올 그룹을 포함하는 리간드로 교환함으로써 음전하, 중성전하, 양전하를 띠는 나노입자를 효율적으로 제작하는 방법을 사용하였다. 리간드 교환에 따른 나노입자의 응집을 방지하기 위해 Sequential Ligand Exchange(SLE) 방법을 도입하였다. 개발된 SLE 방법을 통해 기존의 방법으로는 제작이 어려웠던 양전하로 하전된 단분산 금 나노입자를 비롯하여 다양한 표면 전하를 갖는 나노입자의 제작이 가능해졌다. 제작된 나노입자의 표면 전하는 Zeta Potential 을 측정하여 결정되었고, 나노입자의 분산도 및 크기변화는 Dynamic Light Scattering(DLS)과 UV-Vis spectroscopy 를 통하여 관찰되었다. 제작된 나노입자를 이용하여 나노입자의 표면전하에 따른 세포 독성평가가 수행되었다.

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Isotopic GlcNAc Incorporation by Transglycosylation of Endoglycosidases for the Relative Quantification of N-linked Glycans by Mass Spectrometry

배정은 임재민*

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Glycosylation is attaching the oligosaccharides to proteins or peptides by post-translational modification processing. Various investigations concerning quantitative glycan analysis have been performed because of the importance of the oligosaccharide moieties on glycoproteins that affect a wide range of protein functions such as cellular recognition processes.Endo-β-N-acetylglucosaminidase (Endo-M) is a class of endoglycosedases that releases the N-linked glycans bound to a amide nitrogen of asparagines residue by hydrolyzing the glycosidic bond in N-N’-diacetlychitobiose core. On the other hand, the Endo-M possesses transglycosylation activity and is able to transfer the released N-linked glycans to suitable acceptor such as Glc and GlcNAc. We reported quantitative analysis for fully sialylated N-linked glycans with the normal GlcNAc and the heavy GlcNAc as acceptors by transglycosylation of Endo-M. In this processing, we have performed experimental parameters such as solvent effects and incubation time to optimize the enzymatic reaction conditions.The transglycosylation reaction using Endo-M with heavy GlcNAc as acceptor shows 7 Da difference in comparison with original glycans which can overcome the isotope distribution overlapping. The results provide the use of a quantitative technology for fully sialylated N-linked glycans in biological systems.

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Liquid chromatographic enantiomer separation of rasagiline and its analogues on a chiral stationary phase based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid.

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부산대학교 화학과

The enantiomers of chiral compounds often show different effect on a human body when used as drugs. Therefore it is very important to separate chiral compounds to prevent unwanted side effect. HPLC (High Performance Liquid Chromatography) chiral stationary phase (CSP) method is one of well known and reliable methods for the resolution of the two enantiomers of chiral compounds. In this study, we resolved rasagiline, which is achiral drug for the treatment of Parkinson's disease, and its analogues on a CSP based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid. We synthesized rasagiline and its analogues starting from 1-aminoindan, 6-bromo-1-indanone and 6-methyl-1-indanone. We found that rasagiline and its analogues are generally well resolved on this CSP and the resolution was found to be dependent on the mobile phase composition.

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Determination of Total Dissolved Phosphorus with Microfluidic Chip-Based Absorbance Detection System

나고은 안재훈 한종훈*

포항공과대학교 화학과

We have been developed the compact, sensitive and continuous absorbance detection system for determination of TDP (total dissolved phosphorus) in aqueous media. The measurement of TDP in surface water and wastewater is critical for understanding eutrophication processes and biogeochemical cycling, assessing water quality in drinking water reservoirs. As a common method for determination of TDP, all kinds of dissolved phosphorus should be converted to orthophosphate form which is detectable at 370 nm. At the first step, the conversion process is accomplished by addition of an oxidant under UV irradiation. The system for the UV-oxidative decomposition is a flow reactor made of Teflon capillary. To maximize the efficiency of UV exposure the capillary wound around the UV pen light closely. The following step is for the microfluidic chip-based absorbance detection with color development. The system can be miniaturized by containing a LED (light emitting diode) and PMT (photomultiplier tube) as a light source and detector. To take an advantage on flexibility of a light path length, a LCW (liquid core waveguide) is adopted. The LCW made of Teflon AF-2400 has been used to extend the sensitivity of conventional colorimetric method. The linear range and limit of detection for TDP are 0.5～5 ppm (R^2=0.99) and 0.3 ppm (S/N=3) respectively. The miniaturization of microchip-based analysis system has following characteristics as an ideal *in situ* monitoring system: simplicity, portability, fast analysis, low reagent and power consumption, economic use of stable reagents. Furthermore, the system integrated with wireless communication will be particularly suited for environmental monitoring requiring high spatial or temporal resolution.

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Structural characterization of $0.3Li_2MnO_3 \cdot 0.7LiMn_{0.60}Ni_{0.25}\ Co_{0.15}O_2$ cathode materials for lithium-ion battery

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$LiCoO_2$ is generally used as the cathode material, however, it has the thermal instability, poor rate performance, and the toxicity and high cost. As alternative $LiCoO_2$, $xLi_2M'O_3 \cdot (1-x)\ LiMO_2$ electrode materials (M′= Mn, Ti and M = Mn, Ni, Co) have attracted much attention due to its high rate performance and improved safety. In this work, structural investigations of manganese-rich $0.3Li_2MnO_3?0.7LiMn_{0.60}Ni_{0.25}\ Co_{0.15}O_2$ cathode materials has been performed by 7Li MAS NMR.

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Liquid chromatographic enantiomer separation of iridium(III) complexes on a polysaccharide chiral stationary phase.

김희은 **LIYINAN 탁경미 현명호***

부산대학교 화학과

HPLC (High Performance Liquid Chromatography) chiral stationary phase (CSP) method has been generally used for resolving chiral compounds, especially drugs. However resolution of enantiomers of iridium(III) complexes on HPLC CSPs is rare.In this study, we prepared various iridium(III) complexes starting from 2-phenylpyridine and iridium chloride hydrate and resolved them on a polysaccharide chiral stationary phase. As an effort to find out the optimum resolution condition, various mobile phases were tested.

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All-solid-state Hg(II)-selective electrode using double-layerfilm of polyethylenedioxythiophene(PEDOT) composite and plasticized poly(vinylchloride) containing 4-nitrophenyl urea

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All-solid-state Hg(II)-selective electrodes have been constructed on a Pt disk electrode using a double-layer film of polyethylenedioxythiophene(PEDOT) composite covered with a plasticized poly(vinyl chloride) (PVC) membrane containing 4-nitrophenyl urea(4NPU). The lower composite layer is formed by electropolymerization of EDOT in an acetonitrile containing $LiClO_4$, and the upper PVC layer is formed by casting. The electrode shows a near-Nernstian slope of -31.1 mV/dacade, and low detection limits of 1.0 x $10^{-7.5}$M. The double-layer film electrode using this composite shows no overshoot and lower drift of the standard potential than both a conventional PVC electrode and a single-layer electrode using PEDOT doped with ClO_4^-. This is due to both the highly electrochemical activity of the lower PEDOT and the cation-exchange ability between the PEDOT and the Hg(II)-selective membrane with active sensor elements 4NPU.

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The construction of home-built solid-state NMR probes for special purposes

최성섭 박유근 정지호 김용애*

한국외국어대학교 화학과

The solid-state NMR has been widely used for various insoluble materials like industrial polymers and biological samples, up to now. Analysis of membrane protein using solid-state NMR on lipid bilayer or bicelle for membrane-like environments, is valuable especially for a predominantly their helical secondary structure. But, most of biological lipid samples have high dielectric property due to containing large amounts of lipids, water, and salts. This electrical property causes a loss of probe efficiency. For these reasons, a specific probe with high efficiency is required to study biological samples by using solid-state NMR. The solid-state NMR methodologies originally developed for the study of membrane proteins in lipid bilayers and are also used for the in-situ analysis of liquid crystalline materials in LCD panels and packed Li ion batteries. Since liquid crystals samples in LCD panels could not be analyzed by conventional MAS technique and instruments. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore (NB) 1H-15N solid-state NMR probe with strip-shield coil to prevent heating by high RF power. 1H-15N 2D SAMPI4 spectra from a single crystal and membrane proteins in oriented bicelles was successfully obtained by using these solid-state NMR probe. Also, we present a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil. It was the first application for the in-situ analysis of LCD panel samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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Determination of acetyl content of Cellulose Acetate by HPLC and NMR spectroscopy

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The acetyl content of cellulose acetate can be determined by HPLC and NMR spectroscopy. The number of signals and integration ratio on the 1H-NMR spectrum represents which functional groups have been substituted and the number of signals and integration ratio on the 13C-NMR spectrum represents which sites of cellulose acetate have been substituted with functional groups.Hydrolysis of cellulose acetate has been performed with NaOH and then the amount of functional group have been analyzed with HPLC.

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Design and Structural Characterization of Antibacterial LPcin-I and LPcin Analog Peptides with Enhanced Activities

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한국외국어대학교 화학과

Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of proteose-peptone. LPcin is a good candidate as a peptide antibiotic because it has an antibacterial activity but no hemolytic activity. Three different analogs of LPcin, LPcin-yk2 which has mutant amino acids, LPcin-yk1 and LPcin-yk3 that has shorter mutant amino acids are recently developed by using peptide engineering in our lab. These three LPcin analogs show better antibioitic activities than LPcin and no toxicity at all.In order to understand the correlation between the structure of LPcin analogs and antimicrobial activity interacting with bacterial membrane surface, we tried to express and purify as large as amounts of LPcin and three different LPcin analogs. We finally optimized and succeed to overexpress in the form of fusion protein in Escherichia coli and purified with biophysical techniques like Ni-affinity chromatography, dialysis, centrifuge, chemical cleavage, and reversed-phase semiprep HPLC et al. In order to identify their characteristic structure of the purified peptides in membrane environment, we performed Mass, CD and NMR spectrometry with samples mimicking membrane environments. For identifying antimicrobial mechanisms and dynamics, we use various 1D and 2D NMR techniques using bicelle samples which were similar to bacterial membrane environments.In here, we will present the optimizing processes for high-yield expression and purification and solution NMR spectra and solid state NMR spectra for antimicrobial mechanisms.

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Optimized Expression and NMR Structural Studies of Syndecan-4

송주영 최성섭 김용애*

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Syndecans are involved in a major family of cell surface receptors that participate in cell-cell and cell-matrix interactions. One of the syndecan family peptides, Syndecan-4, has important roles that may affect tissue development and repair as well as the pathogenesis of numerous diseases. Relatively, abundant studies about structural information and biological functions of cytoplasmic and extracellular domain of syndecan-4 have been ascertained, but a lot of efforts to elucidate the structure and function of the syndecan-4 transmembrane domain (Syd4-TM) still has been hindered by insufficient yields and low solubility. Thus, we demonstrate an optimized method for recombinant expression and purification of three kinds of Syd4-TM like wild type Syd4-TM, mutant Syd4-TM, and Syd4-eTC. All peptides were released from the fusion protein, and then purified by semi-preparative reversed-phase HPLC. 5 to 10 mg of purified Syd4-TM peptides was obtained from 1L of M9 minimal media under optimal conditions. Prior to the three dimensional structural determination, biophysical properties of peptides were studied by circular dichroism (CD), MS spectrometry, and nuclear magnetic resonance (NMR) spectroscopy. Analysis of CD spectra presents that Syd4-TM adopts a stable α-helical structure in micelle environments. And solution NMR studies show Syd4-TM forms an asymmetric dimer in micelles. As previously stated, we research mutant Syd4-TM that has a partially modified sequence of Syd4-TM, doesn't show dimerization but consists of monomer, and Syd4-eTC which has extracellular, transmembrane and cytoplasmic domain of syndecan-4. Two peptides also were expressed and purified under optimized conditions and finally we confirmed that mutant Syd4-TM forms a monomer and Syd4-eTC does a dimer.

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Separation and Analysis of Carbon Fiber Sizing Agents by Preparative LC

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Carbon fiber(CF) is widely used in aerospace industry due to its extraordinary properties especially light weight, high specific strength and modulus. However, CF is inert, untreated CF has a poor interfacial bond between fiber and resin matrix. Besides, there tends to arise many problems of filament breakage and fluffs caused by mechanical friction against guides and rollers during manufacturing process because of low expandability and quickly wear and tear by bending of carbon fiber.Sizing method is an efficient method to increase the fiber/matrix adhesion. Sizing agents have been used to insert a polymer interlayer between CF and matrix and to control the level of fiber/matrix adhesion.In this study, we have analyzed several unknown sizing agents through preparative LC system. Each CF sizing component separated by three successive GPC columns has been closely analyzed using H-NMR, FT-IR and GC/MS afterward. We have found that most of the sizing agents mainly consist of epoxy resins, other polymer resins, and emulsifying agents.

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Compositional Analysis of Cu(In,Ga)Se_2 Thin Films using Various Analytical Techniques

이지혜 이연희

한국과학기술연구원(KIST) 특성분석센터

Cu(In,Ga)Se_2 (CIGS) solar cells are very promising films for use in photovoltaic devices, as they feature a high absorption coefficient and a high conversion efficiency at a relatively low manufacturing cost. In order to develop an efficient CIGS solar cell, accurate analysis of the relative atomic fraction of CIGS film is one of the most important factors. In this study, a quantitative analysis of CIGS was investigated using an inductively coupled plasma-optical emission spectrometry (ICP-OES), electron probe micro analysis (EPMA), x-ray fluorescence (XRF), Auger electron spectroscopy (AES), and dynamic secondary ion mass spectrometry (dynamic SIMS). ICP-OES technique is a well-known quantification method and has an advantage in determining the average composition of CIGS film. In order to prevent the loss of Se from a general sample pretreatment process, CIGS samples were treated at room temperature in an hour. The relative sensitivity factors (RSF) of AES and SIMS were obtained by using ungraded CIGS film of known composition as a standard sample. Quantitative analyses of several CIGS samples were performed using the relative sensitivity factor (RSF) value calculated from the depth profile results of the standard film. The Cu/(In+Ga) ratio and the Ga/(In+Ga) ratio of SIMS results are relatively reproducible and close to those of the AES results. Overall, compositional results of CIGS thin films by a variety of analytical methods were compared and their discrepancies were interpreted.

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Authentication of Pinellia ternata and its Adulterants by 1H NMR-based metabolomics

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The tuber of Pinellia ternata is widely used as an oriental medicine in the East Asian regions. Pinellia ternata is known as the herb effective in removing dampness-phlegm, one of the causes of obesity in traditional Korean medicine. Recently, Pinellia ternata is deficient in herb market and its adulterants are used. The adulterants are similar in appearance, but they are different in medicine effect and even have toxic components. Therefore, the discrimination between Pinellia ternata and its adulterants is very important. In this study, Pinellia ternate and its adulterants (Arum flagelliforme and Pinellia pedatisecta)were characterized using 1H nuclear magnetic resonance (NMR) spectroscopy followed by multivariate data analysis. Principal component analysis (PCA) score plots from 1H NMR data showed a clear distinction between three groups. The major metabolites that contributed to the discrimination factor from included various amino acids (arginine, asparagines, glycine, histidine, isoleucine, leucine, phenylalanine, threonine, tyrosine, valine, glutamate), sugars (fructose, glucose, sucrose), organic acids (4-aminobutyrate, acetate, isobutyrate, succinate) and choline. Therefore, our study demonstrates that 1H NMR based profiling coupled with chemometric analysis can be used to effectively discriminate between Pinellia ternata and its adulterants.

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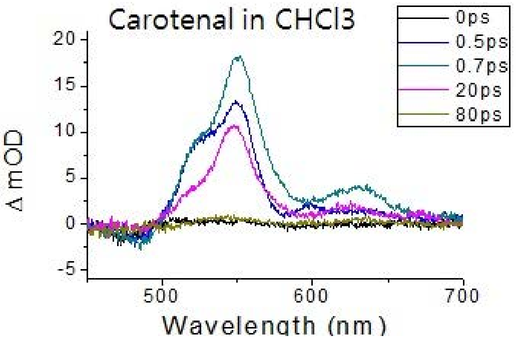
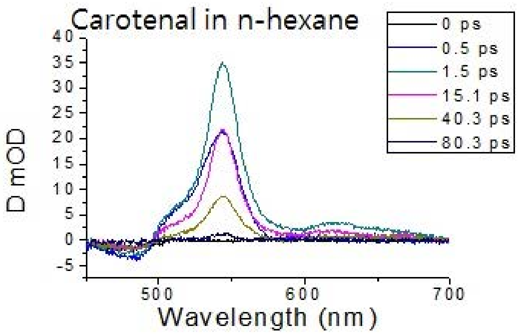
용매에 따른 케로티노이드 화합물의 들뜬상태 동력학연구 Solvent-dependent excited state dynamics of Carotenoids

이인구 이세복 방윤수*

광주과학기술원(GIST) 물리화학부

Carotenoids are light harvesting pigments that play important roles in the photosynthesis. Carotenoids have long conjugated carbon backbones, so the electronic structure of carotenoids is well described by the singlet ground and excited states. Apocarotenoids with a electron-withdrawing group on one side have shown strong solvent dependence in the excited-state dynamics. 8'-Apo-β-caroten-8'-al with carbonyl group has been used in our femtosecond transient absorption measurements. Pump pulses of 510 nm were generated in a noncollinear optical parametric amplifier. White-light probe pulses (450~750 nm) were generated by supercontinuum generation in a sapphire window. Solvent-dependent dynamics were compared between solvents including chloroform (polar) and n-hexane (nonpolar). Excited-state absorption bands of 8'-apo-β-caroten-8'-al in both solvents look similar, but one in chloroform decays faster than that in n-hexane. An excited-state absorption band at 630 nm is stronger in chloroform than that in n-hexane.





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Single C-Reactive Protein Molecule Detection on Nanoarray Biochip Based on Total Internal Reflection Fluorescence

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경희대학교 응용화학과

We detected single molecule of C-reactive protein (CRP), which is known as a non-specific acute phase marker, using a highly sensitive immunosensor. This immunosensor based on gold-nanopatterned chip utilized characteristic of antigen-antibody interaction and lab-made prism-type total internal reflection fluorescence microscopy (TIRFM). The 4×5 gold-nanopattern with a spot diameter of 500 nm was fabricated by using electron beam nanolithography. Unlabeled CRP molecules in human serum were identified by detecting secondary fluorescence which was generated by fluorophores in evanescent field layer. As standard CRP concentrations drop, relative fluorescence intensities decrease in the linear range of 33.3 zM (the theoretical molecule number = 1)-100 pM (the theoretical molecule number = 12.04×10^{8}). Only one single-CRP molecule could be detected on the nanoarray chip by TIRFM. These perspectives could be important to study mechanisms of individual protein dynamics, translation process, and protein-protein interaction at the single-molecule level.

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Characterization of organic components in leachate from animal carcass disposal site over time

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Leachate, is generated by decomposition of animal carcass, has many environmental, sanitary and food safety hazards. However, there is a lack of research on characteristic of leachate. In this study, we identified the characteristic components of cattle leachate from sandy loam soil and sandy soil by 1H-NMR spectroscopy followed by multivariate data analysis. Principal component analysis (PCA) from NMR data is showed similar pattern between samples prepared in two types of soils. The organic components, including organic acids, phenols and methylamine, were identified in leachate, and the levels of their compounds were increased over time. In addition, levels of organic components from sandy soil were higher than those from sandy loam soil, indicating that the biological degradation is faster than sandy loam soil. This study demonstrates that organic components in leachate from animal carcass can be quantitatively evaluated and characterized over time using NMR based profiling approach.

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Chiral Recognition of Amino acid and Amino Acid Derivatives by (R)-Phenylethylamine derived Nickel(II) macrocyclic complexes

유정재 류재정[1,*]

경북대학교 화학과 [1]경북대학교 화학교육과

(R)-Phenylethylamine 을 리간드로 이용한 nickel(II) macrocyclic complexes 는 해당 실험실에서 one pot template condensation reaction 으로 간단하고 효과적인 방법으로 합성되었으며, 해당 생성물을 이용하여 1,1′-Bi-2-naphthol 과 2,2,2-Trifluoro-1-(9-anthryl)ethanol 에 대한 키랄 인지 실험이 진행되었다.[1] 해당 실험을 바탕으로 nickel(II) macrocyclic complexes 가 phenylalanine, N-benzoyl-alanine, N-benzoyl-phenylalanine, N-benzoyl-methionine, N-CBZ-alanine 과 같은 아미노산과 아미노산 유도체들에 대하여 동일한 실험을 진행하여, 키랄 인지 능력을 보이는 지 살펴보았다. [1] J. J. RYOO. Inorg. Chem., 2010, 49 (16), pp 7232?7234

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Integrated analytical approaches for metabolomics study of metastatic cancer cell

이주은 류도현[1,*] 황금숙[2,*]

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The ultimate goal of metabolomics is to obtain the meaningful information and expect the biological events from the metabolome differentiation. Because of the detection ability of diverse metabolites and complementariness between instruments, the integrated analytical technique is a powerful tool for metabolic applications such as biomarker discovery, discrimination of phenotypes, and system biology. In this study, NMR- and MS-based metabolomics was performed to investigate the metabolic difference of metastatic cancer cells dependent on glucose availability. Polar metabolites such as amino acids, organic acids and nucleotides as well as phospholipids in cell extracts were detected using nuclear magnetic resonance (NMR) spectroscopy and ultrahigh-performance liquid chromatography?quadrupole time-of-flight mass spectrometry (UPLC-Q/TOF MS). Principle components analysis (PCA) and metabolite changes showed significant differentiation between groups exposed to different glucose availability. Through these results, we demonstrate that global metabolite profiling using integrated analytical technologies is useful toward discrimination between metastatic cancer cells dependent on glucose availability and interpret the mechanism of metastasis.

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Highly sensitive recognition of various explosive compounds using Raman spectroscopy and Principal component analysis

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With the threat of global terrorism on the rise, various analytical methods to identify of explosives has become an issue of critical national importance. However, limited applicability of several analytical methods such as, the incapability of detecting explosives in a sealed container, the limited portability of instruments, and false alarms due to the inherent lack of selectivity, have motivated the increased interest in the application of Raman spectroscopy for the rapid detection and identification of explosive materials. Raman spectroscopy has received a growing interest due to its stand-off capacity, which allows samples to be analyzed at distance from the instrument. In addition, Raman spectroscopy has the capability to detect explosives in sealed containers such as glass or plastic bottles. We report a rapid and sensitive recognition technique for explosive compounds using Raman spectroscopy and principal component analysis (PCA). Seven hundreds of Raman spectra (50 measurements per sample) for 14 selected explosives were collected, and were pretreated with noise elimination methods. Here, features for discrimination among different explosive compounds were obtained using PCA. The MAP analysis demonstrates an excellent discrimination capability of 99.3% average classification rate. The results show that the combination of the pattern recognition technique of PCA with a Raman detection system can be effectifve to detect explosives over a short period. This expedient and accurate capability to discriminate between explosive compounds wolud be also useful for fast identification of explosives in the field.

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Rapid and sensitive phenotypic marker detection on breast cancer cells using surface-enhanced Raman scattering (SERS) imaging

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We report a SERS-based cellular imaging technique to detect and quantify breast cancer phenotypic markers expressed on cell surfaces. This technique involves the synthesis of SERS nanotags consisting of silica-encapsulated hollow gold nanospheres (SEHGNs) conjugated with specific antibodies. Here we applied a SERS-based imaging technique using SEHGNs in the multiplex imaging of three breast cancer cell phenotypes. Based on results, this technique may enable an earlier diagnosis of breast cancer than is currently possible and offer guidance in treatment.

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The Electrochemical Studies of the glucose biosensor using Fe complexes based on the immobilization of Nickel nanoparticles on the ITO electrode.

이금옥 이수정[1] 이성규[1] 최영봉[1] 김혁한[1]

단국대학교 첨단과학대학 화학과 [1]단국대학교 화학과

Glucose sensors are the most intensively investigated biosensors due to their importance in blood glucose monitoring as well as in industrial application. We have been synthesized Fe complexes having with the 4,4’-bipyridine. Newly synthesized redox mediator presented here are described in shorthand as Fe(CN)5(4,4'-bpy), linked with the nickel nanoparticles onto the ITO electrodes. The surface studies of the immobilized Ni nanoparticle on the ITO electrode was investigated by scanning electron microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). The catalytical currents were amplified by GOx which are electrically mediated by new ferrate redox films, converting the films into an electrocatalysts for the electrooxdation of glucose. The resulting catalyical currents were linearly related with the low concentrations of glucose.

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Electrochemical Immunoassay using Pyridyl-N to Pentacyanoferrate onto the Ni-modified ITO Electrodes.

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단국대학교 나노바이오의과학과 [1]단국대학교 첨단과학대학 화학과 [2]단국대학교 화학과

The coordination of pyridyl-N to pentacyanoferrate for the detection of small organic antigens in solution is presented. The unique contribution of this paper is the direct conjugation of pyridyl-N in small organic antigens to pentacyanoferrate. In addition, an immunoassay methods have been devised using redox-active Fe(Ⅱ/Ⅲ) centers bound to Ni(Ⅱ) cations via cyanide bridges. In this works, Hippuric acid (HA) has been detected competitively on the interaction of free HA and pentacyanoferrate-(4-aminomethylpyridine-hippuric acid) (Fe-HA) to its antibody on the PVI-Ni immobilized ITO electrode. The electrical signals proportional to the Fe-HA was monitored by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The surface morphology of the immobilized PVI-Ni on the ITO electrode was examined by scanning electron microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.

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Intracellular anticancer drug mitoxantrone distribution in cancer cells by fluorescence spectroscopy

윤진하 Ganbold Erdene Ochir 박혜진 주상우

숭실대학교 화학과

We investigated in vitro glutathione (GSH)-induced intracellular anticancer drug release on gold nanoparticle (AuNP) surfaces by means of both label-free confocal resonance Raman and fluorescence spectroscopy. Morphologies of AuNPs were examined by transmission electron microscopy. UV-Vis absorption and infrared spectroscopy were used to check the fabrication of MTX. For Raman, the surface-enhanced Raman scattering (SERS) intensities of MTX were measured to be larger than those of the thiopurine anticancer drugs such as 6-mercaptopurine and 6-thioguanine by a factor of larger than 100. We plan to assemble the PEG moieties and folate targeting unit for an improved drug delivery to cancer cells. GSH-triggered release of MTX was achieved as evidenced by Raman and fluorescence spectroscopy. Our work demonstrates that a simultaneous measurement in the resonance Raman and fluorescence spectroscopic tools are achieved for monitoring of the controlled release of MTX drug molecules in vitro.

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Quantitative analysis of heavy metals and other contaminants in solid and liquid using laser-induced breakdown spectroscopy

buuveidorjbatbold 강위경

숭실대학교 화학과

Laser-induced breakdown spectroscopy (LIBS) is an analytical technique used to determine the elemental composition of samples in all forms. In this study, laser-induced breakdown spectroscopy (LIBS) will be used to determine the contents of heavy metals and other contaminants in solid and liquids. Heavy metals become toxic when they are not metabolized in the body, and will be accumulated in the soft tissues. The experimental setup was designed using a laser Q-switched Minilite II (Nd:YAG, 10Hz, λ=532nm) and the emission signals were collimated by lenses into an optical fiber coupled to charge-coupled device (CCD)-Aurora spectrometer. Prior to the application of LIBS system to actual samples, the LIBS spectrometer was carefully optimized to improve the LIBS efficiency.

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Spectroscopic characterization and cellular uptake behaviors of pegylated porous silica nanoparticle drug delivery system

박혜진 우린토야 주상우

숭실대학교 화학과

We investigate the cellular uptake behaviors and efficacy of pegylated mesoporous nanoparticles (MSNs) for the drug delivery system in human cancer cells by means of spectroscopic tools. The morphologies and physicochemical characterization of pegylated (PEG)-coated MSNs have been examined by infrared, UV-Vis absorption spectroscopy, and transmission electron microscopy (TEM). Live cell imaging of PEG-attached MSNs in cancer cells indicated that the MSNs appeared to enter into the cell with an hour. The cell viability was also compared to estimate the efficacy of PEG-conjugated MSN delivery systems. PEG-assembled MSN systems appeared to decrease cancer cell viability in vitro. We plan to perform a Western blot and FACS analysis to investigate an apoptotic pathway in cancer cells induced by MSNs. Potential applicability of antifungal agent delivery will be performed in the collaboration of other research groups soon and shall be discussed at the meeting.

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Surface-enhanced Raman scattering study of antifungal agent myclobutatil on gold nanoparticle surfaces

SinghDheerajKumar **Ganbold Erdene Ochir 주상우**

숭실대학교 화학과

Metal nanoparticles (especially Ag and Au) are a class of surface-enhanced Raman scattering (SERS) substrates that have proven effective for sensitive, reproducible and analysis of pathogens and have gained enormous attention to protect human health and the enviroments. With this motivation, In the present study, we performed the SERS measurements of antifungal drug myclobutanil (MCB) on the surface of gold nanoparticles (Au NPs). Depending upon the physical environment (concentration, temperature and pH), the spectral changes of marker Raman band of adsorbate on Au NPs surfaces were discussed. Moreover, the quantum chemical calculation, using the density functional theoretical (DFT) was also performed in order to explore geometry configurations, electronic structures, charge populations and interaction energies of MCB with Au ions complexes. We believe that our theoretical calculations may provide some clues for reasonably explain our experimental findings.

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Multiple Nonenzymatic Labels-Based Impedimetric Apatamer Sensor for the Competitive Detection of Thrombin

정봉진 Md. Aminur Rahman[1,*]

충남대학교 분석과학기술대학원 [1]충남대학교 분석과학기술대학원 분석과학기술과

An electrochemical TB aptamer sensor was fabricated by immobilizing a thiolated TB binding aptamer onto the poly-dopamine/AuNPs surface for the competitive detection of TB. The polydopamine/AuNPs surface was characterized using SEM and electrochemical impedance techniques and the conjugate was characterized by TEM, DLS, and UV/Vis. The TB detection was based on the competition between multiple methylene blue-labeled-TB and free TB for the aptamer binding sites. Electrochemical Impedance Spectroscopy (EIS) nyquist plot responses before and after competition suggested that TB can be successfully detected with the poly-dopamine/AuNPs based-TB aptamer sensor. Under the optimized condition, the linear dynamic range and the detection limit were determined to be 10 pM ~ 1.4 nM and 10 pM, respectively.

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Aptamer-based surface-enhanced Raman scattering detection of Ochratoxin A

Ganbold Erdene Ochir **SinghDheerajKumar** 우린토야 윤진하 박혜진 주상우

숭실대학교 화학과

Recently development on detection and quantitation of mycotoxins which produced by fungus in a variety of commodities has received great attention from reseachers. Here, we report a new approach for the detection of Ochratoxin A (OTA) using surface-enhanced Raman scatteing (SERS) that could exhibit lower detection limits than fluorescence method. This approach is based on conformation change of Raman reporter-tagged Ochratoxin A (OTA)'s aptamer. OTA's aptamer could be easily adsorbed onto the surface of metal nanoparticles (NPs), and give good SERS signal. Upon the addition of OTA, however, the conformation of OTA's aptamer is changed from random coil structure to G-quadruplex structure. Thus OTA's aptamer could not be adsorbed onto the surface of NPs, and SERS signal will be decreased.

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Spectroscopic characterization of inclusion complex of drugs or mycotoxins with beta-cyclodextrin thiolate-decorated gold nanoparticles

우린토야 **Ganbold Erdene Ochir** 주상우

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We fabricated doxorubicin (DOX) or other mycotoxin-assembled beta-cyclodextrin thiolate (beta-CD-SH) on gold nanoparticles (AuNPs). The inclusion of DOX to beta-CD-SH and their subsequent adsorption on the AuNP surfaces was characterized using Raman, UV-Vis absorption, quasi-static light scattering, and infrared spectroscopy. A micromolar range of DOX loading is estimated for either 5 nm or 18.5 nm AuNP particle platform covered by beta-CD-SH. The fluorescence recovery test indicated that the attached DOX released from AuNPs after treatment with not serum media but 2 mM glutathione (GSH). Fluorescence microscope imaging indicated that the DOX was released from AuNPs in the cervical cancer HeLa cells after the endocytosis. We performed a cell viability assay for the anticancer drug-AuNP conjugates in the delivery to HeLa cells. A cytotoxicity test indicated that the DOX/beta-CD-SH/AuNPs system reduced the cell viability, whereas a comparable amount of AuNPs did not show any noticeable cytotoxicity. Our characterization may be useful to design the anticancer therapy based on AuNPs and CDs. We plan to develop a new spectroscopic detection method of mycotoxins using these platforms.

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Direct analysis of flame retardants in pellets without sample preparation

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The linear ion trap (LIT) mass spectrometer equipped with Direct Analysis in Real Time (DART) is capable of analyzing flame retardants in pellets of synthetic resins without sample preparation. Since DART is considered a complex thermal desorption ionization process, the optimization of parameters such as helium gas temperature was necessary. It was observed the parameter of helium gas temperature has a significant effect on the intensity of molecular ion on the mass spectra. For most phosphorus-based flame retardants, the major peak is observed as a form of $[\mathrm{M+NH4}]+$. Through this experiment, we have confirmed that DART technique has the potential for direct, simple and rapid analysis of flame retardants in pellets under ambient condition.

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Film sensor for Ni(II) via self-assembled monolayer of receptor on quartz plate surfaces

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Chemical sensing self-assembled monolayers (SAMs) on quartz plate surfaces are developed as new sensing materials for metal ions. This film sensor was designed and prepared by chemically immobilization of a terminal silane group of monomer molecule onto SAM on quartz plates and was used for detection of Ni(II). UV-vis measurements showed the absorption of the N_2O_2 donor macrocycle receptor film was selectively changed by Ni(II) ions and slightly influenced by the presence of other similar divalent metal ions (Pb(II), Zn(II), Cu(II), Co(II), etc.). The advantages of this technique have been demonstrated experimentally by the sensitive response of the presence of small amount of Ni(II). Moreover, the response of the film toward Ni(II) is fully reversible which makes it attractive for sensing application.

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Muti-element and stable isotope analyses in hair for forensic purpose

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The application of IRMS and LA-ICPMS in forensic hair samples was investigated. Identification of forensic hair samples was carried out using stable isotopes and multi elements. As well as, what kind of information to be taken from the unknown hair samples was examined. The scalp hair samples were collected and stored in glass vial on the room temperature. Our isotopic data (C, N, O, S and H) for bulk hair indicated that this signature can be used as an alternative tool of identification for the cases without good results from DNA analysis. The single hair strand was analyzed for getting information like sex, smoking habit and occupation using LA-ICPMS. Even this study was a preliminary test, good results were accquired. We need much more hair samples to be examined and application to LA-ICPMS with Aridus in the future.

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Chemiluminescence system for dissolved oxygen in water

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단국대학교 화학과

The monitoring of dissolved oxygen in water has become of increasing interest, especially in relation to the modern necessity for effective and reliable environmental studies. Conventionally, winkler titration method, polarographic, galvanic method, and fluorescence quenching have been used for many years as analytical techniques to determine dissolved oxygen (DO). Although these techniques are reliable, they have some limitations in terms of high cost, time-consuming, instability, and maintenance. In this work, we developed a highly sensitive, stable, convenient, and cost-efficient chemiluminescence (CL) method for a novel DO sensor. We utilized the mechanism based on the formation of oxygen radical in luminol-metal ion system. Using lab-built chemiluminescence instrument, we obtained the calibration curves and the limit of detection (LOD) for four metal ions (Co2+, Fe2+, Cu2+and Cr3+) that are able to catalyze the CL reaction. Among them, luminol-cobalt ion system was chosen after optimization due to its high sensitivity. According to our experimental results, we concluded that the method we have proposed is feasible to determine the content of DO.

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Evaluation of EGFR expression level on breast cancer cells induced by cetuximab-conjugated nanoprobes using SERS imaging

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EGFR has been recognized as an important biomarker expressed in cancer cells because the activation of EGFR is associated with the key features of cancer including tumor growth, survival, angiogenesis and metastasis. Thus, EGFR has been considered as one of the important prognostic cancer markers. Cetuximab (or Erbitux) is the first monoclonal antibody drug targeting EGFR markers overexpressed in cancer cells. Cetuximab easily binds to EGFR, resulting in the series of reactions: receptor down-regulation, blockage of EGFR-mediated tyrosin kinase activity, and inhibition of cellular proliferation. Thus, EGFR-Cetuximab bindings can be used for the quantitative monitoring of receptor status as well as the prognosis of cancer therapy. In this presentation, we report a new SERS imaging-based EGFR monitoring technique before and after the cetuximab treatment of cancer cells. Here, Raman mapping images were obtained using cetuximab- and hEGF-conjugated Au(core)-Si(shell) nanoprobes. Our experimental results show the potential feasibility of the SERS imaging technique for improving the prognostic efficacy of anti-EGFR treatment

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Development of Simultaneous Multiple Biomarker Detection Method for Early Diagnosis on Acute Myocardial Infarction (AMI) using Surface-Enhanced Raman Scattering (SERS)

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A simultaneous immunoassay technique using surface-enhanced Raman scattering (SERS) has been developed for the multiplex detection of cardiac markers. Troponin I, CK-MB, and myoglobin, were selected as target biomarkers in this work. Here, the detection of single biomarker cannot provide a definitive information about the disease because its sensitivity is very low due to the possibility of the false positive result, different duration and peak elevation time of each biomarker in the blood. To solve this problem, it is necessary to monitor three biomarkers simultaneously. For this purpose, gold nanospheres (GNPs) and magnetic beads wee utilized as detection probes and capturing substrates, respectively. The sandwich immunocomplex format using monoclonal antibody-antigen-monoclonal antibody set has been adopted for this assay. Here we report a preminary result for the multiplex detection of three cardiac markers.

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Synthesis of the new multi-responsive polymer network gels

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In this work, the new multi-responsive polymer network gels (MRPNG) comprising of poly(N-isopropylacrylamide) (PNIPAAm), poly acrylic acid (PA) and carbon nanostructure (CNS) were prepared using ammonium persulfate as an initiator at room temperature. The influence of individual components on the property of resulting hydrogels was investigated. The morphology was investigated by scanning electron microscopy. Fourier transform intra red spectroscopy, thermogravimetric analysis differential scanning calorimetry were employed to examine chemical compositions and microstructures of MRPNG. The hydrogels have large and interconnected porous network structures. The obtained MRPNGs showed multi-reponsive behaviors such as temperature and pH. The thermal and pH responsive equilibrium swelling ratios of the modified hydrogels are reported.

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Development of new carbon nanostructure based drug delivery gel

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Hydrogels have potential applications as structural biomaterials in areas such as tissue engineering and drug delivery. Functionalized carbon nanostructures (f-CNS) can promote gelation and improve properties of the gel. We prepared the new f-CNS incorporated stimuli responsive gel (f-CNS-SRG), comprising of pH responsive and biocompatible polymers. Fourier transform intra red (FTIR) spectroscopy, thermogravimetric analysis, differential scanning calorimetry and scanning electron microscopy were employed to examine chemical compositions and microstructures of f-CNS-SRG. The pH responsive drug release behaviors of the model drug, doxorubicin hydrochloride, have been studied.

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Preparation of new sulfonated poly(ether ether ketone) based organic-inorganic hybrid proton conductive membranes

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It is generally accepted that the use of organic-inorganic hybrid proton conducting membranes would allow formation of inorganic networks and hydrophilic/hydrophobic domains within the polymer matrix. These feature are beneficial for improving the physico-chemical properties of proton exchange membranes. Among the various membranes, sulfonated poly(ether ether ketone) (SPEEK) received considerable attention due to its good mechanical strength and stability. For practical utility as the proton exchange membrane, the properties of plain SPEEK have to be improved. This can be accomplished by blending SPEEK with inorganic and/or organic fillers. In this work, we have prepared the new SPEEK based organic-inorganic hybrid membranes by blending SPEEK with few of the functional particles (FP), such as heteropolyacid (HPA) and carbon nano structures (CNS). The new composite membranes are designated as SPEEK/FP. Degree of FP inclusions in SPEEK was ascertained by Fourier transform infrared spectroscopy and X-ray diffraction analysis. The SPEEK/FP membranes were characterized for morphology, thermal and proton-exchange properties.

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Insitu synthesis of carbon supported palladium - Copper heterogeneous catalysts and their application for the efficient reduction of 4 - nitrophenol

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In the catalytic area, palladium nanoparticles (PdNPs) are of particular importance due to their superior catalytic performance for diverse reactions, Pd based bimetallic catalysts are often used in order to improve the activity, selectivity and stability of simple Pd catalysts. In the present work, carbon supported Pd - Cu catalysts were prepared by simultaneous co-impregnation of Pd and Cu metal salts onto carbon support by a one - step hydrothermal synthesis. The composition and microstructure of C/Pd-Cu catalysts were determined by high resolution scanning electron microscopy and X-ray diffraction analysis. The efficiency of resultant heterogeneous catalysts, C/Pd - Cu, was evaluated towards the reduction of 4 - nitrophenol (4NP), as a model reaction. The reaction kinetics of 4 - nitrophenol to 4 - aminophenol has been studied by UV -Visible spectroscopy. The key findings in this work make the nanotechnology based heterogeneous catalysis platform for the reduction of 4 - NP, a potential industrial intermediate and environmental pollutant.

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Nitric oxide releasing nanofibers based on sol-gel process

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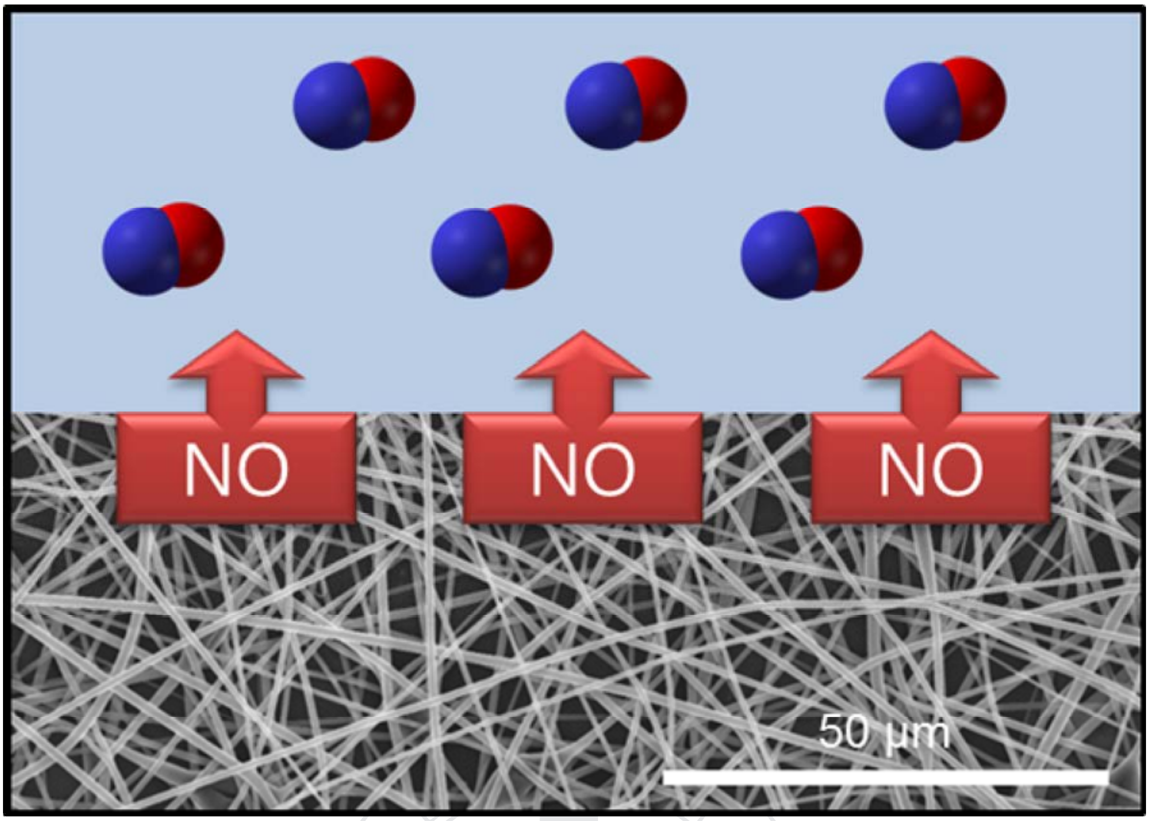
Nitric oxide (NO) and its application have been receving trememdous attention. This is because NO is involved in several physiological processes, such as vasodilation, angiogenesis, immune response, and wound healing. As such, NO has become a widely studied molecule for polymeric materials in biomedical applications. Among them, the use of electrospun materials as NO carriers for preventing from infections and enhancing wound healing has received a surge of interest because of their high surface areas, facile functionalization and tunable mechanical properties in recent years. However, the absence of chemical attachment between NO donors and fabricated fibers restrict their broad therapeutic applications as the physically attached NO donors can be easily leached, eventually serious concerning toward the biomedical application of these materials. It is thus desirable to develop potential nanofibers by electrospinning technique with well-de?ned structural features that can covalently anchor, store and release NO efficiently. In this report, we demonstrate the synthesis of NO releasing nanofibers through sol-gel chemistry for covalent bonding between silyl-modified polymethylmethacrylate (PMMA) and various N-diazeniumdiolate-modified aminoalkoxysilanes by electrospinning technique. Various synthetic parameters were tuned to obtain different diameter of nanofibres, thus controlling the total NO release amount and half-life times successfully. Thus, as-synthesized nanofiber scaffolds show promising results to provide a rational means to store sufficient amount of NO and its controlled release to specific targets and could be potential tool for drug delivery and other similar biological applications.


NO
NO
NO
50 μm

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Targeted Proteomics; Glycan-Targeting Serial Affinity Chromatography

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Glycan-targeting affinity chromatography systems are becoming increasingly important as tools in the purification, enrichment, and identification of glycoproteins. The great advantage of this strategy is that immobilized lectin and antibody selectors allow specific glycan structures to be matched with a particular protein. A problem with single column affinity chromatography is how to obtain information on glycan diversity within the oligosaccharide portions of captured glycoproteins. Although all the glycoprotein species bearing a particular glycan feature will be captured by an affinity column, there is no way of knowing whether the ligand being targeted appears alone or co-resides with a series of other glycan features in the same oligosaccharide conjugate. The utility of serial affinity columns was examined in determining whether individual glycan structures appear alone or together with other glycans in specific proteins. Serial affinity chromatography (SAC) can be a valuable tool in recognizing diversity in protein glycosylation, especially when the order of columns in the SAC series is varied. Two clear types of diversity were recognized. One is the independent occurrence of different affinity targetable glycan features in the same glycoprotein. The second is the case in which multiple targetable glycan features were co-resident in the same glycoprotein. The great advantage of this method is that it couples easily with current methods used in glycoproeomics.

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Quantitative Analysis of Environmental samples Using Laser-Induced Breakdown Spectroscopy (LIBS)

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LIBS is a type of atomic emission spectroscopy that uses a laser beam at high irradiance beyond 10^9 W/cm^2 as an excitation source. In this study, the quantitative laser-induced breakdown spectroscopy (LIBS) analysis was carried out with Standard Reference Materials (SRM). We used 4 SRMs that belong to categoriy of plants. The chemometric method was used for compensation of errors due to matrix effect. The obtained concentration exhibit significant improvement through the chemometric procedure.

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Understanding the N-end Rule Pathway through Development of Heterovalent Inhibitor.

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The N-end rule, which is evolutionarily conserved from yeast to mammals, states that the N-terminal amino acid of a protein determines its in vivo half-life. The degradation signal of the N-end rule pathway (N-degrons) have not been thoroughly examined yet. Here we evaluate the role of N-terminal amino acids as degradation determinants through in vitro translation systems and in silico computational docking analysis. To take advantage of the distinct binding modes of type 1 and type 2 destabilizing residues. we synthesized heterovalent inhibitors(RF-Cn) of the N-end rule pathway. And we optimized that RF-Cn can be internalized and block protein degradation in the primary cardiomyocytes. These results indicate that the inhibitors may be applied to various human diseases, including cardiac diseases, that originate from abnormal N-end rule regulation.

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Role of Proteasome-associated Deubiquitinating Enzymes on N-end Rule Model Substrate Degradation

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The proteasome is a key component of the ubiquitin-proteasome system responsible for the final step of the ubiquitin-mediated irreversible proteolysis. Our knowledge on UPS and its scope in basic biology and clinical sciences are still exponentially expanding. A number of proteasome-associated proteins have been identified, and some of these appear to influence the activity of proteasomes. Among them, there are three deubiquitinating (DUB) enzymes, Rpn11, Usp14, and Uch37, and, here, we examined whether and how these DUB enzymes affect the proteasome activity using N-end rule model substrates. We found that the proteasomal degradation of type 1 N-end rule substrates was significantly inhibited by the dominant negatives of Usp14 and Uch37, while type 2 substrate degradation was delayed by either Usp14 and Uch37 transient overexpression. Knocking-down or nullification of Usp14 significantly upregulated proteasomal activities. Consistently, treatment of Usp14 inhibitor IU1 resulted in mildy decreased ubiquitin chain levels on the proteasome. These data further substantiate the notion of chain trimming effects of Usp14. Although the underlying mechanism is to be determined, the role of Uch37 on proteasomal degradation appeared to be similar to that of Usp14, suggesting that Uch37 might be regulated by another component of mammalian proteasomes.

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In Vitro Biochemical and In Silico Computational Study of Monovalent N-end Rule Inhibitors.

방대인 **JiangYanxialei** 이민재*

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The first two authors are equally contributed to the work as co-first authors.The N-end rule is a recognition mechanism of the ubiquitin-proteasome system (UPS). The rule states that the N-terminal amino acid of a protein determines its half-life. In the N-end rule pathway, N-degrons are recognized and ubiquitinated by the UBR proteins. Simple dipeptides have been used as competitive inhibitors, but only effective near millimolar ranges. We synthesized and examined various N-end rule inhibitors, and we performed in vitro biochemical assay and in silico computational analysis to identify essential structural components of N-degron and to overcome the limitations of existing inhibitors. The L-conformation and protonated alpha-amino group of the first residue were significant for the inhibitors to properly interact with the UBR proteins. The first amide group was important but the carbonyl oxygen was not essential for the type 2 ligand-N-domain interaction. The novel monomeric molecules with minimum interacting motifs showed better inhibitory activities than traditional dipeptide inhibitors. They were also resistant to endopeptidase-mediated degradation. Collectively, our study identifies a pharmacophore of N-end rule inhibitors, which provides a structural platform to improve the efficiency and druggable properties of inhibitors. Considering that the N-end rule have been implicated in many pathophysiological processes in cells, Inhibitors of this pathway may be function as lead compounds for the future drug discovery in various pathological processes derived from abnormal N-end rule pathways.

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Stabilized plasmid-lipid nanoparticle inducing biodegradable polymer

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We performed a study about stabilized plasmid-lipid nanoparticle. It was used to detergent dialysis method which is compose of particle using several 'fusogenic' lipid and detergent in aqueous solution. For formed stable micelle, we use DOPE, which is known to help particle formation and positive charge lipid was DOTAP which induce encapsulation of plasmid-DNA. We characterized block copolymers that consist of poly(ethylene glycol)-b-poly(lysine)-ss-poly(caprolactone). PEG of Hydrophilic block play an important role for protecting any degradation. Poly(lysine) was improved for cell permeability, and poly(caprolactone) was hydrophobic polymer as biodegradable, respectively. Moreover, disulfide bond was reducing by glutathione of intracellular so it was a key that stimuli-sensitive polymer. We removed empty particle or non-encapsulated plasmid DNA by Anion-exchange chromatography, so we observed transfection assay in HEK293 cell.

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Rasatiol, a new phenylpropanoid glycoside from the seed of *Raphanus sativus*.

최병욱* 임진아[1] 이혜숙[1] 이봉호[2]

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The *Raphanus sativus* is an edible root vegetable so-called radish of Brassicaeceae family. It is grown and comsumed worldwide. The seeds of *Raphanus sativus* have been used traditional folk medicine in Asia for chlorhydria, diarrhea, cough, asthma, and constipation. Raphanus sativus has been also known for its various biological activities such as antimicrobial, antiviral, anti-inflammatory, antitumor, hypotensive and platelet aggregation activities. During the search for biologically active metabolites from Korean medicinal plants, we recently isolated a new pnenylpropanoid glycoside, named rasatiol, from the seeds of *R. sativus*. Here we report the isolation, structure determination and its biological activities of rasatiol.

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Stabilized plasmid-lipid particles (SPLP): 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-separose 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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Novel strategy for the high-throughput construction of large DNA molecules

서한나 방두희*

연세대학교 화학과

We developed a highly scalable 'shotgun' DNA synthesis technology by utilizing microchip oligonucleotides, shotgun assembly and next-generation sequencing technology. A pool of microchip oligonucleotides targeting a penicillin biosynthetic gene cluster were assembled into numerous random fragments, and tagged with 20 bp degenerate barcode primer pairs. An optimal set of error-free fragments were identified by high-throughput DNA sequencing, selectively amplified using the barcode sequences, and successfully assembled into the target gene cluster.

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Structural Basis for Genetic Code Expansion by Mutant Saccharomyces cerevisiae Tyrosyl-tRNA synthetase for Incorporation of O-Methyl-L-tyrosine

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한국외국어대학교 화학과

One of the aminoacyl-tRNA synthetases which play a role to assemble amino acids into proteins, Saccharomyces cerevisiae TyrRS (SceTyrRS) was mutated to recognize an unnatural amino acid, O-methyl-L-tyrosine, which is structurally similar to L-tyrosine. The structural change of these mutants was rationalized by the extensive computer-aided simulations. At first, validation of simulation system was carried out using comparison to X-ray crystal structure of SceTyrRS-tRNA^{Tyr} complex. Then, docking of O-methyl-L-tyrosine as a ligand to the mutants of SceTyrRS as a receptor was used to evaluate for generation of virtual protein-ligand complex.

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Specific isoforms of protein kinase G downregulate the transcription of cyclin D1 in NIH3T3

오이진 소재원*

인하대학교 화학과

To elucidate the role of PKG isoforms in transcriptional control of cyclin D1, we employed a series of expression vectors of PKG 1α and PKG 1β which encode HA-tagged wild type and constitutively active (SD and ΔN) mutants. Our present study demonstrates that both the constitutively active mutants of PKG1β downregulate the transcription of cyclin D1 when transiently transfected in NIH3T3 cells, whereas PKG 1α mutants show weak inhibition. We further studied the transcriptional regulators of cyclin D1, such as, c-fos, NF-κB, and CRE by using the luciferase reporter assay. Constitutively active mutants of PKG 1β showed marked transcriptional downregulation of c-fos in NIH3T3 cells, whereas PKG 1α downregulated c-fos to a lesser extent. We also found that the constitutively active mutants of PKG negatively regulated the activation of NF-κB and CRE, suggesting their involvement in the regulation of cyclin D1.

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Single vesicle fusion events mediated by SNAREs using a synthetic host-guest binding pair

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포항공과대학교 화학과 [1]포항공과대학교 물리학과 [2]포항공과대학교 I-BIO/시스템생명공학부 [3]포항공과대학교 시스템생명공학부/물리학

Understanding the molecular mechanism of synaptic vesicle fusion triggered by a conserved family of proteins called SNAREs (N-ethylmaleimide-sensitive factor attachment protein receptors) is a key issue in neuronal communication. In order to study the protein-mediated vesicle fusion mechanism, we designed a synthetic system to observe the synaptic vesicle fusion events at the single-molecular level with the course of time. Here, we report a reliable and efficient single-vesicle content mixing assay for a SNARE-mediated membrane fusion using a fluorophore tagged host-guest pair cucurbit[7]uril-adamentane derivative, on the basis of fluorescence resonance energy transfer (FRET) analysis. Results from this study and their implication in synaptic vesicle fusion will be presented.

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Synthesis and characteristic study with polydiacetylene liposome (conjugated low molecular weight polyethyleneimine) for gene delivery

이영화 최준식*

충남대학교 생화학과

Recently, many people are interested in therapy or diagonosis of diseases. Polydiacetylene liposomes have been used for gene, drug delivery and biosensor research. So we studied for gene delivery with 10,12-pentacosadiynoic acid(PCDA) derivatized polydiacetylene. We made a liposome that was conjugated with low molecular weight polyethyleneimine(PEI) on the 10,12-pentacosadiynoic acid liposome. We used to polymerization PCDA for in this study. PCDA-PEI liposome was confirmed by nuclear magnetic resonance (NMR) spectroscopy and Fourier Transform Infrared Spectrometer (FT-IR). Agarose gel electrophoresis and pico-green reagent assay were ensured to complex formation of the synthesized polymer and plasmid DNA and the size of liposome was measured by dynamic light scattering (DLS). Cytotoxicity of liposome was confirmed by WST-1 assay. We were able to identify transfection efficiency of the PCDA-PEI liposome as protein assay and luciferase assay in HeLa and HEK293 cells. And confocal microscopy images are used to identify for localization of PCDA-PEI liposome in HeLa cells.

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Predicting mutation effect using virtual alanine scanning on aggregation in the bovine CAPN1/CAST4 complex

채한화

농촌진흥청 국립축산과학원/동물유전체과

The activated mammalian CAPN' structures, especially CAPN/CAST complex have also become an invaluable target model using the structure-based virtual screening of drug candidates from discovery phase to development for over-activated CAPN linked to several diseases such as post-ischemic injury and cataract formation. It was proposed that the effect of Ca+2-binding to the enzyme include activation as well as the small regular subunit's dissociation, aggregation, and autolysis. Unfortunately, the enzyme is tends to aggregate when treated divalent ion at the Ca+2ion's high-concentration required for the Ca+2-activated enzyme, which could disturb the regulation of its inhibitor CAST that is recognized only the activated enzyme's structure and leads to a decrease in its proteolysis activity. Extensive researches of protein folding and protein-protein binding were shown that hydrophobic interactions play a key role in protein or antibody aggregation. Indeed, the CAPN large catalytic subunit's aggregation would be expected to promote aqueous solvent-exposed hydrophobic dimerization surface even in the absence of Ca+2, energetically unfavorable and then that's effects are leading to formation of randomly associated aggregates as a result of Ca+2-induced conformational rearrangement and partial dissociation. However the CAPN2/CAST complex's structure from both rats seems to be protected from the CAPN2's aggregation resulting in encompassing exposed hydrophobic regions on the enzyme by the inhibitor. Therefore, we are predicting selective mutation effects and relative importance of hydrophobic interactions on the exposed hydrophobic residue's surfaces across the bovine CAPN1/CAST4 complex of our model structure by calculating the spatial aggregation propensity (SAP).

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Multilayered Adsorption of Human Serum Albumin on Silica Nanoparticles.

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Nanoparticles (NPs) has been a subject of extensive investigation due to its potential applications, particularly in the field of cancer diagnosis and treatment in combination with bioclinical imaging techniques.When NPs are injected in vein, the particles are known to be rapidly coated with serum proteins, forming so called “protein corona”. As the initial interaction of NPs with cells and tissues is primarily related to the surface characteristics of NPs, the protein corona may play an important role in determining the behavior of NPs in living organism. However, the interaction of serum proteins with NPs has rarely been investigated at molecular level.We studied adsorption of human serum albumin (HSA), the most abundant protein in serum, on size-controlled silica nanoparticles using gel electrophoresis (SDS-PAGE) and LC-MS/MS techniques, where the adsorption of HSA were characterized and quantified. This study revealed that HSA adsorbed on silica NPs in multilayers. However, the amount of adsorbed HSA did not show a significant dependence on the size of silica NPs.

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PAMAM-based Gene Deilvery using Nuclear Localization Signal originated from Adenovirus E1a

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Polyamidoamine(PAMAM) is one of the cationic polymer for gene delivery system research and dendrimer consisted of peptide bond between ethylenediamine and methyl acrylate. PAMAM is known to have high biocompatibility and biodegradability. However, It has relatively poor transfection capacity than Polyethyleneimine(PEI). In order to improve such problem, we introduced Nuclear Localization Signal(NLS) Peptide to PAMAM. the NLS peptide is factor assisting entry of external gene into the Nuclear Pore Complex(NPC) via active transport. We selected KRPRP pentapeptide originated from adenovirus e1a protein. In order to verify difference of induced functional status from inversion of N-terminus, we synthesized two type PAMAM-KRPRP and PRPRK(arginine is N-terminus) and performed experiment in several cell line. PAMAM-PRPRK showed similar transfection efficiency with PEI on HEK 293 cell line and indicated comparatively low cytotoxicity than PEI. These experiment results suggest that introduction of NLS peptide provides potential about development of gene carrier having superior gene transfer capacity.

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Enhenced transfection efficiency by cationic amino acid - conjugated PAMAM dendrimer

박정현 최준식

충남대학교 생화학과

Gene therapy is expected to treat genetic disease and cancer. Gene transfer using non-viral gene delivery carrier is being performed instead of viral gene delivery carrier that tend potent cytotoxicity. We introduced Polyamidoamine (PAMAM) dendrimer that is widely used as a non-viral and polycationic vector for gene delivery. We synthesized PAMAM dendrimer (generation 4, G4)-Histidine(H)-Lysine(K) / Ornithine(O) and compared this study with previous results (PAMAM G4-Histidine-Arginine). Amino acid - conjugated PAMAM dendrimer induce not only enhancement of transfection efficiency but also a decrease in toxicity. Cationic amino acid that contribute to condensation of DNA and contact with cell surface. Histidine induce buffer(proton sponge) effect. We experimented the Gel retardation assay and Pico-green Assay for verification of PAMAM-DNA complex. Furthermore Toxicity was confirmed by WST assay. Luciferase assay and Protein quantification were performed for confirmation of Transfection efficiency. Lastly, we used the Confocal microscopy to check movement of polymer in the cell.

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Probing Target Search Pathways of the Protein Complex by NMR Paramagnetic Relaxation Enhancement

유태경 서정용[1,*]

서울대학교 농생명과학대학 바이오모듈레이션 [1]서울대학교 농생명공학부 바이오모듈레이션 전공

In general, specific protein?protein recognition proceeds via a two-step target search process. The first process is a weak association via diffusion-controlled intermolecular collisions, followed by the formation of an ensemble of short-lived, encounter complexes. Secondly, two-dimensional search by translational and rotational rearrangement between the partner proteins results in the specific complex formation. Here we investigated the target search pathways between the N-terminal Domain of Enzyme I (EIN) and the heat-stable histidine phosphocarrier (HPr) protein from bacterial phosphotransferase system using NMR paramagnetic relaxation enhancement (PRE). We examined how mutations away from the binding interface alter the equilibrium binding and also reshape the distribution and/or population of the encounter complex ensemble. We show that encounter complexes are heterogeneous in their contributions toward the specific complex formation, which can be visually monitored and estimated in a quantitative manner.

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Design of sweet-taste peptides based on the relationship between structure and function of sweet-tasting proteins

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중앙대학교 화학과

The importance of sweet-tasting protein continues to rise. To design such optimal sweeteners, knowledge about structural functions and chemicals for sweetness response is required. There are seven sweet proteins: thaumatin, monellin, mabinlin, brazzein, neoculin, miraculin, and egg white lysozyme. Among these proteins, in this study, we are mainly focused on brazzein and thaumatin. The 3D structures of brazzein and thaumatin have been determined by NMR and X-ray, respectively. Brazzein possesses three loops (residues 9-19; 30-33; 38-45). The flexibility of loops is important to make them active conformation when a portion of the large molecule binds to the receptor. Also, in thaumatin, important residues are located in a flexible loop region. Mutagenesis studies have suggested that key sites for interaction between sweet proteins and sweet receptor are nearby the loops. These studies have also suggested that His31 and Glu41 residues of brazzein and Lys67, Arg76, Arg79, and Arg82 residues of thaumatin are involved in eliciting a sweet-taste response. From these results, we designed and synthesized several peptides, and tested sweet tastes towards them.

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Facile Method for Protein Immobilization on the Solid Support

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서울대학교 화학생물공학부

Protein/peptide immobilization is one of the important steps in biochip fabrication. For biochip fabrication, proteins are usually immobilized on each spot with glutaraldehyde, and the desired proteins are identified with their specific location after bioassay. However, when the proteins are to be released from the supports for additional experiments, they cannot be released in this method. Thus, we have developed a facile method for protein immobilization by photo-reactive molecule, which can be activated under UV exposure. With this method, the immobilized target protein/peptide can be easily released from the solid supports under mild condition.

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Study of high affinity ssDNA Aptamer binding to AIV NS1 protein

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Influenza is an infectious disease caused by RNA viruses of the family Orthomyxoviridae, the influenza viruses. Influenza A virus contains 8 segments of (-) ssRNA that encode 11 known proteins. NS1 protein was known for disrupting the induction of IFNs by first inhibiting the intracellular sensor RIG-I. Using a SELEX (systematic evolution of ligand by exponential enrichment) procedure, we selected a high-affinity DNA aptamer capable of binding to NS1 protein with a dissociation constant of 18.91 nM. We investigated the interaction between NS1 protein and aptamer by reverse ELISA. We revealed an intramolecular parallel G-quadruplex structure by Circular dichroism spectrum. The aptamer was incubated with 293T cells expressing NS1 and binding assessed by FACS and Confocal. We measured activation of the INF-β promoter in 293T cells as a reporter gene for IFN induction. The aptamer that was isolated in this study are expected to be new molecular drug candidate.

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ssDNA Aptamers Evolved from Counter-SELEX as Effective Molecular probes for discrimination between Influenza Virus Hemaggutinin Subtype H1 and H5

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Hemagglutinin is appropriate for target to detect the influenza virus because it exists on virus surface and takes part in the first step of viral infection. In this study, we constructed hemagglutinin expression vectors (pGEX-4T-1/HA1(H1N1), pGEX-4T-1/HA1(H5N1)) and purified the GST-tagged HA1 proteins. We performed Counter-SELEX (systematic evolution of ligand by exponential enrichment) procedure to find out the aptamers that have specific affinity for the purified GST-HA1(H1N1). The 14th round ssDNA pool of GST-HA1(H1N1) was cloned 22 aptamer candidates and isolated four ssDNA aptamers, they have high affinity to GST-HA1(H1N1) and low affinity to GST-HA1(H5N1), using a sandwich ELISA and a reverse ELISA. We performed circular dichroism and gel electrophoresis to confirm the G-quadruplex structures of these aptamers and the result shows two distinct classes of secondary structure, G-quadruplex and non-G-quadruplex. The group of aptamer that have G-quadruplex structure were confirmed high affinity with target protein. These selected aptamers would have wide applications in diagnosis, therapy and prevention of influenza virus.

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Glycoprotein functionalization with a Dual Reactive Hydrazide/Click Chemistry

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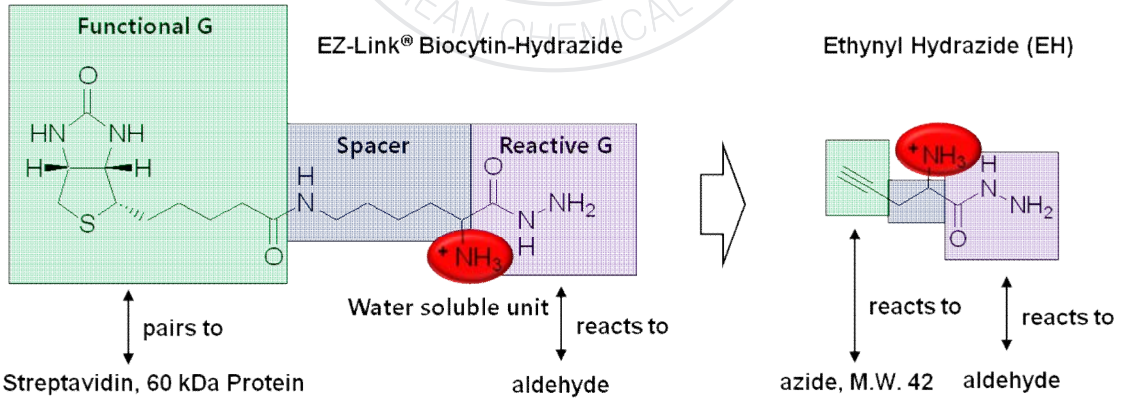
경희대학교 동서의학대학원

A water-soluble, dual reactive hydrazide/click crosslinker (EH) was synthesized and characterized. A model glycoprotein, human IgG was ethynylated by conventional oxidation/hydrazide reactions with the hydrazide moiety of EH. The terminal alkyne conjugated to the glycan of human IgG was easily functionalized by quantitative and bioorthogonal copper(I)-catalyzed azide-alkyne cycloaddition. The potential of the hydrazide/click crosslinker as a reagent to functionalize antibodies was demonstrated with fluorophore labeling and antibody immobilization.



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Syntehsis of PAMAM Dendrimer Derivatives using NLS Peptide

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Polyamidoamine(PAMAM) dendrimer is one of the using cationic polymer in the gene delivery system research and it has advantage such as much less entanglement phenomenon, superior biodegradability and satisfactory transfection efficiency. However, the transgene expression capacity of PAMAM is limited to specific cell line and also shows poor transfection efficiency in comparison with Polyethyleneimine(PEI) or viral vector. In order to solve such expression efficiency problem, we introduced Nuclear Localization Signal(NLS) on the PAMAM surface. The NLS peptide performs guide role facilitating translocation of material above 9nm into the Nuclear Pore Complex(NPC) through active transport. We selected KKKRK peptide originated from simian virus 40 VP3, which is capsid protein enveloping viral gene. Because KKKRK sequence has rich primary amine group, it is expected that PAMAM derivative using KKKRK peptide will have excellent condensation capacity about plasmid DNA and endosome escaping capacity. Therefore, we performed this research.

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Development of Novel Dignostic probe targeting CD44, a breast cancer stem cell biomarker.

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CD44 is a transmembrane glycoprotein specifically associated with plasma membrane protrusions. It was reported that human breast cancer is frequently associated with cells expressing the CD44. Thus, the CD44 has been an attractive biomarker in prevention and vaccinization of breast cancer. In previous study, we have found the peptide binds to the CD44 recombinant protein with phage display and confirm the binding efficiency using FITC labeled peptide to their target.In current study, we found the affinities of single peptides were significantly improved by the synthesized, novel Polyvalent Directed Peptide Polymer (PDPP). Among 7 peptides, 2 peptides show that higher binding affinity and specificity than others. The fabricated PDPP was used to develop a novel ultra-sensitive diagnostic system which could detect lower concentrations than existing probes.The Immunocytochemistry test confirms that, the PDPP exhibits higher specificity towards CD44 at MCF 7 Cell line.

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Chemical compounds that inhibit the activities of Hepatitis C virus NS3 helicase

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Hepatitis C is an infectious disease that affects the liver. The primary route of infection is blood-to-blood contact. The being of HCV was proven in 1989. It caused by Hepatitis C virus (HCV) that is a Hepacivirus within the Flaviviridae family containing a positive sense single strand RNA. The Hepatitis C NS3 helicase has an essential role in viral replication. The purpose of this study is inhibiting the activity of Hepatitis C NS3 helicase to prevent the replication of HCV. We expressed the helicase in E.coli BL21 (DE3) cells and purified it. We confirmed the activity of the helicase as performing ATP hydrolysis and unwinding experiments. To find inhibitors of its activity as drug candidates, we perform screening. We perform two kinds of screening method. The first one is the dsDNA unwinding activity inhibition assay, and the second one is the ATPase activity inhibition assay. As we do these procedures, we find several kinds of compounds inhibiting activity of HCV NS3 helicase. Further we measure IC50 value to find the concentration of inhibitors which is required to inhibit the activity of HCV NS3 helicase by half.

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Cytochrome P450 2A6 Inhibitor Based on the Indole Moiety

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The cytochrome P450 enzymes (CYP 2A6) regulate many endogenous signaling molecules and drugs. Aryl alkynes such as 2-ethynylnaphthalene are important P450 inhibitors which have been extensively studied as medicines or as an effective chemical probes for profiling mouse liver microsomal P450s. Here we have synthesized indole-based novel P450 inhibitor, 5-ethynyl indole 3, and showed that it has successfully inhibited CYP 2A6 by chemical inhibition reaction. By using HPLC equipped with a photo diode array(PDA) detector, all of the peaks derived from the enzymatic reaction have been characterized.

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Tertiary Structure and Thermal Stability of Acyl Carrier Protein from *Enterococcus faecalis*

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Fatty acid synthesis in bacteria is catalyzed by a set of individual enzymes collectively known as type II fatty acid synthase (FASII). Each enzyme interacts with acyl carrier protein (ACP), which shuttles the pathway intermediates between the proteins. *Enterococcus faecalis* is a commensal bacteria now acknowledged to be organisms capable of causing life-threatening infections in humans, especially in the nosocomial (hospital acquired) environment. Structure of acyl carrier protein from *E. faecalis* (*Ef*-ACP) has never been studied yet. To study the structural feature and thermal stability of *Ef*-ACP, we optimized cloning system and the expression condition of *Ef*-ACP. Using circular dichroism (CD) spectroscopy, *Ef*-ACP was characterized to have an alpha helical structure. Thermal stability was studied by measuring melting temperature and *Ef*-ACP showed melting temperature at 70°C, which is much higher than that of ACP from *Escherichia coli* (54°C). We performed multidimensional heteronuclear NMR experiments and completed the backbone resonance assignment. The mutagenesis study revealed that His16 and Phe44 contributed to structural stability of *Ef*-ACP conformations. Preliminary tertiary structure of *Ef*-ACP has been determined, having four α-helices connected by three loops. Tertiary structure will be refined further and dynamics of *Ef*-ACP will be investigated by NMR spectroscopy.

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Relationship of Structures and Functions of Hybrid Antimicrobial peptide, PapMA and its peptoid-substituted analogues

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Papiliocin is consisted of 37-amino acids antimicrobial peptide which is purified from the swallowtail butterfly, *Papilio xuthus*. Magainin 2 is consisted of 23-amino acids antimicrobial peptide which is isolated from *African clawed frog*. PapMA is a 20-residue hybrid peptide incorporating residues 1-8 of papiliocin and residues 1-12 of magainin 2. PapMA have potent antimicrobial activity without toxicity against mammalian cells. PapMA-P2, in which the Gly-Ile-Gly sequence of Pap-MA is substituted with Pro, was designed. According to the results of cytoxicity against bacteria and mammalian cells, and phospholipid membrane permeability, PapMA-P2 with high antimicrobial acitivities targets the bacterial cell membrane. To discover peptide antibiotics having lower toxicity and higher selectivity, we substituted ala, lys and leu peptoid for Pro. Peptoid analogues also showed that high antimicrobial activities and low toxicities against mammalian cells. CD spectra and NMR spectroscopy suggested that PapMA-P2 and its analogues have α-helical conformations in membrane-mimicking environment. DOSY experiments suggested that PapMA-P2 interacts with DPC micelles and diffuses slowly in the bound form. Structure-activity relationships of these peptides will give insights to understand its mechanism of actions and help to develop more potent peptide antibiotics as useful therapeutic agents.

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Intrinsic Dynamics of Heparin-Binding Domain of $\mathbf{VEGF_{165}}$ Provide an Underlying Basis for Its Biological Function

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Vascular endothelial growth factor (VEGF) interacts with Ab by binding to heparin-binding domain (HBD) at C-terminus of VEGF and is accumulated in the senile plaques of Alzheimer’s disease patients’ brains. Triamterene (Trm), which is a well-known potassium-sparing diuretic, is an inhibitor of interaction between VEGF and Aβ with a moderate activity (IC_{50} of 50 μM). Heparin acts as an antiangiogenic, antimetastatic, and anti-inflammatory agent and heparin-binding is important for the stability and mitogenic activity of VEGF. Binding models based on measurements of chemical shift changes and docking study showed that the disordered loop region at N-terminus of HBD constitute Trm binding site while heparin-binding site was composed of two basic clusters (R13/R14/K15 and K30/R35/R49). Spin relaxation data, CPMG data and model-free analysis showed that the residues in the Trm binding site as well as residues near heparin binding site exhibited conformational exchanges in free HBD and these flexibility decreased dramatically upon binding to Trm and heparin, respectively. It can be suggested that Aβ as well as heparin and inhibitor may recognize these unique dynamic features of the HBD. The flexibility of HBD should be essential for VEGF function and interaction with other protein partners.

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Functional importance of N-terminal and C-terminal helix of papiliocin with antimicrobial and anti-inflammatory activities isolated from *Papilio xuthus*

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The 37-residue, cecropin-like peptide papiliocin, isolated from the swallowtail butterfly, *Papilio xuthus.* Papiliocin is a potent antibiotic possessing very low cytotoxicity against mammalian cells and high bacteria cell selectivity, particularly against Gram-negative bacteria. The three-dimensional structure of papiliocin shows that papiliocin in 300 mM dodecylphosphocholin (DPC) micelle has α-helical structure from Lys^{3} to Lys^{21} and from Ala^{25} to Val^{36} and hinge structure in between. To investigate functional importance of N-terminal helix and C-terminal helix as well as the aromatic residues, five papiliocin analogs were designed. Two 22mer analogs composed of N-terminal helix, PapN including N-terminal helix from Arg^{1} to Ala^{22} of papiliocin and PapN-FW with exchange of Trp^{2} and Phe^{5} in PapN, showed outstanding anti-inflammatory activity as well as antimicrobial activity against Gram-negative bacteria without toxicity against mammalian cells. Through tryptophan blue-shift and STD-NMR experiments, it was proved that Trp and Phe at the N-terminal helix of papiliocin and its analogs play key roles in targeting the bacterial cytoplasmic membrane and interaction with LPS. Furthermore, hydrophobic interactions between the C-terminal helix of papiliocin and the hydrophobic portion of LPS or other Gram-negative bacteria cell components provide papiliocin with selectivity against Gram-negative bacterial membranes.

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Structures and Dynamics of apo- and holo-Phosphatases of Regenerating Liver-3 (PRL-3): Catalytic Sites and Regions to Undergo Conformational Change Exhibit Diverse Dynamical Features

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Phosphatases of regenerating liver (PRL) constitute a prenylated phosphatase with oncogenic activity. PRL-3 is overexpressed in liver metastasis of colorectal cancer cells, and it represents a new therapeutic target. With the aim of verifying the functional importance of the inherent structural flexibility of PRL-3, we investigated the structural and dynamic features of apo- and holo-PRL-3. Apo- and holo-PRL-3 have substantial differences in the general acid loop. Moreover, Cys104, Arg110, and Asp72, which participate in the enzymatic reaction, are close together in holo-PRL-3. Based on the spin relaxation, CPMG data and model-free analysis, we found that microsecond to millisecond time scale motions on the general acid loop and α5-α6 as well as P-loop are important in ligand recognition and the differences between loops flexibilities in apo- and holo-PRL-3 may control the protein-ligand interaction. Flexibility of PRL-3 shown in this study may be essential for its ability to dephosphorylate the enzyme partners.

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Structure and function of coprisin with antimicrobial and anti-inflammatory activities isolated from the dung beetle, *Copris tripartitus*

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The 43-residue defensin-like peptide, coprisin isolated from the Dung Beetle, *Copris tripartitus* exhibits antimicrobial activities against bacteria. We determined the three-dimensional structure of coprisin in aqueous solution by NMR spectroscopy, showing that coprisin has an amphipathic α-helical structure from Ala^{19} to Arg^{28} and β-sheet from Gly^{31} to Gln^{35} and Val^{38} to Arg^{42}. Coprisin has a highly electropositive regions positioned at the end of the helix (Arg^{28}), turns between the helix and the first strand of the sheet (Lys^{29}, Lys^{30}), and C-terminus (Arg^{42}). As coprisin was treated in LPS-stimulated macrophage cells, inflammatory cytokines was inhibited. We have demonstrated that coprisin shows profound antibacterial activities since coprisin has an amphipathic helix and electropositive surface which may play important role in its structure stability and effective interaction with bacterial lipid membrane. Since a short antimicrobial peptide would be an attractive candidate for a therapeutic agent, we designed several 9-mer analogs on the basis of its sequence from Leu^{22} to Lys^{30}. The peptide analogs exhibit antibacterial activities as well as anti-inflammatory effects. Therefore, positively charged surface plays a key role in anti-bacterial activities. Furthermore, coprisin is a potent anti-inflammatory peptide with antibacterial activities, and this work may help to understand its mechanism of action.

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Sentinel Lymph Node Imaging by a Fluorescently Labeled DNA Nanostructure.

김경란 안대로[1,*]

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Sentinel lymph nodes (SLNs) are the first lymph nodes which cancer cells reach after traveling through lymphatic vessels from the primary tumor. Evaluating the nodal status is crucial in accurate staging of human cancers and accordingly determines prognosis and the most appropriate treatment. The commonly used methods for SLN identification in clinics are based on employment of a colloid of radionuclide or injection of a small dye. Although these methods have certainly contributed to improve surgical practice, new imaging materials are still required to overcome drawbacks of the techniques such as inconvenience of handling radioactive materials and short retention time of small dyes in SLNs. Here, we perform SLN imaging by using a fluorescence-labeled DNA nanostructure.With a successful identification of SLNs by the DNA nanoconstruct, we suggest that DNA nanoconstruct hold great promises for clinical applications.

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Identification of novel regulatory peptides against Sox2 in cancer stem cells

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Earlier research proved that human cancer is frequently associated with overexpression of the cancer stem cell marker, Sox2 transcription factor. Therefore, the Sox2 has been a fascinating biomarker in prevention and vaccinization for various cancer tumors. In the present study, the Sox2 gene was amplified from the Human lung small cell carcinoma leaves by polymerase chain reaction (PCR) and cloned into a pET28a expression vector. The Sox2 gene was expressed in E. coli and purified to homogeneity. The purified recombinant Sox2 provides a basis to screen novel Sox2 binding peptides (SBP), which bind with higher affinity and specificity to Sox2. The specificity is also confirmed in U87 glioma cell with SBP by using immunocytochemistry (ICC) method. Future studies of the candidate peptides ability to detect Sox2 and regulate several protein expression such as Nanog were in progress and we believe these studies would significantly contribute in cancer tumor prevention and vaccinizations.

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Solution Structure and Backbone Dynamics of the Cold Shock Proteins (CSPs) and Its Complex with Single-Stranded Nucleic acids from Psychrophilic Bacterium, *Listeria monocytogenes*

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Cold shock proteins (Csps) are proteins expressed when growth temperature drops below physiological temperature. They bind to single-stranded nucleic acids and act as RNA chaperones to regulate translation. *Listeria monocytogenes* is a psychrophilic foodborne pathogen that is problematic for the food industry because it can grow at low temperatures. Here, we investigated the structural and dynamic features as well as the thermostability of *L. monocytogenes* CspA (*Lm*-CspA). *Lm*-CspA has a five-stranded β-barrel structure and flexible loop regions. Upon binding heptathymidine (dT_7), heteronuclear NOE values and order parameters of residues in surface loop regions dT_7 binding sites increased dramatically. Moreover, Carr-Purcell-Meiboom-Gill experiments showed that slow motions observed for the dT_7 binding residues K7, W8, F15, F27, and R56 disappeared in *Lm*-CspA-dT_7. *Lm*-CspA is less thermostable with a lower melting temperature (40˚C) compared with mesophilic and thermophilic Csps. The structural flexibility with longer surface loops and less hydrophobiccore packing as well as unfavorable electrostatic interactions may be key factors in determining the low thermostability of *Lm*-CspA. This implies that the large conformational flexibility of psychrophilic *Lm*-CspA, which more easily accommodates nucleic acids at lowtemperature, is required for RNA chaperone function under cold-shock conditions and for the cold adaptation of *L. monocytogenes*.

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Photo-activatable Fluorescent Labeling of Target Proteins in Live Cells

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Spectroscopic monitoring of proteins of interaction in live cells provides valuable information on function, interactions, and trafficking of proteins in their native context. Here, we describe a method to introduce spectroscopic probes to target proteins with a spatio-temporal control. We are utilizing split-intein mediated protein trans-splicing reaction for fluorescent labeling of target proteins. We also adopted a molecular switch to control the intein mediated reaction by using external stimuli.

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Extracellular Matrix Protein Adsorption on Immobilized Giant Unilamellar Vesicles

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The tissue-specific nature of native ECM through in vivo tissue development is leading to a great variety of compositional heterogeneities and the structural complexities at levels, which could have not been comparable to those reproduced by the in vitro models even in the current state-of-the art tissue engineering methods. Although many researches on regeneration of, cell-free, in vitro ECM were performed successfully, the mechanisms are far from the reality. ECM incorporated giant unilamellar vesicles (GUV) is a novel artificial cell model, having an ideal native. Especially, immobilized stable GUVs provide ideal in vivo model surface which has a similar dimension to in vivo cellular membranes enable us to fibronectin (FN) network formation. Streptavidin micro-patterns achieved by μCP technique provide selectively immobilized biotinylated GUV patterns. Time-dependence observation during FN incubation may detail the FN assembly process, firstly short FN molecular adhesion on cell membrane, and may convert later to larger insoluble fibril network. The connective FN network may change physical, and mechanical properties of lipid-based vesicles dramatically, and can be observed by a single-cell manipulator technique. Study would be extended to the FN-encapsulated freely-mobile GUVs, which have pharmaceutical potentials in tissue engineering.

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Generation of Light induced Membrane Potentials from Proteorhodopsin incorporated lipid vesicles

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Proteorhodopsin (PR) is a photoactive transmembrane protein, which is functioning as a light-driven proton pump in marine bacteria. In biological systems, light stimulates the PR to pump out cytoplasmic protons to extracellular space, lowering cytoplasmic potential. Therefore, one may utilize the PRs to functionalize liposomes as light driven proton capacitors if one can incorporate the PRs into liposomes with unidirectional manner, which remains as a technological obstacle yet. In order to control the direction of PR incorporation, we varied the lipid compositions, i.e. head group charges, chain lengths, and preparation processes. pH sensitive dyes and a computerized pH meter have been used to monitor the cytoplasmic potential of proteoliposomes in situ, and their light-driven pH variation will be presented. Furthermore, fundamental understanding on a light-induced proton trafficking mechanism and effective transmembrane reconstitution methods will be discussed.

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Near-Infrared 조사를 통해 Graphene quantumdots/Elastin-like polypeptides 복합 하이드로겔의 약물방출 조절이 가능한 GQDs 스위치

박종보

서울대학교 화학과

그래핀은 우수한 기계적 성질 및 열 안정성, 뛰어난 전기전도성 등의 장점으로 인해, 트랜지스터, 태양전지, 센서 등의 다양한 응용분야에서 활발히 연구되고 있으며, 최근에는 그래핀 옥사이드와 그래핀 양자점 (GQDs)를 이용한 암 치료 및 바이오 센싱, 약물 전달 등의 biological application 관련된 연구들도 많이 이루어지고 있다. 또한, 그래핀 기반 물질들의 NIR light irradiation 흡수에 의한 열 방출 특성을 이용한 cancer therapy, antibacterial treatment 등의 연구도 최근 들어 각광을 받고 있다. ELP 는 poly(N-isopropylacrylamide)와 더불어 대표적인 온도 감응성 물질로서 전이 온도 (transition temperature)를 기점으로 물질의 용해성이 변하며, 이로 인해 sol/gel transition 이 가능하다. 본 발표에서는, 이러한 ELP 의 온도를 조절할 수 있는 스위치로서 GQDs 를 이용하였으며, GQDs/ELP 복합 하이드로겔의 sol/gel transition 및 약물방출 거동을 NIR 을 통해 조절가능한지를 확인하였다.

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Synthesis and Evaluation of Small Molecule-Peptide Conjugates as Potential Whitening Agents

이혜숙 김한영*

애경산업(주) 중앙연구소

Hyperpigmentation which usually presents as age spots, uneven color, freckles and sometimes melasma has become an object of public concern. Hyperpigmentation was resulted from over-production of melanin by melanocytes within the skin, and this process was called melanogenesis.*p*-coumaric acid conjugated peptides were prepared by solid-phase synthesis as potential whitening agents. Their anti-melanogenic activities were performed by melanin inhibitory assay using B16F1 melanoma cell line. We found that *p*-coumaric acid conjugated peptides showed superior melanin inhibitory activities than arbutin. Also, through MTT assay and LDH release assay, we found that *p*-coumaric acid conjugated peptides showed very low cytotoxicity. We established HPLC analysis condition to identify *p*-coumaric acid conjugated peptides. Using this method, we found that *p*-coumaric acid conjugated peptides were stable in condition of high temperature (43℃) or direct sunlight.

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Generation and characterization of engineered split-inteins

전용권 정덕호 권영은*

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Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. While the PTS became a useful tool for various biological studies, the difficulties associated with the synthesis of 40mer peptide became a drawback in its applications. Here we have generated several engineered split-inteins by shifting the split-site of naturally split-inteins to new positions. We utilized Npu DnaE intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate how the lengths of N and C-intein affect the PTS kinetics, we prepared multiple pairs of split-inteins that consist of various lengths of N and C-inteins. The kinetics of reaction between each engineered pairs and the cross-reactivity were studied.

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The effect of extein pI values on the kinetics of split-intein mediated protein trans-splicing reaction

전용권 정덕호 권영은*

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Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. As the PTS became a useful tool for various biological studies, it is important to understand the factors that affect the kinetics of the PTS. For this study, we have chosen Npu DnaE intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate the effect of extein pI's on the PTS kinetics, we prepared multiple pairs of split-inteins that carry exteins of various pI's. We observed accelerated reaction rates as the pI's of exteins decrease. This result provides a good guideline in designing efficient PTS.

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One step detection of circulating tumor cells in ovarian cancer with enhanced fluorescent silica nanoparticles

송미령 정민숙 박수진 김준성 김진현

(주)바이테리얼즈 부설연구소

Ovarian cancer is the fifth leading cause of cancer-related deaths among women because of late diagnosis. For this reason, more sensitive and specific methods should be needed to detect ovarian cancer earlier to improve survival. Here, we developed a one-step circulating tumor cells(CTCs) detection technology in ovarian cancer based on multifunctional silica nanoparticles which can be detected CTCs in whole blood with high sensitivity with in 1hour by using flow cytometry. We prepared MNP-SiO2(RITC) which in corporated with organic dyes(rhodamine B isothiocyanate, RITC, λmax(ex/em)= 543/580 nm) in the silica shell. And then, we controlled amount of organic dye in the silica shell of MNP-SiO2(RITC) for the increased fluorescence intensity to overcome the autofluorescence of blood and increased sensitivity of CTCs detection in whole blood. Next, we modified surface function group of MNP-SiO2(RITC) from ?OH to PEG/COOH and conjugated MCU1 antibody on the surface of MNP-SiO2(RITC) for the CTC detection. To study the specific targeting effeciency of MUC1-MNP-SiO2(RITC), we demonstrated by using immunocytochemistry with MUC1 positive cell line (OVCAR-3) and negative cell line (HEK293T). Based on these results, , we developed one-step detection of CTCs with MUC1- MNP-SiO2(RITC) by using flow cytometry in whole blood CTCs model. Fortunately, we can detected small amount CTCs in whole blood.

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Multifunctional Collagen Hydrogels for the Sustained Release of Biomolecules in the Reconstruction of Human Gingiva

최종훈* 박호영[1]

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We present in vitro release profiles of fluorescently labeled dextran and ferritin nanoparticles from engineered collagen constructs while maintaining the collagen constructs designed as biocompatible inserts into a wounded area of human gingiva. Collagen scaffolds were fabricated under different conditions for optimizing the release profile. When collagen constructs containing ferritin nanoparticles decorated with quantum dots were incubated under a physiological condition (i.e., 37°C and 5% $CO2$) for 24 hours, the hydrogel released 20-70% of initially loaded biomolecules (depending on the size, structure or surface charges) to culture media in a controlled manner. The release profiles can be tuned by varying gelation conditions of the collagen constructs. The amounts of released nanoparticles were quantified by imaging fluorescent quantum dots. This implantable collagen constructs could serve as an efficient platform in releasing biomolecules and imaging agents in human gingiva to facilitate the regeneration of oral tissues.

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Binding Pattern of Capsid Proteins and DNAs in M13 Bacteriophage using Coarse Grained Simulation

정환원* 석차옥[1]

한국과학기술연구원(KIST) 다원물질연구소/계산과학연구단 [1]서울대학교 화학부

A Coarse grained (CG) model was used to investigate the binding pattern between single-stranded (ss) DNAs and major capsid proteins in M13 filamentous bacteriophage. An all-atom model of the capsid protein was mapped to the CG model with several beads using Martini force field. For DNA, we developed a new CG model with three beads per each nucleotide which could be used to predict the binding process of proteins and DNAs. We performed several molecular dynamics simulations and examined the structural changes and dynamics of the capsid proteins and DNAs. Two major interactions were essential for the binding process: the attraction between the capsid protein's basic domain and the phosphate backbone of the viral ss DNA, the entropic gain due to the aggregation of the capsid's hydrophobic domains.

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Purification and Characterization of Mammalian Proteasomes

최원훈 신승균 황민혜 **JiangYanxialei** 이민재*

경희대학교 응용화학과

The ubiquitin-proteasome system (UPS) is a major cellular mechanism that regulates most short-lived intracellular protein levels. Protein substrates labeled with polyubiquitin chains are mostly degraded by 26S proteasomes into small peptides of 3 to 24 amino acids. The proteasome is a ~2.5 MDa holoenzyme complex consisting of at least 33 distinct subunits with, structurally and functionally distinctive, two distinguishable the 28-subunit core particle (CP, also known as the 20S) and the 19-subunit regulatory particle (RP, also known as the 19S). Here we present a novel and more efficient method to purify mammalian proteasome from 293 cells using a tandem-affinity tag, which is stably incorporated into beta4/Pre1 subunit of the proteasome. The proteasome showed good proteolytic characteristics toward chymotrypsin-like and trypsin-like activities. Moreover, we observed that Usp14, a deubiquitinating enzyme (DUB) is significantly associated with the proteasomes. Through a biochemical assays using purified mammalian proteasomes and recombinant Usp14 proteins from yeast, we discovered that 1) the Usp14 DUB activity is required proteasomal activation through unidentified mechanism, 2) a proteasome inhibitor MG132 diminished the DUB activity, and, however, 3) a Usp14 inhibitor IU1 abolished the effect of MG132. These results indicate that our proteasome purification system is an invaluable tool to understand the regulatory mechanisms of the UPS-mediated protein degradation.

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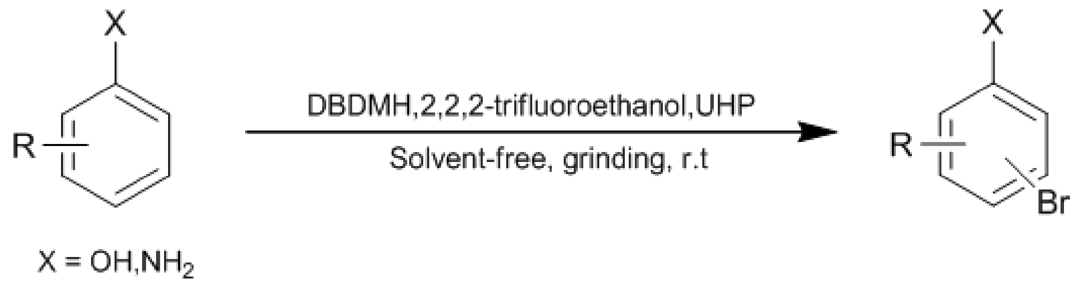
Regioselective and Efficient Bromination of Activated Aromatic Compounds with DBDMH (1,3-Dibromo-5,5-dimethylhydrantoin) under Solvent-free conditions

이란 이종찬*

중앙대학교 화학과

Selective bromination of various industrially and pharmaceutically important substituted aromatics using a DBDMH (1,3-Dibromo-5,5-dimethylhydrantoin) as an efficient reagents is disclosed. General bromination methods of aromatic compounds involve the use of hazardous molecular bromine which has nature. We describe the procedure for bromination of anilines and phenols with DBDMH and TFE (2,2,2-Trifluoroethanol) under solvent free condition by grinding the reactants in a mortar with pestle at room temperature. The reactions afforded corresponding bromo derivatives in excellent yield with high regioselectivity.

<Scheme>



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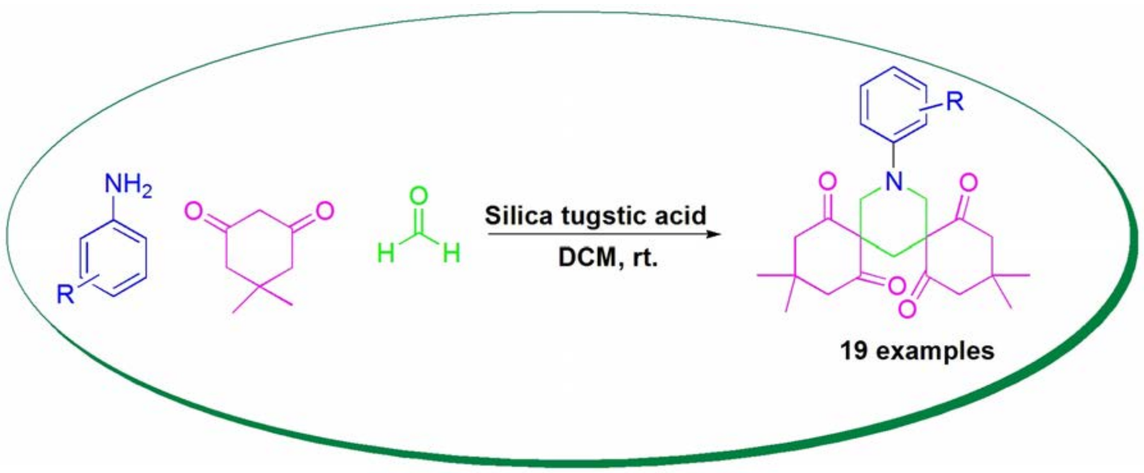
General and Efficient Silica supported tungstic acid (STA)-Catalyzed Three-Component protocol for the synthesis of bis-spiro piperidine derivatives under milder condition

<u>Atar Amol Balu</u> 현동균 정연태*

부경대학교 이미지시스템공학과

A mild, efficient and expeditious method has been developed for the synthesis of 3,5-dispirosubstituted piperidine via a three component, one-pot cyclocondensation reaction of aromatic amines, formaldehyde and dimedone using Silica supported tungstic acid as heterogeneous catalyst for the first time. The reaction involving formation of six new covalent bonds was conveniently promoted by Silica supported tungstic acid and the catalyst could be recovered easily after the reaction and reused without any loss of its catalytic activity. The advantageous features of this methodology are high atom-economy, operational simplicity, shorter reaction time, convergence and facile automation.



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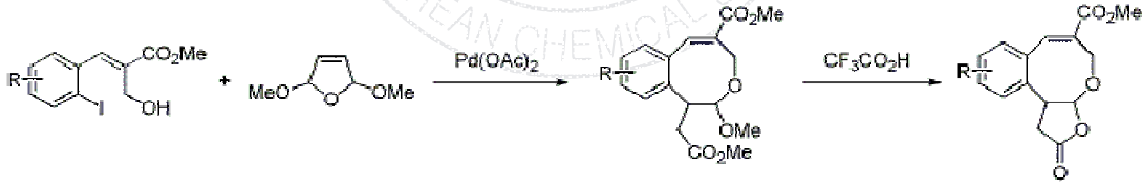
Synthesis of 1,4-Dihydro-2*H*-3-benzoxocine derivatives via the Heck reaction of Methyl 2-(hydroxymethyl)-3-(2-iodophenyl)propenoates with 2,5-Dimethoxy-2,5-dihydrofuran

현지나 안상현 이기정*

한양대학교 화학공학과

A new synthetic method for methyl 2-methoxy-1-(methoxycarbonylmethyl)-1,4-dihydro-2*H*-3-benzoxocine-5-carboxylates via the Heck reaction of 2,5-dimethoxy-2,5-dihydrofuran with methyl 2-(hydroxymethyl)-3-(2-iodophenyl)propenoates, has been developed. The benzoxocine derivatives were converted into methyl 2-oxo-1,2,5,11b-tetrahydro-3a*H*-furo[3,2-*a*][3]benzoxocine-6-carboxylates on exposure to excess trifluoroacetic acid.



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Synthesis of Solution Processable Small Molecules for Ambipolar Organic Field Effect Transistors

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π-conjugated organic semiconductors have attracted great attention as active layers in organic field effect transistors (OFETs) due to their several advantages such as low-cost, flexibility and solution processability. Recently, there are interests in the application of ambipolar OFETs which can transport both holes and electrons in single component. Low band-gap organic semiconductors are commonly selected as active layers for ambipolar OFETs due to energy level alignment between semiconductors and source/drain electrodes. In addition, quinoidal structure is known to reduce the band-gap dramatically. Therefore, quinoidal molecules have been considered as promising candidates for ambipolar OFETs. In this research, we synthesized low band-gap small molecules containing thiophene and selenophene. We characterized their thermal, optical and electrochemical properties and fabricated OFET devices. These materials clearly showed well-balanced ambipolar properties. In addition, we fabricated ambipolar complementary-metal-oxide (CMOS) inverter and investigated the device performance.

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In situ generation of hydroperoxide by oxidation of benzhydrols tobenzophenones using sodium hydride under oxygen atmosphere: use forthe oxidative cleavage of cyclic 1,2-diketones to dicarboxylic acids

강선혜 전민주 한호규 양정운[1]

고려대학교 화학과 [1]성균관대학교 에너지과학과

A facile oxidative cleavage of cyclic 1,2-diketones 1 to dicarboxylic acids 3 with hydroperoxide generatedin situ has been developed. In situ generation of hydroperoxide was effected by the oxidation of 4,40-dichlorobenzhydrol 2f to 4,40-dichlorobenzophenone 4f using sodium hydride under oxygen atmosphere.

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Indium Tri(isopropoxide)-Catalyzed Selective Meerwein-Ponndorf-Verley Reduction

류태규 김상혁 서보람 이필호*

강원대학교 화학과

Indium tri(isopropoxide)-catalyzed Meerwein-Ponndorf-Verley reduction of aliphatic and aromatic aldehydes in 2-propanol gave selectively the corresponding primary alcohols in good to excellent yields at room temperature. A wide range of functional groups including alkene, ether, ketone, ester, nitrile, and nitro were tolerated under the optimum reaction conditions. Chemoselective reductions were also achieved not only between aromatic aldehyde, aromatic ketone, and epoxide but also between aliphatic aldehyde and alkene.

1. Lee, J.; Ryu, T.; Park, S.; Lee, P. H. *J. Org. Chem.* 2012, *77*, 4821.

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Efficient Conia-Ene Cyclization of 2-Alkynic 1,3-Dicarbonyl Compounds

박영철 김상혁 이필호*

강원대학교 화학과

A cheap, simple, and effective $FeCl_3$-catalyzed Conia?ene cyclization of 2-alkynic 1,3-dicarbonyl compounds was stereospecific to afford alkylidenecyclopentanes in (*E*)-isomers via the 5-*exo-dig* pathway. The 5-*endo-dig* and 6-*exo-dig* cyclizations were also possible, depending on the structure of the substrates.

1. Chan, L. Y.; Kim, S.; Park, Y.; Lee, P. H. *J. Org. Chem.* 2012, *77*, 5239.

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Synthesis of Naphthalenes via Platinum-Catalyzed Hydroarylation

강동진 류태규 임수진 이필호*

강원대학교 화학과

An efficient synthetic method of functionalized naphthalenes having hydrogen, alkyl, alkenyl, aryl, or heteroaryl groups on the 4-position and ethoxycarbonyl group on the 2-position was developed through selective Pt-catalyzed 6-*endo* intramolecular hydroarylation of ethyl (*E*)-2-ethynyl/alkynyl cinnamates.

1. Kang, D.; Kim, J.; Oh, S.; Lee, P. H. *Org. Lett.* 2012, *14*, 5636.

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Synthesis of Vinyl Sulfides and Vinylamines through Catalytic Intramolecular Hydroarylation in the Presence of $FeCl_3$ and AgOTf

김상혁 김예린 이필호*

강원대학교 화학과

A synthetic method was developed for the preparation of vinyl sulfides and vinylamines from arylalkynyl phenyl sulfides and sulfonamides. Under mild conditions, a catalytic intramolecular hydroarylation reaction was carried out in the presence of $FeCl_3$ and AgOTf (OTf = trifluoromethanesulfonate) in 1,2-dichloroethane. A variety of 1,2-dihydronaphthalenes, 2*H*-chromenes, and 1,2-dihydroquinolines containing a phenylsulfenyl or *N*-phenyl-*N*-tosyl group on the sp^2-hybridized benzylic carbon were prepared in good to excellent yields. The present method could be extended to the preparation of dihydropyrano[2,3-*g*]chromenes through a twofold Fe-catalyzed hydroarylation by a selective 6-*endo* mode.

1. Eom, D.; Mo, J.; Lee, P. H.; Gao, Z.; Kim, S. *Eur. J. Org. Chem.* 2013, 533

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Brønsted Acid-Catalyzed Intramolecular Hydroarylation Driving Cycloalkenyl Selenides and Tellurides

엄다한 류태규 이필호*

강원대학교 화학과

Trifluoromethanesulfonic acid-catalyzed intramolecular hydroarylation of alkynyl selenides and tellurides was developed for the preparation of cycloalkenyl selenide and telluride derivatives through a selective 6- and 7-*endo* mode. The cycloalkenyl selenides and tellurides can easily be converted to a wide range of other valuable functionalities.

Reference:
1. Eom, D.; Park, S.; Park, Y.; Lee, K.; Hong, G.; Lee, P. H. *Eur. J. Org. Chem.* 2013, ASAP

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Metal/Brønsted Acid Relay Catalysis for the Double Hydroarylation and Cationic Cyclization

모준태 김재은 이필호*

강원대학교 화학과

We have developed a hybrid system of metal/Brønsted acid relay catalysis for the intramolecular double hydroarylation and cationic cyclization of diyne diethers and diamines to give 4,4`-bi(2*H*-chromene), bi(2*H*-quinoline), and dioxafluoranthenes starting from 2,4-diyne-1,6-diethers and diamines in one reaction vessel under mild conditions.

1. Mo, J.; Eom, D.; Lee, E.; Lee, P. H. *Org. Lett.* 2012, *14*, 3684.

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New Synthetic Method of Substituted Coumarin Derivatives

박상준 김철의 민지애 이필호*

강원대학교 화학과

Coumarins were obtained from the condensation of electron-rich arenes with allenes in the presence of TfOH in good yield. Depending on the substituent pattern of allenes employed, the general synthetic method of 4- and 3,4-di-substituted 3-arylcoumarins has been developed. Readily available allenes were employed as the three carbon atom sources constituting the coumarin skeleton for the first time.

1. Lee, P. H.; Mo, J.; Kang, D.; Eom, D.; Park, C.; Lee, C.-H.; Jung, Y. M.; Hwang, H. *J. Org. Chem.* 2011, *76*, 312.
2. Kim, S.; Kang, D.; Lee, C.-H.; Lee, P. H. *J. Org. Chem.* 2012, *77*, 6530.

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Synthesis of Indenes *via* Brønsted Acid Catalyzed Cyclization of Diaryl- and Alkyl Aryl-1,3-dienes

엄다한 박상준 신서현 이필호*

강원대학교 화학과

Substituted indenes can be synthesized *via* the Brønsted acid catalyzed cyclization of diaryl- and alkyl aryl-1,3-dienes. In this approach, treatment of symmetric or unsymmetric diaryl- and alkyl aryl-1,3-dienes with a catalytic amount of trifluoromethanesulfonic acid gives a variety of indene derivatives in good to excellent yields under mild conditions.

1. Eom, D.; Park, S.; Park, Y.; Ryu, T.; Lee, P. H. *Org. Lett.* 2012, *14*, 5392.

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Copper-Catalyzed Intramolecular Hydroalkoxylation

김상혁 박상준 이필호*

강원대학교 화학과

Ethyl *α*-(1-hydroxy-1-alkyl)methylallenoates and *α*-(1-hydroxy-1-aryl)methyl allenoates containing not only electron-donating groups but also an electron-withdrawing group on the aryl group at the *α*-position have been shown to undergo an efficient and selective copper-catalyzed intramolecular hydroalkoxylation to give functionalized 3-ethoxycarbonyl-2-alkyl- and -aryl-2,5-dihydrofurans in good to excellent yields through a 5-*endo* mode.

1. Kim, S.; Lee, P. H. *J. Org. Chem.* 2012, *77*, 215.

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Hydrosilyloxylation Driving Tandem Aldol and Mannich Reactions

강동진 류태규 이필호[*]

강원대학교 화학과

The chemoselective formation of an enolate from alkyne in the presence of a carbonyl and imine group was realized, which constructed a variety of structural motifs under exceedingly mild reaction conditions in a tandem process. Reaction driving tandem hydrosilyloxylation/aldol reactions was achieved through the formation of enol silyl ethers catalytically generated in situ from readily available alkynes. These reactions were expanded to obtain *β*-amino enol silyl ethers in good yields via the tandem hydrosilyloxylation/isomerization/Mannich reaction.

1. Kang, D.; Park, S.; Ryu, T.; Lee, P. H. *Org. Lett.* 2012, *14*, 3912.

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Gold-Catalyzed Sequential Alkyne Activation for the Synthesis of 4,6-Disubstituted Phosphorus 2-Pyrones

모준태 박영철 이필호*

강원대학교 화학과

Tandem gold-catalyzed addition of alkynyl phosphonic acid monoethyl esters to terminal alkynes and cyclization were developed for the synthesis of 4,6-disubstituted phosphorus 2-pyrones in one reaction vessel based on the concept of sequential alkyne activation. Alkynyl enol phosphonates were selectively obtained through the gold catalyzed addition reaction in the presence of a catalytic amount of triethylamine. Also, gold-catalyzed cyclization of alkynyl enol phosphonates was successful in giving a variety of 4,6-disubstituted phosphorus 2-pyrones.

1. Mo, J.; Kang, D.; Eom, D.; Kim, S. H.; Lee, P. H. *Org. Lett.* 2013, *15*, 26.

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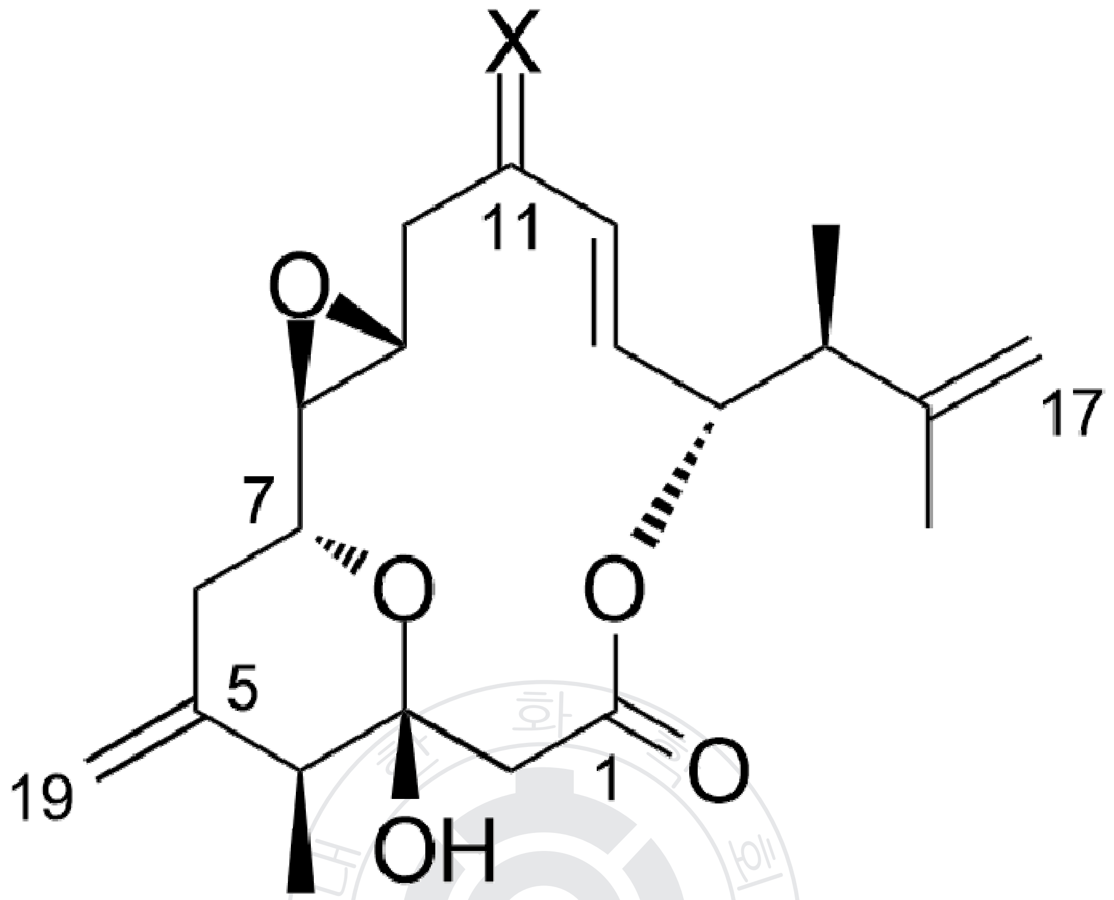
Total Synthesis of (-)-Amphidinolide O and (-)-Amphidinolide P

황민호 한서정[1] 이덕형*

서강대학교 화학과 [1]California Institute of Technology, U.S.A.

Anmphidinolides O and P were isolated from Okinawan marine dinoflagelate amphidinium sp. by Kobayashi group. They have shown in vitro cytotoxicity against murine lymphoma L1210 (IC50 = 1.7 and 3.6 ?g/mL, respectively) and human epidermoid carcinoma KB cells (IC50 = 1.6 and 5.8 ?g/mL, respectively). Two natural products have a very closely related structure except the functional group at C11 (the carbonyl group in amphidinolide O vs. the exo-methylene group in amphidinolide P). To date, total synthesis of amphidinolide P was reported by Williams and Trost, and total synthesis of amphidinolide O has not been reported yet. Herein we report the first total synthesis of (-)-amphidinolide O and the its conversion to (-)-amphidinolide P



X = O : (-)-Amphidinolide O

X = CH_2 : (-)-Amphidinolide P

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Controlled synthesis of 1-vinylnaphthalenes versus (*E*)-α-(1,3-enyn-4-yl)-α,β-unsaturated esters from Morita-Baylis-Hillman bromides: a sequential alkynylation and competitive 6π-electrocyclization versus conjugative transposition of a triple bond

임진우 김고훈 김세희 김재녕*

전남대학교 화학과

The synthesis of α-ethynyl-α,β-unsaturated esters has received much attention due to their wide synthetic applicability. However, the synthesis of α,β-unsaturated esters bearing a 1,3-enyne tether at the α-position has not been reported. This prompted us to investigate the synthesis of α-(1,3-enyn-4-yl)-α,β-unsaturated esters starting from the bromides of Morita-Baylis-Hillman (MBH) adducts. An expedient controlled synthesis of 1-vinylnaphthalenes and various dienyne derivatives has been carried out from the Morita-Baylis-Hillman bromides and propargyl acetate or *p*-nitrophenyl propargyl ether. By judicious choice of base, reaction temperature and leaving group, a selective synthesis of 1-vinylnaphthalenes and dienynes, (*E*)-α-(1,3-enyn-4-yl)-α,β-unsaturated esters, could be performed.

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Novel blue organic-light emitting materials of tert-Butylated spirofluorene derivatives with arylamino-vinyl groups

김혜정 윤승수*

성균관대학교 화학과

A series of tert-butylated spirofluorene derivatives with a arylamino-vinyl group were synthesized to serve as blue organic-light emitting materials via the Horner-Wadsworth-Emmons olefination. Also, a variety of electron-withdrawing groups in tert-butylated spirofluorene derivatives were introduced by a Suzuki cross-coupling reaction. To explore EL performances of these materials 1-5 as blue dopant, we have fabricated blue OLEDs with the following device structure: ITO/DNTPD(60 nm)/NPB (30nm)/MADN:blue dopant materials 1-5 (3, 5, 10%) (30nm)/TPBi (15nm)/Liq (1.0nm)/Al. All blue OLEDs using these materials 1-5 showed deep-blue emission. Particularly, the device using dopant 3 with MADN as the host exhibited a luminance of 10630 cd/m^2 at 7.0 V, a luminous efficiency of 15.1 cd/A at 20 mA/cm^2, power efficiency of 8.60 lm/W at 20 mA/cm^2 and an external quantum efficiency of 8.90 %, respectively. Moreover, the device using dopant 2 showed a deep-blue emission with the CIE$_{x,y}$ coordinates of (0.142, 0.156) at 8.0 V, and a luminance of 6355 cd/m^2 at 7.0 V, an external quantum efficiency of 7.65 % at 20 mA/cm^2, respectively. In conclusion, these results demonstrate that the excellent properties of a tert-butylated spirofluorene with arylamino-vinyl groups as deep-blue dopants for OLED applications.

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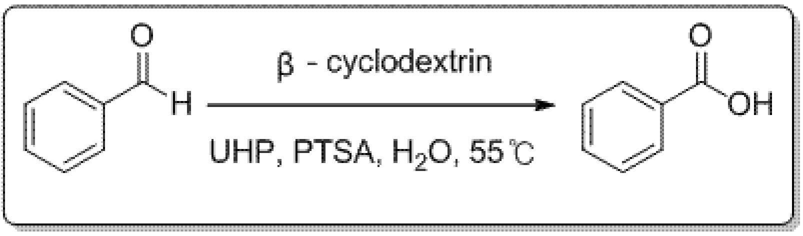
One-pot Oxidation of aldehyde in water Using UHP and β-cyclodextrin

정세영 이종찬*

중앙대학교 화학과

Simple, mild and hightly efficient oxidation of aromatic aldehyde with UHP(urea hydrogen peroxide) and PTSA(p-Toluenesulfonic acid) Nearly complete conversion of benzaldehyde to corresponds benzoic acid could be achieved within 20h at 60 ℃. This method is a direct one-pot transformation under mild condition using water as solvent and has many advantages over the exsting methodologies. also we are under investigation as well as the solvent ethylene glycol.



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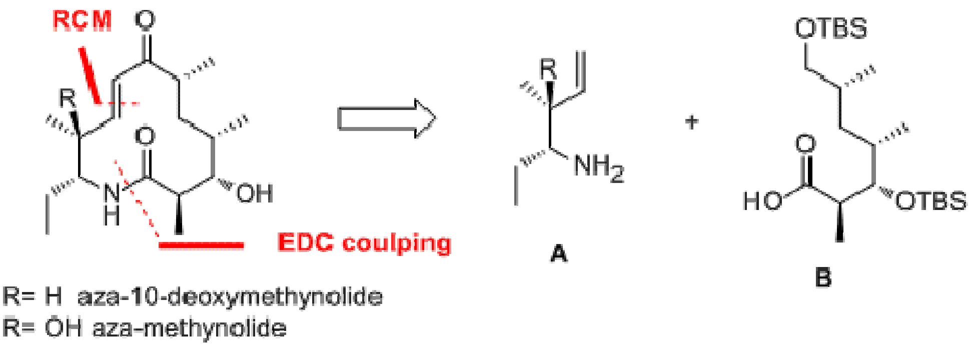
Synthesis of the Lactam Analogues of 10-Deoxymethynolide and Methynolide

강한영[*] <u>오홍세</u>[1]

충북대학교 화학과 [1]서울대학교 화학부

Converting the lactone moiety to the corresponding lactam structure has been a well-known strategy to improve biological activities of the compounds that contain lactone rings. An excellent example can be found in the case of Ixabepilone, that is, an aza-analogue of epothilone B. We hoped to extend this strategy to the corresponding lactam analogue of methymycin and pikromycin. For the synthesis of lactam analogues of the methymycin family we first decided to synthesize the aza-analogues of the corresponding aglycones, that is, aza-10-deoxymethynolide and aza-methynolide. Based on the developed synthetic strategy the desired 12-membered lactams could be divided retrosynthetically into two parts. The two parts were synthesized asymmetrically and assembled by the key reactions, that is, EDC coupling, and ring-closing metathesis by Grubb's second-generation catalyst.



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One-Pot Synthesis of Diaryl Alkynones Through Pd-Catalyzed Selective Carbonylative and Non-Carbonylative Couplings of Propiolic Acid

김원영 민홍근 이선우*

전남대학교 화학과

The synthesis of ynone is one of the most important tools in the medical and material fields which is based on organic chemistry. Because ynones are easily transformed into heterocylic compounds such as pyrimidine, quinolone, furan, pyrazole, flavone and oxime. There are major two ways to synthesized the diaryl alkynones. One way is from the acyl halides and the other is by using Sonogashira type carbonylation. However, they have some drawbacks in the instability and limitation of substrates and the requirement of multistep process. Thus the development of the simple, general and efficient synthesis is desired.To reach this goal, we develop the one-pot synthesis of diaryl alkynone from the palladium-catalyzed selective non-carbonylative and carbonyltive couplings toward propiolic acid with aryl halides. Diaryl alkynones were synthesized from one-pot Pd-catalyzed carbonylative and non-carbonylative coupling reactions of propiolic acid with aryl iodides under carbon monoxide atmosphere. The optimized condition is that aryl iodide (2.0 equiv), propiolic acid (1.0 equiv), $Pd(PPh_3)_2Cl_2$(5mol%), CuCl(10mol%), Et_3N(5.0equiv), CO(8atm) were reacted in CH_3CN at 80^{o}C for 3h. It showed good yields and functional group tolerance.

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pH-Sensitive Fluorescent Probes Based on 6-Membered Rhodamine B Derivatives

변지민 태진성*

연세대학교 화학과

We report new pH-sensitive fluorescence chemosensors based on rhodamine B base. The mechanism of the probe to monitor H+ is based on the structural change of rhodamine amides from the spirocyclic to the open form in response of proton. Typically rhodamine amide probes exist in colorless and non-fluorescent spirocyclic forms, however, they turn to pink colored and strongly fluorescent open forms in the presence of H+. To facilitate this structural change, we modified the rhodamine amide to a 6-membered amide possessing hydroxylamine unit. This new structure proved to be highly sensitive to proton in aqueous media. In the pH range of 3.6-3.8, the probes display very sharp fluorescence intensity changes and clear color changes from colorless to red. In addition, this probe shows strong fluorescecnce intensity increase in acidic aqueous solutions such as acetic acid and acidic amino acids.

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Synthesis and Charaterization of Hybrid azo compounds for Colorants

최우근 정연태[1,*]

부경대학교 이미지 시스템 공학 [1]부경대학교 이미지시스템공학과

Hybrid azo compounds 는 염,안료가 가진는 단점을 보완한 material 로 기존 염료가 가지는 내열,내광성을 개선하고 안료가 가지는 단점인 용해성을 증가시켜 열 안정성이 우수한 azo compounds 를 합성하였다. Hybrid azo compounds 를 합성하기 위하여 amino 그룹으로 발색단으로 하고 Aniline,Naphtol,benzoimidazol 계로 조색단으로 하여 UV- visible, TGA, FT-IR, H-NMR 통해 그 특성을 보았다.

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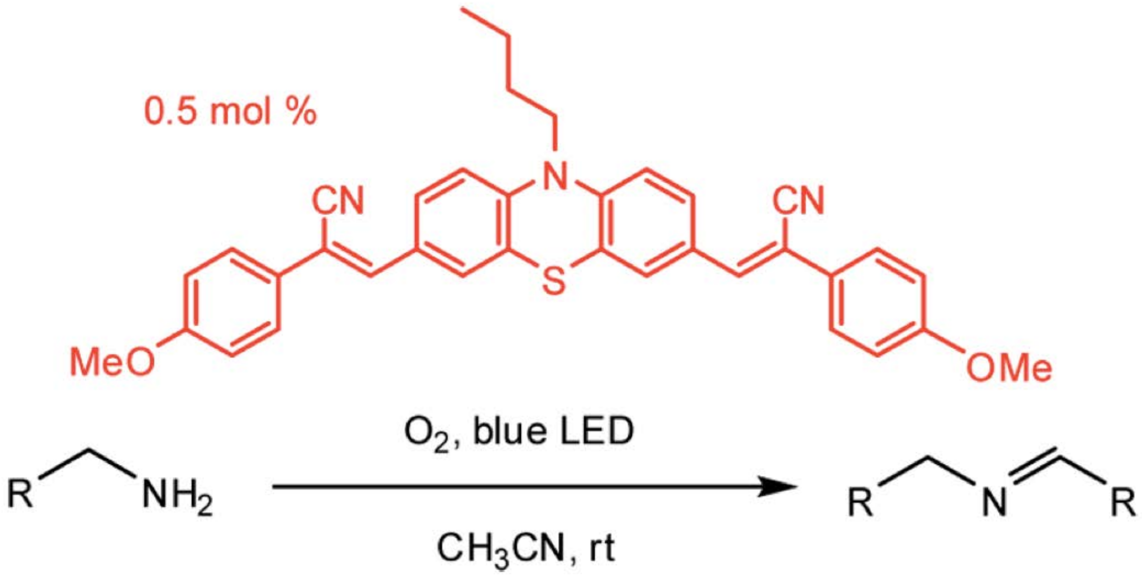
Visible-Light-Driven Photoredox Catalysis by Phenothiazine dyes for Oxidative Coupling of Primary Amines at Ambient Temperature

박지훈 박노진[1] 손성욱[*]

성균관대학교 화학과 [1]성균관대학교 에너지과학과

Recently, new photoredox catalysis using visible light harvesting dyes has shown successful results in variety range of chemical transformations. Usually, ruthenium or iridium complexes have been used as dyes in these reactions. In addition to efforts for the expansion of the range of organic reactions, more studies are required for the development of more diverse dyes, including organic dyes.In this work, new phenothiazine based organic dyes were prepared for visible-light-driven organic transformations. The 3,7-disubstituted phenothiazine derivatives showed visible light absorption and reversible one-electron oxidation behavior. In the presence of 0.5 mol % of 3,7-disubstituted phenothiazines, primary benzylamines showed oxidative coupling under visible light irradiation from a blue LED at room temperature. As far as we are aware, this is the most active visible light driven photocatalytic system for oxidative coupling of primary amines. The high activity of phenothiazine dyes was rationalized based on their optical and electrochemical properties. The reaction mechanism was discussed based on the detection of H_2O_2 as a byproduct after the reaction.


0.5 mol %
CN
CN
N
S
MeO
OMe
R
NH$_2$
O$_2$, blue LED
CH$_3$CN, rt
R
N
R

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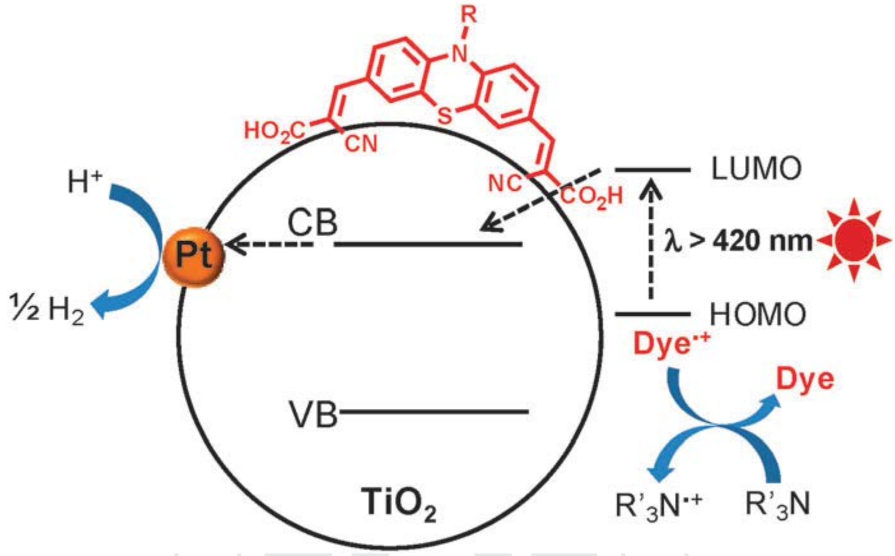
Highly efficient visible light-induced water splitting by phenothiazine-based organic dyes with two anchoring groups on TiO2

박노진 손성욱[1]

성균관대학교 에너지과학과 [1]성균관대학교 화학과

Phenothiazines are cyclic compounds with amine and sulfide moieties. One of the interesting aspects of phenothiazines is the intriguing stability of their cationic radical formed by one electron oxidation. Thus, it can be speculated that the phenothiazine-based dyes can have enhanced stability in photo-induced electron transfer from dyes to TiO2.In this work, new phenothiazine-based organic dyes with two anchoring groups at 3,7 positions and systematic alkyl chains on nitrogen are prepared. Their TiO2?Pt composites showed excellent photo-catalytic activities in visible light-induced water splitting. Interestingly, phenothiazine dyes with longer alkyl chains showed better stability in catalytic systems. The alkyl chains on the nitrogen of the phenothiazine ring further enhanced the TON values up to 1016 after 5 hours. This work shows that phenothiazines are promising building blocks for visible light harvesting materials in photocatalytic water splitting.


Control of Chemical Property
R
N
S
HO2C
CN
NC
CO2H
Anchoring Sites
Electronic Effect
R
N
S
- e-
+ e-
R
N
+•
S


R
N
S
HO2C
CN
NC
CO2H
LUMO
λ > 420 nm
HOMO
Dye•+
Dye
R'3N•+
R'3N
H+
Pt
½ H2
CB
VB
TiO2

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Construction of Linear Hybrid Peptides Containing Sugar Derived Gamma Amino Acids for Studying Foldameric Properties

DASADHIKARYNIRMAL 권순정 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

We have developed an understanding of the importance of non-covalent interactions in regulating protein folding. However, the rules used in these studies have been largely developed with peptides and proteins composed of α-amino acids, which lead to the question of whether our understanding is overly parameterized and specific to conventional peptides, or whether it is truly molecular in nature. Therefore, the development of small, easy-to-functionalize building blocks and oligomers with backbones of discrete and predictable folding patterns is required to design and develop molecules with biological functions. Sugar Amino Acids (SAAs) are sugar moieties containing at least one amino and one carboxyl group. Herein, we want to report the synthesis of linear hybrid peptides containing sugar derived gamma amino acids to study their folameric properties.

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The synthesis of heterocyclic compound initiated by Mn(OAc)3 from 1,3-dicarbonyl derivatives

<u>Ju Yeming</u> MIAO DI 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Heterocyclic structure containing compounds are of great importance in our life, which exhibit anticancer, antiseptic, disinfectant, and pesticide properties. The hetero-Diels-Alder reaction has been proven to a powerful method for introducing the heteroatom. The 1,3-dicarbonyl compounds have been known to be the excellent candidate for radical formation initiated by Manganese acetate. In our reaction system, the air was utilized as the source of oxygen. The Manganese triggered carbon radical was then trapped with oxygen instead of carrying out the radical addition reaction to unsaturated bond, which followed with deacetylation, double bond migration and hydroxyl introduction accomplished the formation of various aliphatic cyclic structure and aromatic furan derivatives.

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A highly efficient synthetic method of carotenoid Zeaxanthin.

이규상 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Zeaxanthin is one of the most common carotenoid alcohols found in nature. It is the pigment that gives paprika, corn, saffron, wolfberries, and many other plants their characteristic color. A highly efficient synthetic method of carotenoid compounds has been developed by our group on the basis of the sulfone coupling / double-elimination and Ramberg-B?cklund reaction strategy.Zeaxanthin requires the controlled allylic oxidation in the terminal cyclohexene ring moiety to produce the hydroxyl group.Proper protection, coupling with C10 di-aldehyde and the double elimination were required to synthesize Zeaxanthin.

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A study on the synthesis, characteristics and properties of Carotenoids.

김영훈 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

The carotenoids are important class of organic molecules with delocalized π-electrons, which show electric conductance. We have researched the synthesis of natural carotenoids, which can be extended to the synthesis of unnatural carotenoid wires. We designed the unnatural carotenoids by attaching aromatic substituents of different electronic nature. The unnatural carotenoids can be assembled by allylic sulfone and dialdehyde. These two parts can be connected by following reactions ; sulfone-mediated coupling reaction, protecting of alcohol, and double elimination. The conjugated polyene chains of the unnatural carotenoids would show an extra stability and improved electronic characteristics compared with those of the natural carotenoids.

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

Regioselective construction of 1-α-tocopheryl-3-glyceride for the synthesis of phosphatidylcholine compounds.

최정애 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Phosphatidylcholine is the major component of cell membranes.A universal phosphatidylcholine is composed of a choline head group that is polar part and two fatty esters being nonpolar part.We decide to replace one of the ester by α-tocopherol, which is a well known anti-oxidant. We synthesized 1-α-tocopheryl-3-glyceride of various carboxylic acids by the regioselctive ring opening reaction of the α-tocopherylglycidylether. Then the phosphatidylcholine part were synthesized by transferring the hydroxy to the polar group. We synthesized various 1-α-tocopheryl-3-glycerides, which would be efficiently utilized for the formation of diversely substituted phosphatidylcholine derivatives.

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A Study on the synthetic method of Unnatural carotenoid

임보람 구상호[1]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Conjugated poylene chains containing phenyl substituents which are almost perpendicular to the chain are not fully conjugated. If two phenyl substituents can provide the proper distance, we can anticipate that they can coordinate with metal ions. So, It may be possible to design efficient metal ion sensors based on the carotenoid polyene chain. Under the sequence of Indium mediated addition and oxonia-cope rearrangement reaction, chloro sulfone unit containing phenyl substituents can be readily prepared from acetophenone derivatives. Then, the chloro sulfone unit is strategy for the carotenoid synthesis, the conjugated polyene chain with di-phenyl substituents could be synthesized as a metal ion sensors.

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Synthesis of 2,5-Disubstituted Tetrahydrofuran-3-ones via Gold(I)-catalyzed [2,3]-Sigmatropic Rearrangement

한미연 배주희 태진성*

연세대학교 화학과

The tetrahydrofuran ring is an important common structure found in numerous natural products and biologically active compounds. Especially, 2,5-disubstituted tetrahydrofuran rings can serve as versatile starting substrates for the synthesis of various synthetic transformations. We have developed an efficient synthetic method for 2,5-disubstituted tetrahydrofuran-3-one by using a gold(I)-catalyzed cyclization method. Reaction of homopropargyl allyl ethers with gold(I)-catalyst in the presence of amine oxide generates gold-carbene complex which is trapped by allyl ether and subsequently rearranges to 2-allyl tetrahydrofuran-3-one structures. The overall strategy could be efficiently applied for the synthesis of various biologically active natural products.

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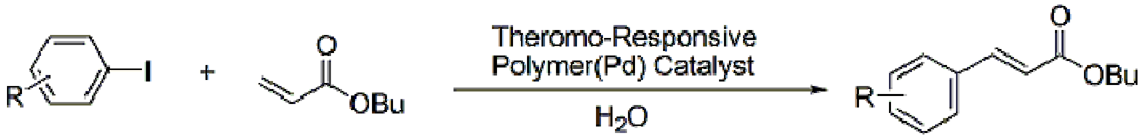
Mizoroki-Heck Coupling Reaction in Water with Poly(*N*-isopropylacrylamide)-co-4-Vinylpyridine copolymer as Solid-Support of Pd Nanoparticles

홍명찬 이학준*

한양대학교 응용화학과

One of a well known temperature-responsive polymers is Poly(*N*-isopropylacrylamide)(PNIPAM). In other words, PNIPAM has hydrophilic character below LCST but upper LCST, PNIPAM changes hydrophobic character in water. Also, pyridine is well known ligand that forms complexes with transition metal ions. So, we have prepared co-polymer by polymerization of PNIPAM and 4-vinylpyridne(4-VP). Pd nanoparticles were immobilized on synthesized PNIPAM-co-4-VP co-polymer. Pd@PNIPAM-co-4-VP catalyst was applied for Mizoroki-Heck reaction in water. We have developed an efficient heterogeneous Pd nano catalyst system.



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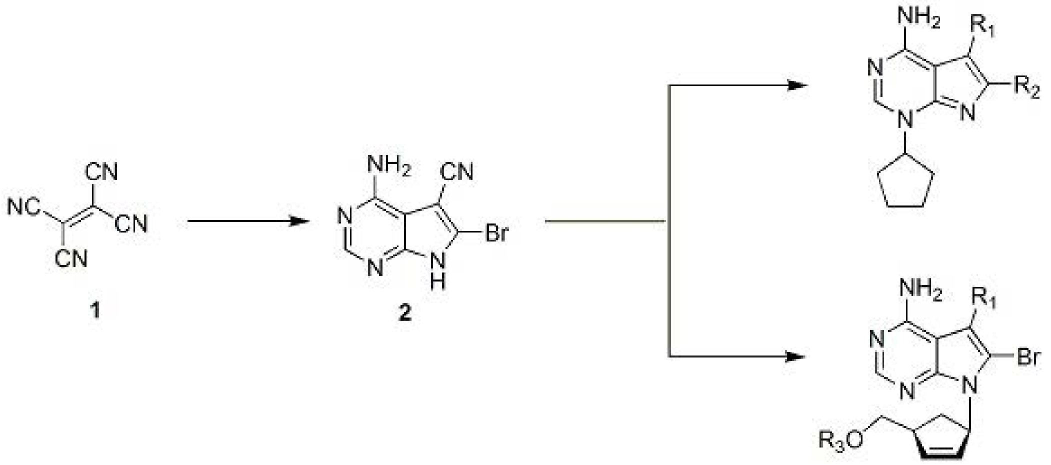
The Synthesis and Evaluation of Carbocyclic Pyrrolo[2,3-d]pyrimidine Nucleoside Analogs.

윤상은 이종복[1] 이학준[*]

한양대학교 응용화학과 [1]한양대학교 바이오나노학과

New carbocyclic pyrrolo[2,3-d]pyrimidine nucleoside analogs were synthesized with the key heterocyclic compound, 4-amino-6-bromo-5-cyanopyrrolo[2,3-d]pyrimidine (2). One of the products, compound 3 (R1=-CONH2, R2=-Br), showed significant anticancer activity to the human ovarian cancer PA-1 cells (IC50: 3.9 μM). Based on the biological effects and the functional group characteristics of this compound, the synthesis of carbocyclic nucleoside analogs has been tried by a Pd(0)-catalyzed coupling reaction with key intermediate 2 and cyclopentenyl dicarbonate. One of the coupling products, compound 4 (R1=-CONH2, R2=-Br, R3=-CH3), showed very similar anticancer activity to the human ovarian cancer PA-1 cells (IC50: 2.6 μM). According to the biological activity data, the amide functional group, the existence of the bromine atom, and the position of the hydrophobic character would have an effect on the anticancer activity.



R_1 = -CN, -$CONH_2$
R_2 = -H, -Br
R_3 = -CO_2CH_3, -$COCH_3$, -CH_3

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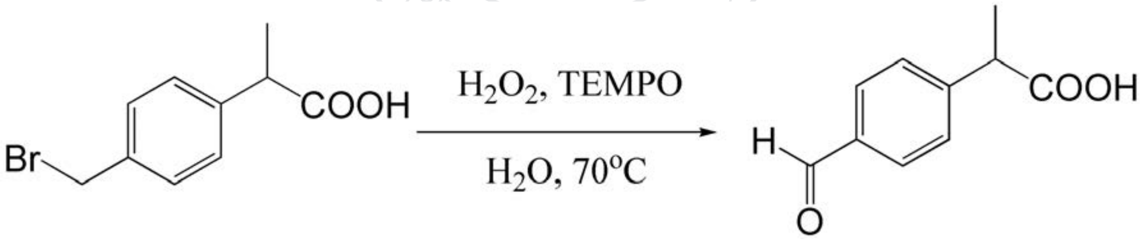
A green process for preparing 2-(4-formylphenyl)propionic acid in water solution

이용우 **shabbir saira** 이학준

한양대학교 응용화학과

The 2-(4-formylphenyl)propionic acid is the key intermediate of Pelubiprofen which is NSAID (nonsteroidal antiinflammatory drug).We successfully synthesized the 2-(4-formylphenyl)propionic acid using Hydrogen Peroxide and TEMPO (2,2,6,6-Tetramethyl-1-piperidinyloxy, free radical).This method is a one-pot reaction from 2-{4-(bromomethyl)phenyl}propionic acid to 2-(4-formylphenyl)propionic acid through the hydrolysis of benzyl bromide and consequential oxidation of benzyl alcohol.It is economic and eco-friendly reaction methodology.



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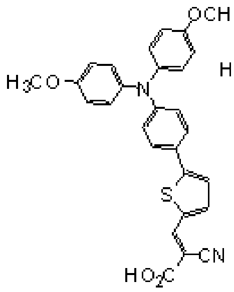
Bridging Effect of Dye on Cell Efficiency of DSSC

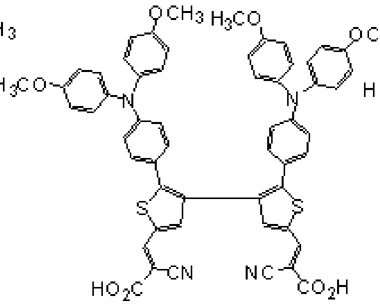
이상희* 김동희 김가영 Mannix Balanay

군산대학교 화학과

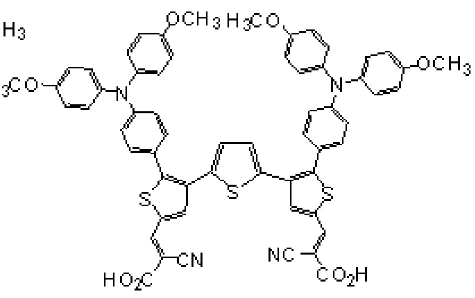
Dye L1 was bridged to give to KS-11 and KS-13. Synthesis and of cell performance of KS-11, and KS-13 will be described. Bridging of dye can affect on binding strength on TiO2 surface because Bridged dyes have two anchoring groups which bind to TiO2 efficiently. In addition, bridging of dye can affect on dye aggregation and dye amount on TiO2, finally cell efficiency of DSSC.



L1



KS-11



KS-13

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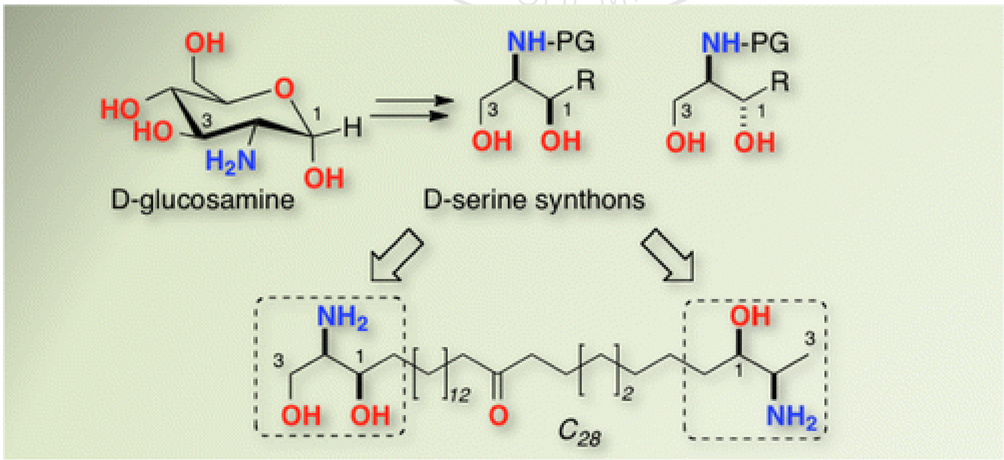
D-Glucosamine-Derived Synthons for Assembly of l-threo-Sphingoid Bases. Total Synthesis of Rhizochalinin C

고재영 Tadeusz F. Molinski[1,*]

아모레퍼시픽 피부소재팀 [1]*University of California at San Diego*

A five-step transformation of d-glucosamine, commencing with indium-mediated Barbier reaction without isolation of intermediates, into (R,R)-2-aminohex-5-ene-1,3-diol in 45?51% is described. The latter is a useful synthon for assembly of l-threo-sphingoid bases: long-chain aminoalkanols and aminoalkanediols with configurations antipodal to that found in mammalian D-erythro-sphingosine but prevalent among invertebrate-derived sphingolipids. The utility of the method is demonstrated by the first total synthesis of rhizochalinin C, the long-chain, “two-headed” sphingoid base aglycon of the natural product rhizochalin C from the marine sponge Rhizochalina incrustata.



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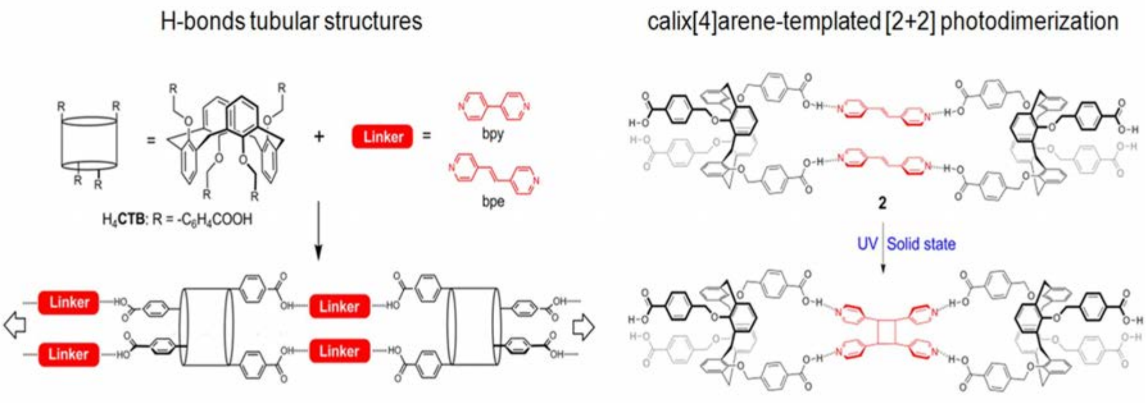
H-bonds tubular structures based on 1,3-Alternate calix[4]arene with bipyridines: calix[4]arene-templated [2+2] photodimerization

이은지 주희영 이심성 박기민*

경상대학교 화학과

From the reaction of calix[4]arene tetrabenzoic acids with bipyridyl derivatives (bpy and bpe) the cocrystallized 1D tubular products in which the two bipyridyl linkers are aligned parallel via H bonds were prepared. We confirmed that the olefinic tube incorporating bpe molecules undergoes the [2 + 2] photodimerization in solid state. Such tubular structures based on the combination of calixarene and bipyridyl derivatives and their uses in the photodimerization of the olefinic system have not been reported before. Consequently, the specific conformation of calix[4]arene derivatives can act not only as platforms for the construction of the novel supramolecular networks but also as templates for the photoreactive solid-state system.



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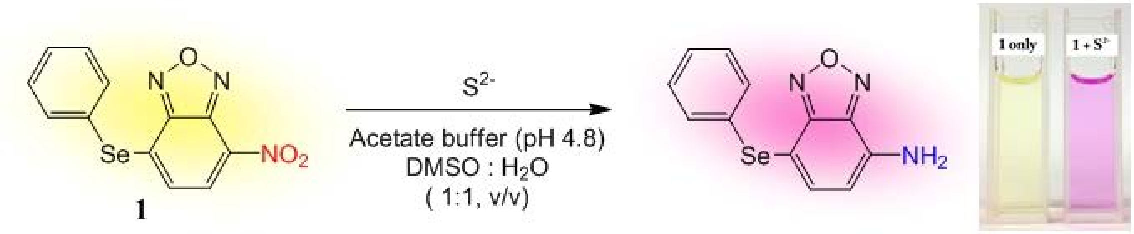
Colorimetric Signaling of Hydrogen Sulfide by Reduction of Phenylseleno- nitrobenzoxadiazole (NBD) Derivative.

<u>배지희</u> 장석규*

중앙대학교 화학과

A new reaction-based probe for the highly selective colorimetric signaling of hydrogen sulfide was investigated. Reduction of nitro group of NBD moiety to amino group by hydrogen sulfide resulted in a pronounced chromogenic signaling from yellow to pink color change. Selective hydrogen sulfide signaling was possible by the probe in the presence of commonly encountered metal ions and anions. The detection limit for the determination of hydrogen sulfide in 50% aqueous DMSO was 2.1 x 10^{-6} M. The designed probe could be useful for the determination of hydrogen sulfide in environmental samples.



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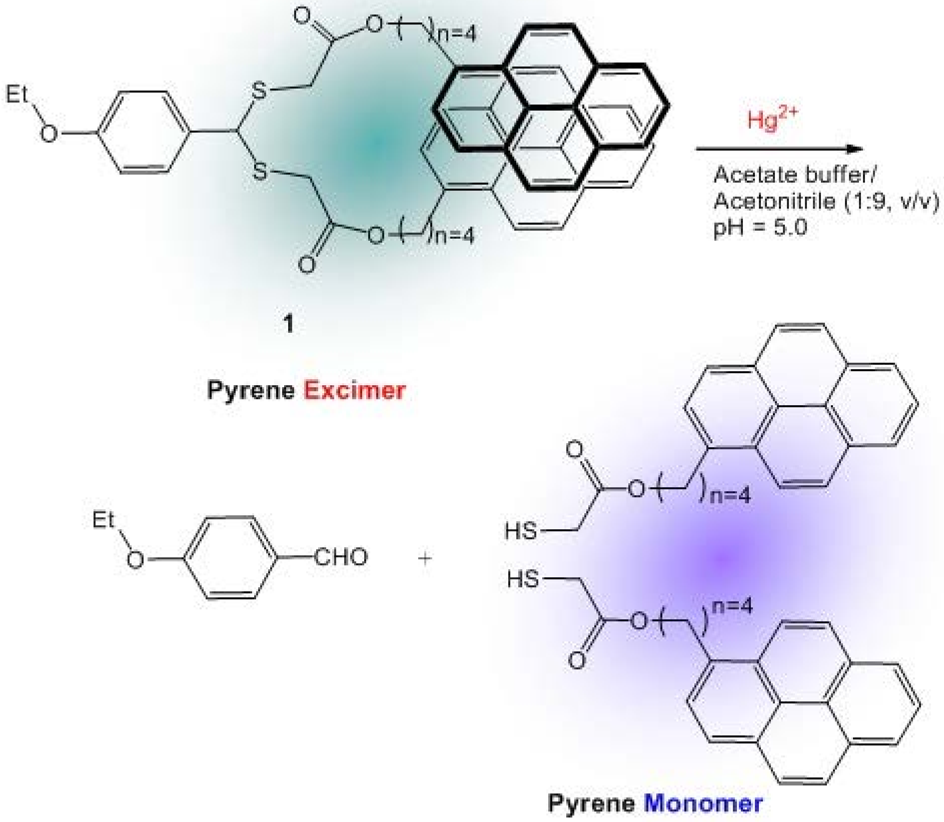
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reaction-based Hg(II) signaling by excimer?monomer switching of bis-pyrene dithioacetal

조윤하 장석규*

중앙대학교 화학과

A novel reaction-based probe for the fluorescence signaling of Hg^{2+} ions was developed. The probe having two pyrene fluorophores and dithioacetal linking moiety was designed to allow a conformation in which two pyrene moieties are in close proximity for the excimer emission. Selective Hg^{2+}-induced cleavage of dithioacetal that resulted in the switching of pyrene excimer to monomer emission was used for the signaling. The reaction based excimer-monomer switching of pyrene moieties was readily used for the ratiometric signaling of Hg^{2+} ions in aqueous acetonitrile. Selective signaling of Hg^{2+} ions was possible over other common metal ions and anions with a detection limit of 9.82×10^{-7}M.


Et
O
S
S
O
O
n=4
n=4
Hg^{2+}
Acetate buffer/
Acetonitrile (1:9, v/v)
pH = 5.0
1
Pyrene Excimer
Et
O
CHO
+
HS
HS
O
O
n=4
n=4
Pyrene Monomer

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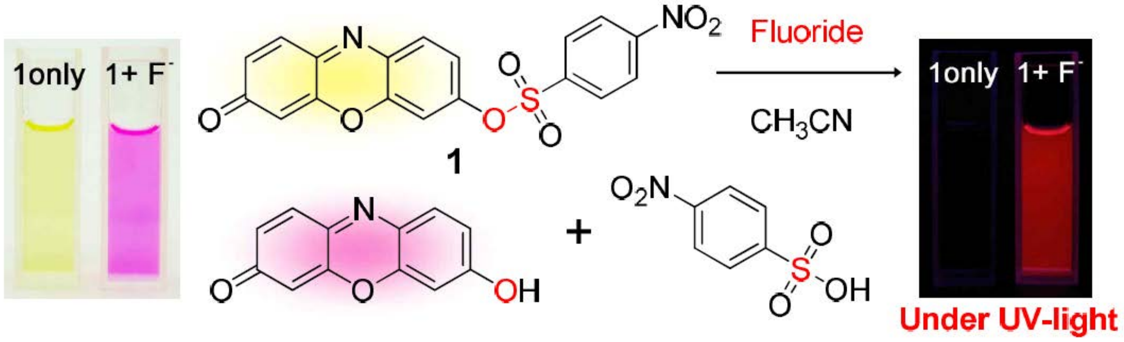
Reaction-based dual signaling of fluoride ions by resorufin sulfonates

임현규 장석규*

중앙대학교 화학과

New reaction-based probes for dual signaling of fluoride ions were investigated. Selective fluoride-assisted deprotection of resorufin nosylate to generate resorufin fluorochrome was used for signaling. Resorufin nosylate exhibited selective colorimetric and fluorogenic signaling of fluoride in acetonitrile. The interference from sulfide ions was successfully removed by using TPEN-Cu^{2+} complex as a source of Cu^{2+} ions for masking sulfide. Selective optical signaling of fluoride with a detection limit of 1.9 x 10^{-6} M in the presence of commonly encountered anions was possible.



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Synthesis and Characterization of Amphiphilic Diblock DendrimersContaining Carbazole as a Core Chromophore

최인화 윤성희 한승철 이재욱*

동아대학교 화학과

In the convergent synthesis of the dendrimers, two feasible methods are the fusion of two dendrons and the stitch of multi-functional group with dendrons. We have developed the fusion and stitching methods for the synthesis of symmetric and unsymmetric dendrimers and diblock codendrimers using click chemistry between an alkyne and an azide. The well-known click chemistry which is useful tool for synthesis of dendrimers, is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition proved to be an ideal reaction in very good to excellent yields. Taking advantage of these facts, we will present the efficient strategy for the convergent synthesis of amphiphilic diblock dendrimers having the core chromophore via the double click chemistry. The absorption and emission of the dendrimers will be disclosed.

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Triphenylsilane End-Capped Anthracene Derivatives For Highly Efficient Organic Light-Emitting Diodes

송지영 김영관[1,*] 윤승수[*]

성균관대학교 화학과 [1]홍익대학교 기초과학과

A novel series of anthracene derivatives with a triphenylsilane end-capping group were designed and synthesized for application as new blue emitting materials in organic light emitting diodes (OLEDs). The silicon is located in the center of a tetrahedron formed by the phenyl group. Therefore, we expected that triphenylsilane end-capping group disrupt intermolecular interaction and reduce self-aggregation through steric hindrance of the non-coplaner structure. To evaluate their electroluminescent properties, OLED devices with the structure of ITO (180 nm) / NPB (50 nm) / blue materials (30 nm) / Bphen (30 nm) / Liq (2 nm) / Al (100 nm) were fabricated. All devices using these materials showed the efficient blue emissions. In particular, the device using S-4 exhibited maximum luminance efficiency, power efficiency and quantum efficiency of 2.71 cd/A, 2.43 lm/W and 2.64% respectively. Also, the device incorporating S-1 shows a deep-blue emission with the CIEx,y coordinates of (0.16, 0.09) at 6.0V.

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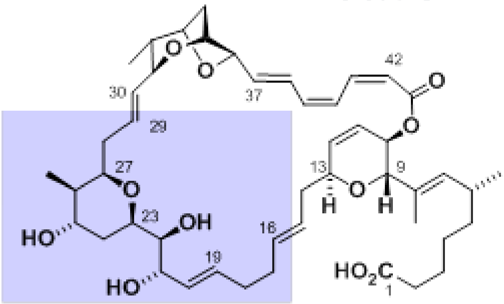
Synthetic Approach to the C16-C29 Subunit of Antibiotic Sorangicin A

이유진 최일영[1] 이효원

충북대학교 화학과 [1]한국화학연구원 의약화학연구센터

Sorangicin A, isolated from myxobacterium *Sorangium cellulosum*, is a 31-membered macrolide with potent antibiotic activity against both Gram negative and Gram positive bacteria. The structural feature of sorgangicin A involves a signatural dioxabicyclo[3.2.1]octane, a tetrahydropyran ring, a dihydropyran ring and a (*Z*,*Z*,*E*)-trienoate ester unit.Our synthetic efforts toward the subunit of C16-C29 comprising a tetrahydropyran subunit utilized the Prins reaction as well as the Evans protocol of aldol reaction will be disclosed.



(+)-Sorangicin (1)

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Regioselectivity of Alkylation of 5-Aminotetrazole : Synthesis of 1,2,-Bis(5-aminotetrazol-1-yl)ethane

이세진 임영권[1]

국방과학연구소 제4기술연구본부 2부 [1]국방과학연구소 4-2

5-Aminotetrazole-based compounds are fascinated as high energy density materials (HEDMs) for high explosives and propellants because they have high nitrogen content and thermal stability despite large positive enthalpies of formation. The key factors driving the requirement for a candidate for the chemical energetic materials include not only improved performance for high energy density but also high stabilities and low sensitivities to external stimuli. In recent developments, the introduction of methyl groups helps to reduce sensitivity of the compounds while concomitantly increasing their thermal stability at the cost of performance and makes interesting compounds accessible. Since the alkylation of 5-aminotetrazole was reported in 1885, there are several reports of alkylation of 5-aminotetrazole. However, alkylation of 5-aminotetrazole gives, as a rule, mixtures of isomeric 1- and 2-alkylated-5-aminotetrazoles, the latter often being the major products. Moreover, few reports have been reported about alkylation of 5-aminotetrazole. Herein, regioselectivity of alkylation of 5-aminotetrazole with 2-bromoethanol using various conditions and synthesis of 1,2-bis(5-aminotetrazol-1-yl)ethane with improving yield will be presented.

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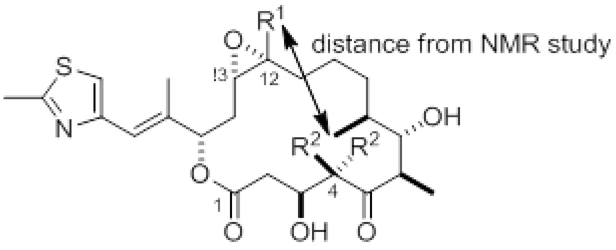
Synthesis of an Epothilone Derivative with Fluorine and Deuterium Substituents

이재호 최일영[1] 백윤기[2] 이효원

충북대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]한국기초과학지원연구원 대구센터

Antimiotic epotilones exert their cytotoxicity through the interruption of cancer cell division. Epotilones were isolated from myxobacterium *Sorangium cellulosum* strain So ce90 and *S. cellulosum* SMP44. For the examining the conformation of binding epothilones in the biological system through solid NMR study, deuterium and fluorine substituted epothilone derivative is required. The resulting distance between the deuterium and fluorine atoms will lead to the required conformaton for the binding. Our synthetic plan towards this derivative from epothilone B was envisoned from the coupplig of the northern fragment of C7-C21 with a fluoromethyl group and the southern fragment C1-C6 with two germinal trideuteromethyl groups. The aldol reaction and the following lactonization would lead to the required product. Further details will be disclosed



Epo A (R^1 = H)
Epo B (R^1 = CH_3)
Epo Derivative (R^1 = CH_2F, R^2 = CD_3)

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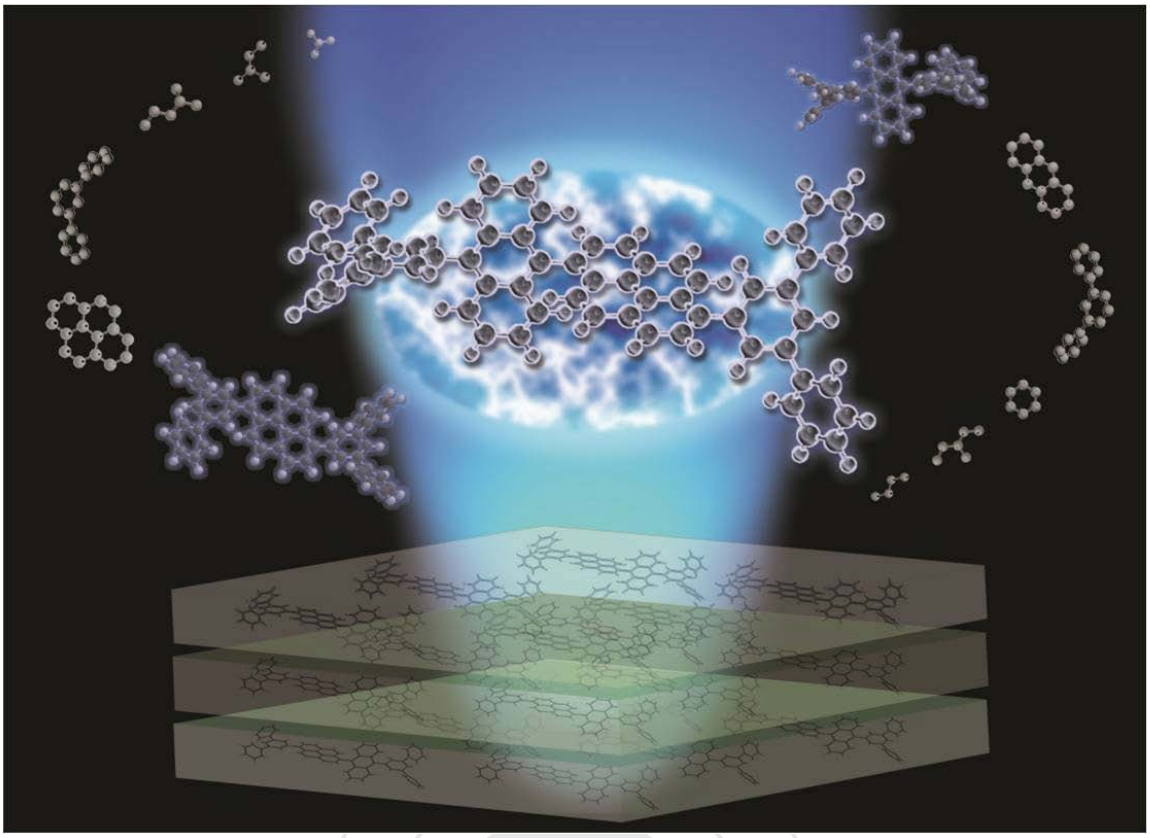
Synthesis and electroluminescence properties of highly efficient blue fluorescence emitters using dual core chromophores

김범진 박종욱

가톨릭대학교 화학과

Organic light-emitting diodes (OLEDs) based on organic small molecules are currently the subject of intense research efforts due to their promise in full-color large display applications.We have synthesized new dual core chromophore materials that are created by introducing an additional chromophore into a single core chromophore; this approach is based on our experience with the core-side concept of mono- and dimer-core materials.3,15 The dihedral angle between the two core chromophores in these dual core chromophore materials is 90 degree, which means that excimer formation is reduced and the efficiency and lifetime of the devices are greatly improved.We synthesized and systematically examined the characteristics of the anthracene single core chromophore material 9-(3',5'-diphenylphenyl)-1'-(3''',5'''-diphenylbiphenyl-4''-yl)anthracene(MAM), the pyrene single core chromophore material 1,6-bis-[1,1';3',1'']terphenyl-5'-yl-pyrene (TP-P-TP), and the dual core chromophore compounds 1-phenyl-6-(10-phenyl-anthracen-9-yl)-pyrene (Ph-AP-Ph) and 1-[1,1';3',1'']terphenyl-5'-yl-6-(10-[1,1';3',1'']terphenyl-5'-yl-anthracen-9-yl)-pyrene (TP-AP-TP).One of the dual core derivatives, TP-AP-TP, exhibited an ELmax value of 456 nm and a high luminance EQE of 7.51% when used in an EL device. The dual core chromophore materials had narrower PL and EL spectra and better thermal properties than the single core chromophore materials. A device based on TP-AP-TP showed twice the lifetime of a device based on the commercialized material, 2-methyl-9,10-bis(naphthalen-2-yl)anthracene (MADN).



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Novel Fluorescent Probes for Ratiometric Detection of Singlet Oxygen

한예지 류승연[1] 유영민[2,*] 남원우[3,*]

이화여자대학교 바이오융합과학과 [1]이화여자대학교 바이오융합과학과/화학 [2]한국과학기술연구원(KIST) 의공학연구소 [3]이화여자대학교 화학과

Singlet oxygen ($^1O_2$), a highly reactive oxygen species (hROS), is linked to a variety of pathological and physiological processes in the human body. However, efforts to the elucidation of molecular mechanisms underlying the biological actions of $^1O_2$ suffer from lack of suitable probes. We synthesized a series of ratiometric fluorescent probes, which are capable of detection of intracellular $^1O_2$. The $^1O_2$ probes were constructed based on 1,3-diarylisobenzofuran that undergoes the [2+4] pericyclic reaction with $^1O_2$. The reaction produces fluorescence ratiometric changes, and was selective to $^1O_2$ over other ROSs. The pseudo-first order reaction rate increased in proportional to the pi-conjugation length of the probes. We demonstrated the biological utility of the probes by successful visualization of the cellular production of $^1O_2$ in RAW 264.7 cells under phorbol 12-myristate 13-acetate (PMA) stimulation.

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How Much the Hybridization of Carbon Atom Affects the Transmission of the Substituent Effect?

한인숙* 정은정[1]

강원대학교 과학교육학부 [1]강원대학교 화학과

M- and p-substituted phenyl esters of propanoic acid, acrylic acid, and propiolic acid were prepared and their 1H and 13C NMR spectra were obtained in 0.1 M - CDCl3 solution. The chemical shift values of the α- and β-protons and carbon atoms as well as the carbonyl carbon atoms were correlated with the Hammett substituent constant (σ). The carbonyl carbon atoms show inverse correlations and the magnitudes of the slopes are increased as the s character of the carbon atom increases. On the other hand, the substituent increments in the chemical shifts of the C atoms of the benzene ring by the propionoxy and acryloxy groups are about same whereas those by the propioloxy group are significantly changed.

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Copper(II) Ion-Selective Sensing with Spiropyran-Cored PAMAM Dendron

신은주* 허대영

순천대학교 화학과

Copper is one of the three most abundant and physiologically essential transition metal ions(including zinc and ion) in the human body. However, excessive amounts of copper can cause serious health problems such as kidney failure, nerve system damage, or even death. Therefore, developing better sensors for the detection of environmentally and biologically important copper has been an important subject in the field of chemical sensors for several decades. Spiropyran(SP) is an important class of photo- and thermo-chromic compounds, which show reversible structural transformation upon optical, chemical, or thermal stimulation. Colorless SP of nonpolar closed form can be converted on UV irradiation by heterolytic C-O bond cleavage into colored MC of extendedly conjugated zwitterionic open form, and then the MC returns to the SP by ring closure thermally or on irradiation of visible light. The negatively charged phenolic oxygen atom in the MC form could bind to a metal ion in cooperation with other chelating functional group. Dendimers have been attracted much attention because of the most appealing characteristics such as low viscosity, flexibility, pH-dependent contraction and swell, ample interior voids, amphiphilicity, high biocompatibility, thermal stability, and peripheral functional density. Incorporating photochromic molecules into PAMAM dendron might lead to a light-modulated sensor. Spiropyran-cored PAMAM dendron shows reversible photochromic reaction, solvatochromic behavior in various solvents, and copper(II) ion-selective sensing ability.

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Light-Induced Unusual Behavior of Porphyrin-Spiropyran Dyad in Dichloromethane

신은주* 허대영

순천대학교 화학과

It is expected that combination of most frequently employed photoactive molecule porphyrin(Por) and well-known photochromic compound spiropyran(SP) could lead to an interesting light-controllable molecular device. In dichloromethane, Por-SP dyad shows unusual red-shifted absorption spectral changes completely different from normal conversion of spiropyran(SP) into merocyanine(MC). Absorption maxima in dichloromethane are shifted from 418(Soret band), 515, 550, 590, 645(four Q bands) nm into 450 and 665 nm. Also, fluorescence maxima are also shifted from 650 and 715 nm to 692 nm. Forward reaction is completed after around one hour. In the dark, original absorption and fluorescence spectra are recovered very slowly over about 15 hours by ring closing reaction. To search for the origin of these spectral changes, reversible photochromic reaction of Por-SP dyad has been investigated under a variety of reaction condition such as concentration and solvent. Unexpectedly, on UV irradiation, Por-SP dyad shows strikingly different spectral changes in two solvents of dichloromethane and tetrahydrofuran. In addition, comparative study of Por-SP dyad and porphyrin was conducted with TEM and AFM as well as absorption and fluorescence spectroscopy.

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Solvent-dependent Photochromic Reaction of Porphyrin-Spiropyran Hybrid Compounds

신은주* 허대영

순천대학교 화학과

Spiropyran(SP) is well-known photochromic compound accomplishing reversible molecular structural change to merocyanine(MC) by the photochemical ring opening on UV irradiation. In turn, MC is transformed to SP by ring closure, thermally or on irradiation of visible light. Reversible photochromic SP-MC transformation is one of subjects of active research on switch, sensor and optical memory.On the other hand, porphyrin(Por) is one of most frequently employed photoactive molecules because of it's photophysical and redox properties. Incorporating a photochromic molecule SP into porphyrin could lead to interesting photoresponsive system, the properties of which can be manipulated by light. In this study, absorption and fluorescence spectral changes for various porphyrin-spiropyran(Por-SPn) hybrid compounds such as Por-SP, Por-SP2, and Por-SP4 have been investigated to explore their photochromic reaction behavior. Unexpectedly, on UV irradiation, Por-SPn hybrid compounds shows strikingly different spectral changes in two solvents of dichloromethane and tetrahydrofuran.

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Biological Properties Synthesis and Characterization of Morpholino and Di(methoxyethyl)amino Substituted 1,3,5-Triazine Derivatives.

이채호* 이종대[1] 강상욱[2]

원광대학교 생명나노화학부 [1]조선대학교 화학과 [2]고려대학교 소재화학과

The delivery of boron-containing molecular fragments to tumor tissues and the accumulation of these agents within the framework of boron neutron capture therapy (BNCT) is the subject of a great deal of attention. We report the biological properties , synthesisand characterization of s-triazinyl morpholine and di(methoxyethyl)amine derivatives and their related o-carborane moieties with good yields as potential BNCT agents as an extension of our ongoing inevestigations into the biological behavior of bio-molecules based on o-carboranes.

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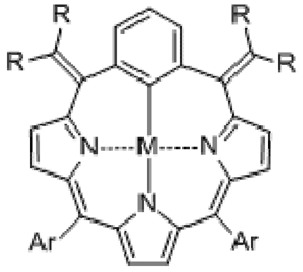
meso-Alkylidene porphyrins and their metal complexes: Structures and Properties

이창희* 박도우 김진경

강원대학교 화학과

Since the Pd(II)-complexes of meso-alkylidene-(m-benzi)-porphyrin show promising catalytic activity toward C-C bond forming reactions such as Sonogashira coupling, we extend the metallation chemistry of meso-alkylidene-(m-benzi)-porphyrin to other transition metal ions. The reaction is straight forward and column chromatographic separation usually results in pure metal complexes. Pd(II), Cu(II) and Ni(II) form stable complexes. However, the Ag(I) need axial ligands to stabilize the metal complex. The inner aromatic sp2-carbon participates in the coordination with metal ion in the case of Pd(II) and Ni(II), however, in the case of Cu(II), only three core nitrogens participate in the coordination. All adducts were characterized by spectroscopic means. The current metal complexes can be used as catalysts in the various C-C bond forming reactions as well as C-H activations.



M = Pd(II), Ni(II), Ag(I), Cu(II)

R = ethoxy carbonyl, -CN

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non-Aromatic, Expanded meso-Alkylidene Porphyrins: Dibenzo-hexaphyrins Containing Four Exocyclic Double Bonds at meso-Positions

박도우 이가원 이창희*

강원대학교 화학과

We have reported that the meso-alkylidene porphyrins are non-aromatic and show very interesting site-selective protonation depending on the number of core-hydrogen. For example, the compounds containing no core hydrogen are protonated at core nitrogen, but the compounds bearing core-hydrogens are protonated at meso-(α)-position with concomitant hypsochromic shift of the absorption maxima. As a part of our efforts for the construction of the new expanded version of the macrocycles, we here report the synthesis, characterization and spectroscopic properties. The synthesis was accomplished by a typical ‘3+1’ type of the mixed-condensation. Synthesized compounds contain multiple exocyclic carbon-carbon double bonds at meso-positions. The compounds show asymmetric nature in proton NMR spectra, which is a strong indication of the twisted conformation of the molecules. The protonation site upon addition of acid will be extensively discussed.

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Anion binding property of the alkynyl extended, picket calix[4]pyrroles

김진주 하민지 이창희*

강원대학교 화학과

Series of calix[4]pyrroles containing aromatic pickets with various dimensions at crossing meso-positions have been synthesized and characterized. The binding pocket created by the two crossing meso-positions and four pyrrole N-Hs with different dimension is expected to exhibit different affinity and anion selectivity. Anion binding studies confirmed that the synthesized receptors form stable complex with various anions in organic media. The binding affinities are directly related with the distance between aromatic and the meso-carbon. The compounds synthesized here would be good model systems for dimensional probes for the role of the aromatic picket to the binding affinity and the contribution of anion-pi interaction.

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Core-modified analogues of expanded porphyrins containing β,β'-linked o-phenylene bridges

shettivijayendra 이창희*

강원대학교 화학과

Rubyrins are a family of expanded porphyrins containing six pyrrole rings and 26π aromatic system. Due to the conformational flexibility of the individual pyrrole rings, variety of the conformational isomers can exist. The ring flipping usually depends on the degree of protonation and leads to the existence of various conformers, which hampered the systematic studies of these compounds. With these regards, we here report the synthesis and properties of the core-modified rubyrins containing β,β'-linkage that completely restrict the conformational changes. The naphthorubyrin and dithia-naphthorubyrin have been synthesized and characterized by spectroscopic means. The ground state properties of core-modified naphthorubyrins are probed by means of Absorption spectroscopy and electrochemical redox measurements and compared with the normal naphthorubyrin. The role of rigid pyrrole linkage on the structure and properties of these new macrocycles and the possible application of these macrocycles in the area of anion sensing will be described.

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Palladium-Catalyzed Hydrodehalogenation of Aryl Halides Using Paraformaldehyde as the Hydride Source: High Throughput Screening by PBCIS.

변아름 표아영 한민수[1] 이선우

전남대학교 화학과 [1]중앙대학교 화학과

Paraformaldehyde was employed as a hydride source in the palladium-catalyzed hydrodehalogenation of aryl iodides and bromides. High throughput screening by paper-based colorimetric iodide sensor (PBCIS) showed that $Pd(OAc)_2$ and Cs_2CO_3 were the best catalyst and base, respectively. Aryl iodides and bromides were hydrohalogenated to produce the reduced arenes by $Pd(OAc)_2$ and $Pd(PPh_3)_4$ catalyst.

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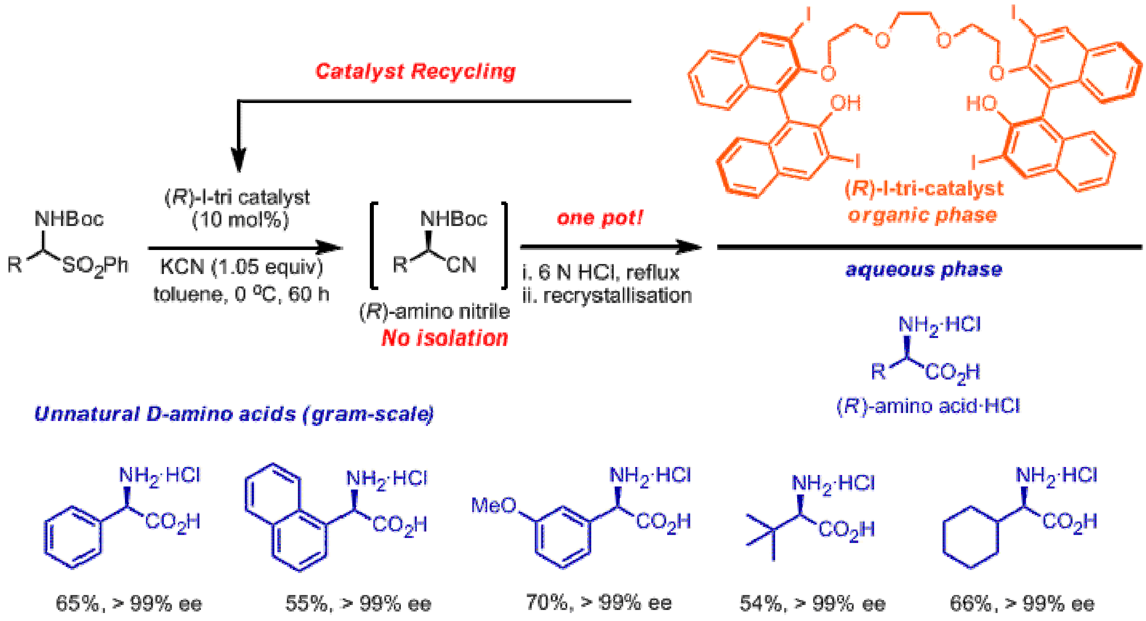
Organocatalytic Asymmetric Strecker Reactions Catalyzed by a Chiral Cyanide Generator: a Practical Route to Enantiomerically Pure α-Amino Acids

오중석 송충의*

성균관대학교 화학과

We have developed a highly efficient organocatalytic Strecker reaction utilizing easily accessible α-amino sulfones as imine precursors and potassium cyanide as a safe cyanide source. By using a highly accessible chiral variant of oligoethylene glycols as a catalyst , and KCN, a chiral cyanide anion could be generated for an asymmetric Strecker reaction. Various α-amido sulfone substrates (alkyl, aryl and heteroaryl) could be transformed to the optically enriched Strecker products, α-amino nitriles, with excellent yields and ees. Moreover, the robust nature of the catalyst toward chemicals enables “one-pot” synthesis of enantiomerically pure α-amino acids starting from α-amido sulfones and easy catalyst recycling; all this can make this protocol easily adaptable to the practical synthesis of unnatural amino acids.


Catalyst Recycling
NHBoc
R
SO2Ph
(R)-I-tri catalyst
(10 mol%)
KCN (1.05 equiv)
toluene, 0 °C, 60 h
NHBoc
R
CN
(R)-amino nitrile
No isolation
one pot!
i. 6 N HCl, reflux
ii. recrystallisation
I
O
O
O
O
I
OH
HO
I
I
(R)-I-tri-catalyst
organic phase
aqueous phase
NH2·HCl
R
CO2H
(R)-amino acid·HCl
Unnatural D-amino acids (gram-scale)
NH2·HCl
CO2H
65%, > 99% ee
NH2·HCl
CO2H
55%, > 99% ee
MeO
NH2·HCl
CO2H
70%, > 99% ee
NH2·HCl
CO2H
54%, > 99% ee
NH2·HCl
CO2H
66%, > 99% ee

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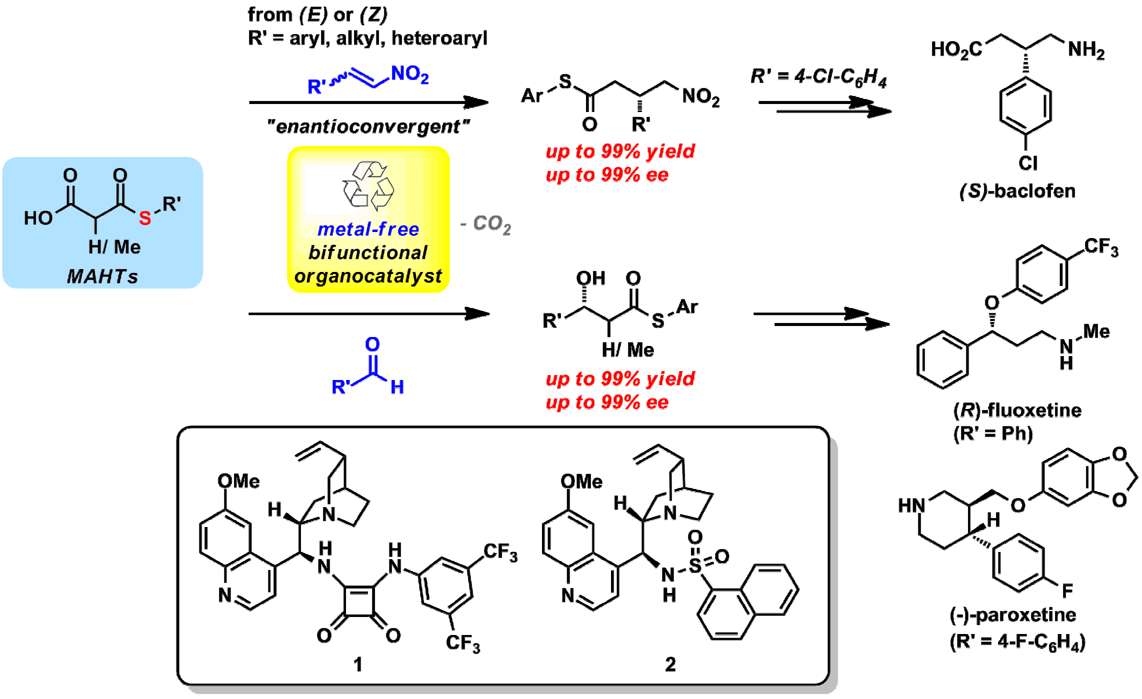
Bioinspired Organocatalytic Reactions using Malonic Acid Half-Thioesters (MAHTs) as Enolate Precursors: From Mimicry of Polyketide Synthases to Scalable Synthesis of Some Pharmaceuticals

배한용 심재훈 박상연 **Ji-Woong Lee[1] Benjamin List[1,*]** 송충의[*]

성균관대학교 화학과 [1]Max-Planck-Institut fuer Kohlenforschung

In this symposium, we present that some cinchona-based organocatalysts 1 and 2 can serve as remarkably effective catalysts for biomimetic organocatalytic reactions using malonic acid half thioesters (MAHTs) as enolate precursors (e.g., up to 99% yield and 99% ee in the Michael reaction of MAHT with nitroalkenes; up to 99% yield and 99% ee in the aldol reaction of MAHT with aldehydes). In addition, the synthetic utilities of these biomimetic protocols are demonstrated in the formal synthesis of some pharmaceutically important compounds. Details of the mechanistic hypothesis and the basis for enantioselectivity will also be presented.


from (E) or (Z)
R' = aryl, alkyl, heteroaryl
R' NO2
"enantioconvergent"
metal-free
bifunctional
organocatalyst
- CO2
HO
O
O
S
R'
H/ Me
MAHTs
Ar
S
O
R'
NO2
up to 99% yield
up to 99% ee
R' = 4-Cl-C6H4
HO2C
NH2
Cl
(S)-baclofen
OH
O
R'
S
Ar
H/ Me
up to 99% yield
up to 99% ee
R'
O
H
CF3
O
N
Me
H
(R)-fluoxetine
(R' = Ph)
HN
O
O
O
H
F
(-)-paroxetine
(R' = 4-F-C6H4)
OMe
H
N
H
N
H
N
CF3
CF3
O
O
N
1
OMe
H
N
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S
O
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H
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2

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Diversification of azaindole with palladium-catalyst coupling reaction

김재원 염을균

충남대학교 화학과

Pyrrolopyridines (azaindoles) have shown attractive attentions as a various bioactive compounds. However, the reported Madelung, Fischer synthesis method of azaindole moiety required harsh reaction conditions such as strong base, high temperature, and limited functional groups. Recently, lots of azaindole compounds showed potent biological activities in literatures. So we tried to diversification of azaindole derivatives for bioactive compounds, Specially, diversification of 3-position at azaindole is quiet limited until now. So we focused palladium catalyzed coupling reaction with Suzuki, Heck , etc ,

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SYNTHETIC METHODS OF MONO AZO COMPOUNDS AND ECOFRIENDLYMONO AZO COMPOUNDS SYNTHESIZED THEREFROM

최우근 이동훈[1,*]

부경대학교 이미지 시스템 공학 [1]욱성화학주식회사 기술연구소

모노 아조 화합물의 제조 방법 및 이로부터 제조되는 친환경 모노 아조 화합물에 관한 것으로서, 환경 위해물질인 PCBs(Poly ChlorinatedBiphenyls), 나프톨(Naphthol) 및 PAA(Primary aromatic amines)의 함량이 낮은 친환경 모노 아조 화합물의 제조 방법 및 이로부터 제조되는 친환경 모노 아조 화합물에 관한 것이다. 본 합성으로 해결하고자 하는 과제는 PCBs, 나프톨, PAA 를 포함하는 모노 아조 안료가 포장재용으로 많이 사용되어 왔으며, 최근 그 규제 물질과규제 범위가 좀 더 명확해지고 좀 더 구체화됨에 따라 모노 아조 안료에서 발생하는 PCBs 를 규정에 맞게 25ppm 이하로 하고, 나프톨도 1% 이하로 하며, PAA 는 500ppm 이하 낮춘 모노 아조 화합물 및 이의 합성 방법을 제공하고자 하는 것이다.

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Aminocarbohydrates Recognition with Cucurbit[7]uril

장윤정 고영호[1] 김기문[*]

포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

Carbohydrates play crucial role in many biological processes. Carbohydrate binding proteins, namely lectins, recognize and bind the carbohydrates with great affinity and selectivity, thus mediate cell-cell adhesion, fertilization, infection and protein transport. Mimicking the carbohydrate recognition, exhibited by natural lectins, with synthetic receptors in water through non-covalent interaction is a great challenge. Such synthetic lectins have potential applications such as biomarkers to detect cancer in early stage, as pharmaceutical inhibitors between cell and pathogens, and many others. Synthetic receptors which bind carbohydrates through non-covalent interactions are scarce, and they rely on laborious, non-trivial and low-yielding synthesis. We have uncovered that cucurbit[7]uril (CB[7]) binds aminocarbohydrates such as galactosamine with excellent affinity and selectivity, as revealed by isothermal titration calorimetry (ITC). Further, 2D NMR studies confirmed that CB[7] stabilizes the α-anomers of the aminocarbohydrates with >99% de through strong host-guest binding. Such supramolecular stabilization of specific anomer is unprecedented. CB[7] also binds several antibiotic aminoglycosides, thus can be used as potential delivery vehicle for them.

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Synthesis of Deoxoartemisinin-chalcone hybrids for anticancer activities

고유진 민동국 정만길*

연세대학교 화학과

The chalcone constitutes a biologically important group of natural products and serve as precursors for the synthesis of different classes of various flavonoids, which are common substances in plants that have an array of biological activities such as brain dysfunction, cancer, infection and cardiovascular risk. Non acetal-type derivatives at C-12 of artemisinin have also been reported to have anti-angiogenic activity. We recently reported that 12β (C?C)-type artemisinin show strong anti-angiogenic activity. In this study, we have synthesized new deoxoartemisinin-chalcone hybrid compounds for anticancer activities.

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Direct one-pot synthesis of naphthoxindoles via Suzuki-Miyaura coupling/aldol condensation cascade reaction

박경용 허정녕[1,*]

충남대학교 신약전문대학원 [1]한국화학연구원 의약화학연구센터

The oxindole scaffold is the common core of a large family of alkaloids and medicinally relevant compounds. A direct one-pot synthesis of naphthoxindoles via a Suzuki-Miyaura coupling/aldol condensation cascade reaction of 4-bromo-1-methyl-oxindole with 2-formylphenylboronic acid has been developed. The reaction in the presence of a palladium catalyst and a base provided a biaryl intermediate, which underwent in situ cyclization to afford the corresponding naphthoxindole in high yield. Especially, the counterion of the base plays a critical role in the efficiency of the coupling process.

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Selective fluorescence sensing of salicylic acid by a cooperative π-π and hydrogen bond interactions

김보연 김홍석

경북대학교 응용화학과

The recognition of both mono- and dicarboxylic acids by a large number of receptors of different architectures is known. In relation to this, imidazole as a binding motif is less explored in carboxylic acid recognition. To explore the imidazole receptor further we have reported a series of steroid-based imidazole receptors for aliphatic carboxylic acids.A pyrene appended imidazole sensor (1) has been synthesized for the sensing of salicylic acid (SA) derivatives. The sensing ability of 1 toward various salicylic acid derivatives has been examined by UV-vis and fluorescence spectroscopy. The sensing of salicylic acid derivatives resulted in significant monomer emission. Sensor 1 showed the highest binding constant with 5-nitrosalicylic acid among all the tested salicylic acid derivatives ($K_a = 7.18 \times 10^4 M^{-1}$). 5-Nitrosalicylic acid formed a complex with 1 in 1:1 ratio in EtOH.

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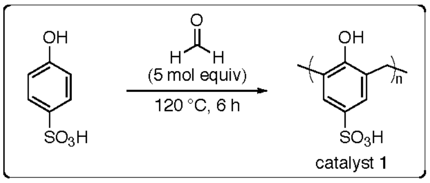
Direct Esterification with a Mesoporous Phenol Sulfonic Acid-Formaldehyde Resin Catalyst

백희열 Maki Minakawa[1] Yoichi M. A. Yamada[1,*] 한진욱 Yasuhiro Uozumi[2,*]

한양대학교 화학과 [1]RIKEN, Wako, Saitama [2]RIKEN, Wako, Saitama, Institute for Molecular Science (IMS), Okazaki, Aichi

Direct esterification of alcohols with carboxylic acids is an important transformation reaction in organic synthesis. Although several methods have been explored and developed, in most cases, large excess amount of either carboxylic acids or alcohols are required in order to obtain quantitative products. Here, a novel heterogeneous polymer acid catalyst 1 was readily prepared for the direct esterification. Thus, condensation polymerization of p-phenolsulfonic acid with formaldehyde was performed at 120 °C for 6 h to give brownish acid catalyst 1 as hardly soluble precipitates (Eq. 1). The direct esterification of various alcohols (Eq. 2) and carboxylic acids (Eq. 3) was carried out with 3 mol% (SO3H residue) of 1 at 50-80 °C under solvent-free conditions without removal of water to afford the corresponding esters in 91-95% isolated yield. Moreover, direct lactonization of hydroxycarboxylic acids with the polymeric acid catalyst 1 will be discussed in this poster session.

Preparation of Polymeric Acid Catalyst



catalyst **1**

(1)

Direct Esterification

$$R^1\text{-OH} \quad + \quad \underset{1.2\text{ mol equiv}}{\text{AcOH}} \quad \xrightarrow[\text{50-80 °C, 12 h}]{\text{catalyst 1 (3 mol\%)}} \quad R^1\text{-OAc} \tag{2}$$

R^1 = $CH_3(CH_2)_7$: 92%, $CH_3(CH_2)_9$: 92%, $CH_3(CH_2)_{11}$:93%, $C_6H_5CH_2$: 94%, $C_6H_5(CH_2)_2$: 93%,
$C_6H_5(CH_2)_3$: 93%, $CH_3CH(CH_2)_5CH_3$: 94%, $(CH_2)_5CH$: 94%, $(CH_2)_7CH$: 91%

$$R^2\text{-COOH} \quad + \quad \underset{5.0\text{ mol equiv}}{\text{MeOH}} \quad \xrightarrow[\text{50-60 °C, 12 h}]{\text{catalyst 1 (3 mol\%)}} \quad R^2\text{-COOMe} \tag{3}$$

R^2 = $CH_3(CH_2)_6$: 94%, $CH_3(CH_2)_8$: 95%, $CH_3(CH_2)_{10}$:93%, $CH_3(CH_2)_{14}$: 95%, $CH_3(CH_2)_{16}$: 94%,
$CH_3(CH_2)_7CH{=}CH(CH_2)_7$: 93%

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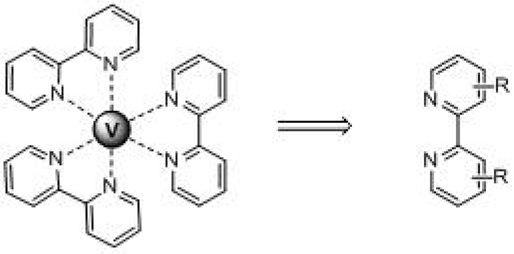
Development of Bipyridine Ligand Derivatives for Vanadium: Application for Redox Flow Battery

김은선 안철진*

창원대학교 화학과

The vanadium redox flow battery is a type of rechargeable flow battery that employs vanadium ions in different oxidation states to store chemical potential energy. Current production vanadium redox batteries achieve an energy density of about 25 Wh/kg of electrolyte. To improve the energy density, we try to prepare vanadium complex including bipyridine ligand. In this paper, we will present the efficient preparation of various bipyridine derivatives.



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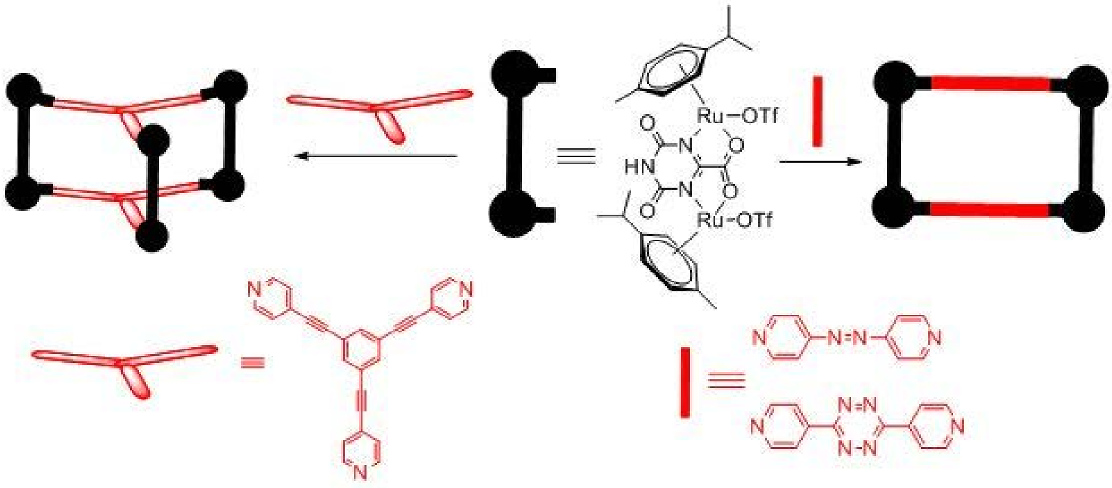
Tetranuclear (2D) and Hexanuclear (3D) Self-Assemblies Based on Half-Sandwich Ruthenium(II) Complexes

DUBEY ABHISHEK 송영호 지기환

울산대학교 화학과

To effect and maintain biological functions, natural systems assemble a variety of specialized supramolecular nanostructures from multiple subunits with high efficiency. In the past two decades, coordination-driven self-assembly has emerged as an effective tool for constructing functionalized metalla-supramolecules with the aim of better understanding and mimicking their biological analogues. It has been well demonstrated that two-dimensional (2-D) macrocycles and three-dimensional (3-D) cages can form by the self-assembly of molecular subunits encoded with specific directional information (controlling their sizes and shapes) and appropriate chemical functionalities (tuning their physical and chemical properties). Such functionalized metallosupramolecules lend themselves to various applications, from supramolecular catalysis to chemical sensing, biological studies and host-guest chemistry.



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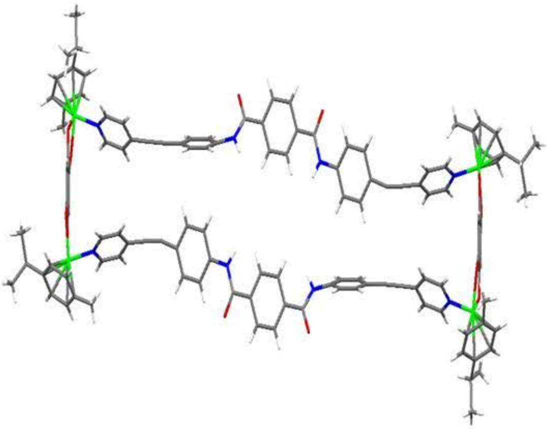
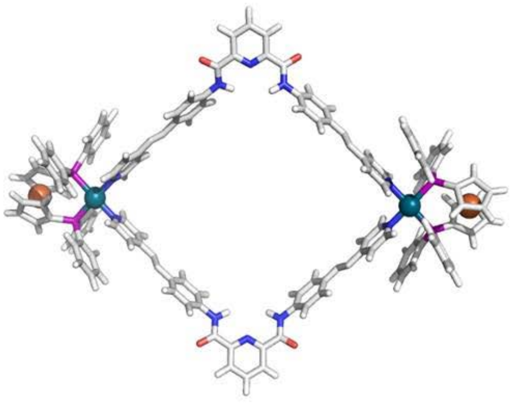
Fullerene binding study by supramolecular metallacycles self-assembled with N-donor ligands and different metal acceptors

ANURAG MISHRA 이승창 지기환

울산대학교 화학과

The coordination-driven self-assembly of metallacyclic structures has attracted interest for promising applications in molecular recognition, separation, catalysis, encapsulation of guests and biological systems. The present work demonstrates the coordination behavior of N donor ligands with different functionality (ferrocene and arene) to synthesized new self-assembled supramolecular metallacycles. These complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. The crystal structures of these complexes show that the metal ion coordinate between two nitrogen containing donor ligands. These self-assembled metallacycles were further explored Fullerene binding study. The poster will address a detail comprehensive account of the mentioned work.





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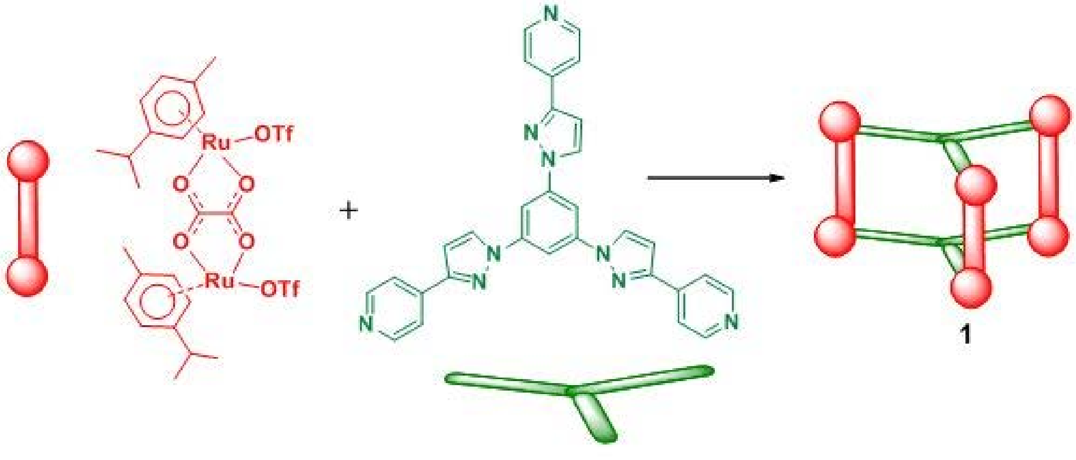
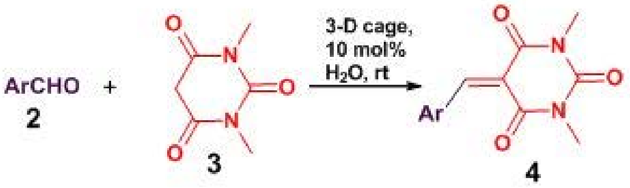
Cage-Catalyzed Knoevenagel Condensation under Neutral Conditions in Water

DUBEY ABHISHEK 민진욱 지기환

울산대학교 화학과

A cationic coordination cage 1 dramatically accelerates the Knoevenagel condensation of aromatic aldehydes 2 in water under neutral conditions. The addition of a nucleophile 3 to the aldehyde to generate anionic intermediates seems to be facilitated by the cationic environment of the cavity. The products are ejected from the cage as a result of the host?guest size discrepancy. As a result, the condensation is promoted by a catalytic amount of the cage.





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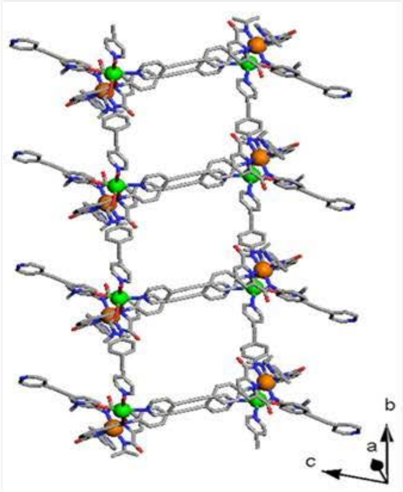
Luminescent metal-organic frameworks for highly sensitive and selective detection of Hg^{2+} ion

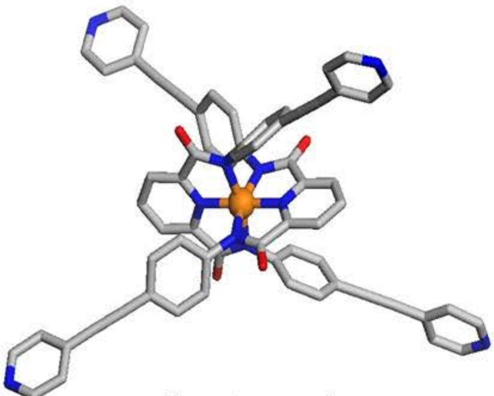
ANURAG MISHRA 조재호 지기환

울산대학교 화학과

Luminescent metal-organic frameworks (MOFs) with one-, two-, and three-dimensional (1D, 2D, and 3D) networks are of great current interest due to their potential applications in fluorescent sensors. Through constructing well-designed MOFs, some intriguing examples with remarkable luminescence selectivity have been reported. However, it was found that most complexes reported to date were heavily dependent on the special pore sizes or open metal sites. Moreover, the luminescent behavior of a MOF is highly dependent on the organic ligand and metal ion. Hence, enhanced performance can be achieved by careful selection of the organic building block and the nature of the metal. Herein, we report ethynyl pyridine amide based two different structural cobalt complexes. The discrete complex show enhanced levels of selectivity and very strong sensitivity of Hg^{2+} ion, while other ions such as K^{+}, Mg^{2+}, Ca^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, and Cd^{2+}, do not show any notable effects.



1 D coordination complex



discrete complex

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Direct Asymmetric Aldol Reactions Co-catalyzed By (L)-Proline and Isothiouronium Salts Under Solvent-free Conditions.

조은 김택현[1]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

The direct asymmetric aldol reaction is a powerful C-C bond-forming transformation in organic chemistry. Among asymmetric catalytic methods, the proline-catalyzed version, which proceeds via in situ generated enamine intermediates, has attracted much attention, since it affords aldol products with a high level of selectivity under very mild reaction conditions. Isothiouronium salts have been explored as prospective replacements of thioureas in the area of the anion binding to enhance the acidity of the NH moieties and allow more hydrogen bonding. Considering the probed ability of isothiouronium salts in anion recognitions, we contemplated the possibility of using isothiouronium salts as new additives in the aldol reactions. The combined activity of (L)-proline and an achiral isothiouronium salt allow direct aldol reactions to be carried out with high diastereoselectivity and enantioselectivity (up to 99.5 : 0.5) under solvent-free conditions with a rather simple reaction setup.

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Non-cross-linked polystyrene supported 2-imidazolidinone chiral auxiliary: synthesis and Asymmetric alkylation reations

강병선 김택현[1]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

Chiral auxiliary-derived asymmetric alkylations have been extensively studied and are now important and general methods for asymmetric carbon-carbon bond formation. 2-imidazolidinone chiral auxiliary has been proven as a powerful tool for the asymmetric synthesis of highly pure compounds used in pharmaceuticals or agrochemicals. Soluble polymer supports allow expeditious transfer of solution-based synthetic protocols, circumventing the extensive optimization process often required in heterogeneous reactions. In this study, asymmetric alkylation reactions using the non-cross-linked polystyrene(NCPS11)-supported 2-imidazolidinone chiral auxiliaries will be introduced with high stereoselectivity and yields. In addition, the good recycling of our chiral auxiliaries will be discussed.

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Development of Cysteine selective probes

하수라 이희윤*

한국과학기술원(KAIST) 화학과

In order to understand the role of cysteine oxidation in biological system, it is important to analyze cysteine levels in proteins. To this end, we focused on capturing the cysteine in thiol stage before oxidized. General cysteine capture probes, Iodoacetamide(IAA), N-ethylmaleimide(NEM) capture not only cysteine but also sulfenic acids and carbon, nitrogen nucleophiles. These are not selective probes to analyze the cysteine. To overcome the problem of general electrophilic probes, IAA and NEM, we designed and synthesized the new probes to capture only the unmodified cysteines.

NosP1 (Nosyl piperidine) has a specific electrophile for thiols. The probe showed only to capture the free thiols in the model thiol system and cysteine analogs. Based on these result, biotinylated probes were prepared and tested on the various peptides for oxidation sites and oxidation level of cysteines in proteins.

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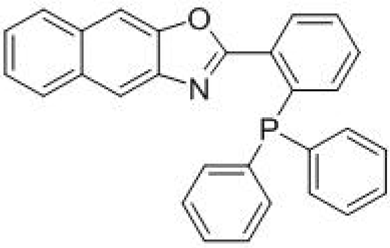
OLED Property of 2-(2-(Diphenylphosphino)phenyl)naphtho[2,3-d]oxazole (PPN) as Blue-Emitting Material

김익환 강은국 이범종[1,*]

인제대학교 화학과 [1]인제대학교 의생명화학과

In the course of investigation for finding new light-emitting materials based on the phosphino-oxazole structure, we have employed 3-amino-2-naphthol and 2-(diphenylphosphino)benzoic acid as starting materials for synthesizing 2-(2-(diphenylphosphino)phenyl)naphtho[2,3-d]oxazole (PPN). The chemical structure of PPN was determined by ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-Vis and elementary analysis (EA). Photoluminescence (PL) and electroluminescence (EL) of PPN were respectively characterized. PPN shows a strong blue emission under excitation by UV-lamp of 365nm. The PPN also shows blue PL emission around 441nm in chloroform solution. Two different OLED devices were fabricated with the structure of ITO / NPB[50nm] / PPN[50nm] / Liq[0.5nm] / Al[120nm] and ITO / NPB[50nm] / PPN[50nm] / Alq3[15nm] / Liq[0.5nm] / Al[120nm]. The electroluminescence (EL) of the devices showed a green emission with the maximum wavelength of 498nm.



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Practical and Versatile Synthesis of Thioflavones from 2-Bromobenzoic Acids

최진선 송윤주[1] 홍효정 이재인

덕성여자대학교 화학과 [1]덕성여자대학교 건강기능신소재

Thioflavones are of current interest due to their pharmacological activities such as antibacterial, antimicrobial, and anticancer effects. A synthetic route of thioflavones from 2-bromobenzoic acids is described. The treatment of 2-bromobenzoic acids with oxalyl chloride in the presence of pyridine afforded 2-bromobenzoyl chlorides, which were acylated with half equiv of 4,6-dihydroxypyrimidine in the presence of triethylamine to give 4,6-pyrimidyl di(2-bromobenzoates). These activated esters were reacted with (hetero)arylethynylmagnesium bromides to afford 1-(2-bromophenyl)-3- (hetero)aryl-2-propyn-1-ones. The resulting alkynones were treated with sodium hydrosulfide in EtOH to form unsaturated thiolate adducts, which underwent subsequently intramolecular nucleophilic substitution at reflux to give thioflavones in high yields.

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Novel Synthetic Methodology to Fullerene Derivatives Using SET-Promoted Photoaddition Reactions of Fullerene Acceptor-α-Silyl tert-Amine Donor.

유현지 김지나 윤웅찬*

부산대학교 화학과

The exploration of fundamental and applied aspects of fullerene (C_{60}) has gained intense interest and a large number of fullerene derivatives containing an array of functionalities have been synthesized in recent years[1]. Fullerene has low solubility in common organic solvents, which makes handling in solution processing during device fabrication difficult. The recent efforts in this area have shown that structural modifications, made by introducing of a variety of substituents on the fullerene moiety, lead to increases in the energies of the fullerene LUMO level and solubilities in organic solvents. Our past studies led to the discovery that single electron transfer (SET) induced photochemical reactions of α-silyl electron donors generate α-carbon radical in a highly chemoselective and regioselective manner. Consequently, this process can be used as a highly efficient methodology to generate useful molecular targets. In a recent investigation, we have used this SET-photochemistry as the foundation for the development of a novel and efficient methodology to prepare new functionalized fullerenes. In this effort, we observed that fullerene, serving as an electron acceptor, undergoes high yielding photoaddition reactions when irradiated in the presence of α-silyl-tert-amines to produce 1,2-adducts, 1-(diakylamino)methyl-2-hydrofullerenes α-silyl in toluene-methanol solvent. The new SET process produces 1,2-adducts between fullerene and α-silyl tert-amines in short reaction times (5 min) and in high chemical yields (>62%), in contrast to photoaddition reactions employing non-silicon containing aromatic[2(a)] and non-aromatic tertiary amines[2(b)], and other types of donors[2(c)]. Moreover the reverse of these reaction does not occur to regenerate fullerene when the α-aminofullerene adducts are irradiated. Additional details of this study will be discussed in the poster presentation session.

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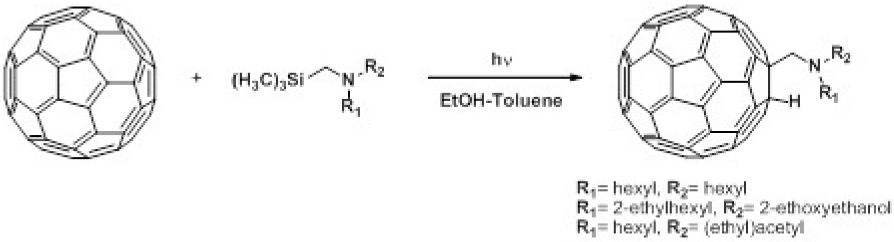

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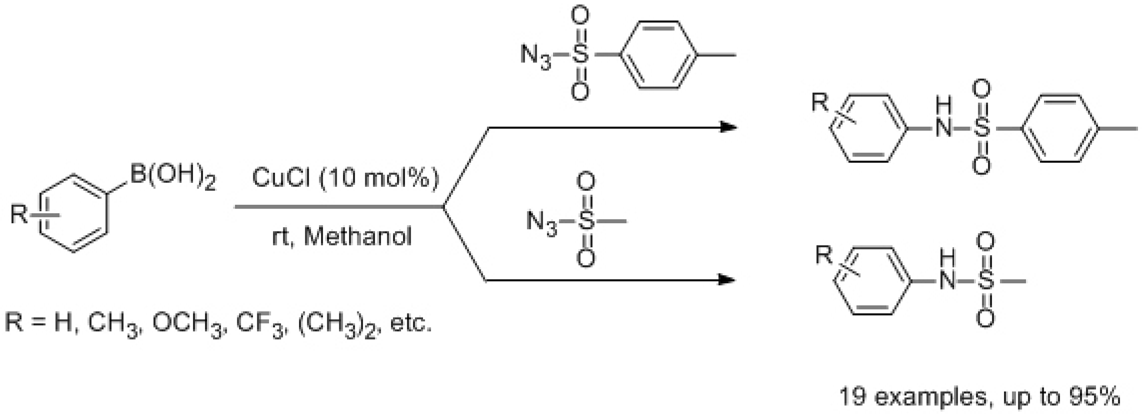
A New Approach to the Synthesis of N-Aryl Sulfonamides

남정수 문수연[1] 김원석[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 첨단유기합성연구실 [2]이화여자대학교 화학나노과학과

The copper-catalyzed coupling of arylboronic acids with sulfonyl azides has been employed for the synthesis of N-aryl sulfonamides. The use of this method avoids the potential mutagenic byproducts that can occur from the aniline and the sulfonyl chloride. Importantly, in the presence of 10 mol% of CuCl, a variety of arylboronic acids were transformed into N-aryl sulfonamides at room temperature without the use of any base, ligand or additive.



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A Novel Synthesis of 1-Alkyl-2-phenyl-4-quinolones from 2-Halobenzoyl Chlorides

송윤주 최진선[1] 이재인[1]

덕성여자대학교 건강기능신소재 [1]덕성여자대학교 화학과

1-Alkyl-2-phenyl-4-quinolones are distributed in the plant family Rutaceae and have attracted attention due to their antibacterial and antitumor activities. A synthetic route of 1-alkyl-2-phenyl-4-quinolones from 2-halobenzoyl chlorides is described. The benzoylation of half equiv of 4,6-dihydroxypyrimidine with 2-halobenzoyl chlorides in the presence of triethylamine afforded 4,6-pyrimidyl di(2-halobenzoates), which were reacted with (hetero)arylethynylmagnesium bromides to give 1-(2-halophenyl)-3-(hetero)aryl-2-propyn-1-ones. These alkynones were treated with primary amines to afford 1-(2-halophenyl)-3-phenyl-3-(N-alkylamino)-2-propyn-1-ones in situ by 1,4-addition, which were further converted to 1-alkyl-2-phenyl-4-quinolones with sodium hydride in refluxing DME in high yields.

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Rhodium-Catalyzed Oxygenative Addition of Alcohols and Amines to Terminal Alkynes for the Synthesis of Esters and Amides

김인수 이철범*

서울대학교 화학부

A rhodium-catalyzed reaction has been developed, in which terminal alkynes undergo an oxygenative addition with alcohols and amines to produce the corresponding esters and amides as the products. In this process, the rhodium vinylidene generated from a terminal alkyne is converted to a rhodium ketene complex by oxygen transfer from sulfoxides or N-oxides. Subsequently, the addition of nucleophiles such as alcohols and amines to the ketene complex gives esters and amides. Mechanistic studies suggest that the catalytic reaction involves the formation of a rhodium ketene complex via the oxidation of the metal-bound unsaturated carbene.

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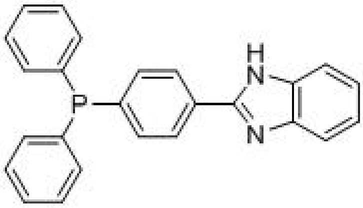
Synthesis and PL Property of 2-(4-(Diphenylphosphino)phenyl)-1H-benzo[d]imidazole (DPI)as Blue-Emitting OLED material

강은국 김익환 이범종[1,*]

인제대학교 화학과 [1]인제대학교 의생명화학과

We have designed and synthesized a novel blue-emitting OLED material based on the phosphino-benzimidazole structure. 2-(4-(Diphenylphosphino)phenyl)-1H-benzo[d]imidazole (DPI) was synthesized from o-diaminobenzene and 4-(diphenylphosphino)benzoic acid. Polyphosphoric acid (PPA) was employed straightforward as solvent and catalyst for the cyclization reaction. The chemical structure of DPI was determined by ^{1}H-NMR, ^{12}C-NMR, FT-IR and UV-vis. The DPI showed a strong blue emission under excitation by UV-lamp of 365 nm. The photoluminescence (PL) property of DPI will be discussed.



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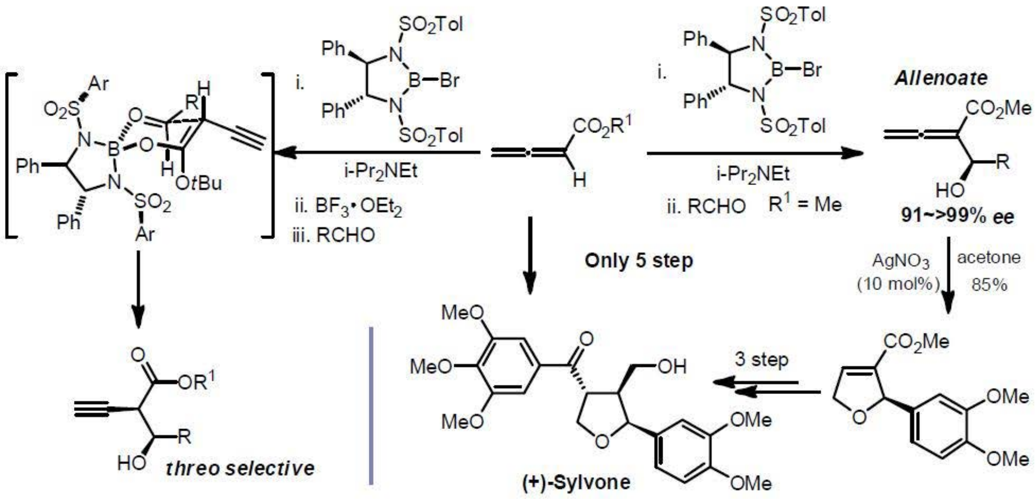
Highly Diastereo- and enantioselective Aldol Reaction of Allenoates with Aldehydes for the Synthesis of Alkynyl Aldol Adduct

김현아 방지윤 유찬모*

성균관대학교 화학과

Recently, we have developed a new aldol method of the allenoate process in forming 2-hydroxy allenoate in high levels of enantioselectivity. In light of this progress, we turned our attention to achieve alkynyl addut without isomerization to allenyl ester. After conversion of allenoate to borone enolate in the presence of chiral bromoborane complex, 1 equivalent of trifluoroborane etherate complex followed by aldehyde resulted in the formation of alkynyl aldol adduct without any allenyl species. We would like to present herein the scope of reaction, stereoselectivity, and its applications.


SO2Tol
Ph
N
B—Br
Ph
N
SO2Tol
i.
i-Pr2NEt
ii. BF3• OEt2
iii. RCHO
CO2R1
H
i.
i-Pr2NEt
ii. RCHO R1 = Me
Allenoate
CO2Me
R
HO
91~>99% ee
O2S
Ar
N
B
O
R
H
Ph
N
H
OtBu
Ph
SO2
Ar
O
OR1
R
HO
threo selective
Only 5 step
AgNO3
(10 mol%)
acetone
85%
CO2Me
O
OMe
OMe
3 step
MeO
MeO
MeO
O
OH
O
OMe
OMe
(+)-Sylvone

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The Investigation of Chemoselective O-Acylation of β-mercaptoalcohols with Acid Chloride Derivatives

장지성 김예진 안철진*

창원대학교 화학과

Molecules including free -SH are important to prepare gold nanoparticle(GNP) encapsulating with organic ligand. The selective O-acylation of mercaptoalcohols is synthetically important to prepare the organic compounds with free -SH. In this paper, the investigation to the chemoselective O-acylation of β-mercaptoalcohols with acid chloride derivatives is reported.

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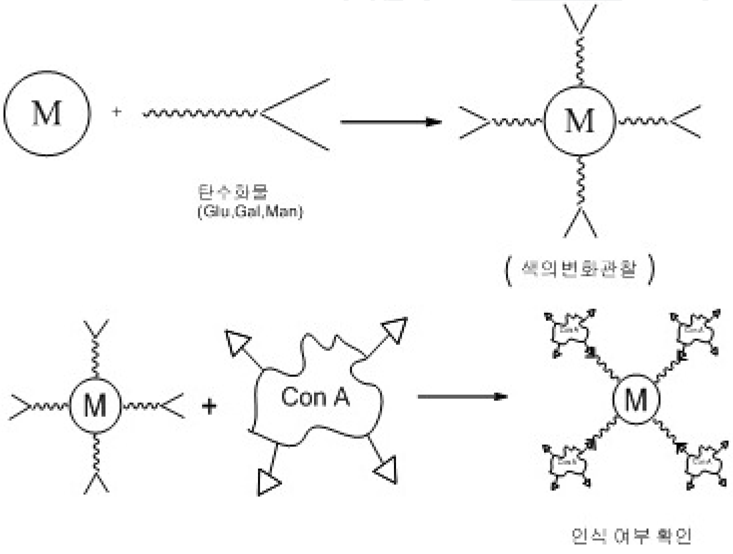
The Preparation of Vanadium(V) or Molybdenum(Mo) Complexes of Carbohydrates and Their Recognition of Con A

김기우 안철진*

창원대학교 화학과

Although in recent years an increasing amount of data regarding the interaction of vanadium or molybdenum species with carbohydrate has been accumulated, information regarding these complexes remains relatively scarce.In our lab, we have investigated the interaction of the vanadium or molybdenum with carbohydrates and the recognition of Con A with these vanadium or molybdenum complexes containing carbohydrates.



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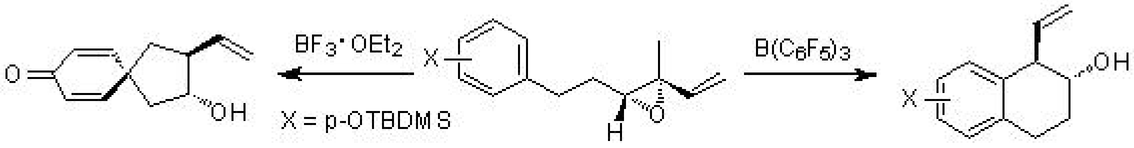
Dearomatizative Cyclization of Vinyl Oxiranes through Fridel-Crafts Type Reaction by Lewis Acid Catalysis

최미라 유찬모

성균관대학교 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of Lewis acid catalysts are some of the most attractive methodologies. A highly diastereoselective synthesis of trans adduct is achieved from the reaction of vinyl oxiranes with 10 mol% of tris(pentafluorophenyl)borane as a Lewis acid catalyst, whereas dearomatized product is formed from para-hydroxyl derivatives by trifluoroborane etherate complex. The method described herein is successful with various substrates in good yields and high levels of diastereoselectivity.



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Palladium-Catalyzed Synthesis of (*Z*)-3-Arylthioacrylic Acids and Thiochromenones

Thiruvengadam Palani 최주석 송광호[1,*] 이선우[*]

전남대학교 화학과 [1]고려대학교 화공생명공학과

1-Alkenyl sulfides are important intermediates in the synthesis of organic and polymeric materials due to their ease of transformation and are key structure units in natural products and biologically active compounds. Recently, we reported on transition-metal-catalyzed C-S bond formation using sulfur surrogates and a variety of the coupling reactions of propiolic acid. As an expansion of these methodologies, we envisioned that the combination of two concepts would provide an efficient method for the synthesis of stereoselective 1-alkenyl sulfide. Three-component reaction of aryl halide, Na_2S?$5H_2O$, and propiolic acid in the presence of 2.5% $Pd(PPh_3)_2Cl_2$, 5% 1,4-bis(diphenylphosphino)-butane (dppb) and 2 equiv. of 1,8-Diazabicyclounde-7-ene (DBU) produced stereoselectively (*Z*)-3-arylthioacrylic acids in good yields. Study of the reaction pathway suggested that the C-S bond formation of aryl halides and Na_2S?$5H_2O$ proceeded first, and the resulting intermediate reacted with propiolic acid to produce the desired product. We found that Na_2S?$5H_2O$ has key role in the highly stereoselective formation of (*Z*)-isomer. In addition, when the resulting product was treated with acid, the desired thiochromenones were formed in good yields.

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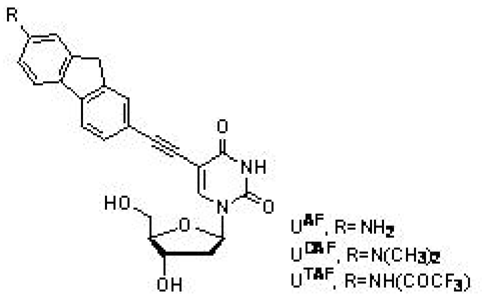
Synthesis and photophysical properties of 2'-deoxyuridine labeled with fluorene derivatives

이지원 황길태*

경북대학교 화학과

To monitor microenvironment in a cell, various methods have been proposed. Among these, fluorescent probes are very attractive because they are simple and sensitive. In this study, we utilized fluorene derivatives which have moderate quantum yields and are less bulky than other commonly used fluorophores. We synthesized 5-(2-amino-7-ethynyl)-2’-deoxyuridine (UAF), 5-(2-dimethylamino-7-ethynyl)-2’-deoxyuridine (UDAF), and 5-(2-ethynyl-7-trifluoroacetylamino)-2’-deoxyuridine (UTAF). To investigate the photophysical characterization of these fluorescent nucleosides, we measured the fluorescent spectra in various pH buffer solutions.



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Bis(carbazoyl arylamine)과 fluorenyl arylamine group을 갖는 OLED 전공수송층 arylamine 합성

백승지 채규윤* 이덕희[1,*] 김보미 백오현

원광대학교 화학과 [1]원광대학교 생명나노화학과

단일 starburst 에 기존의 물성이 좋은 것으로 알려진 spiro 와 fluorene 화합물을 도입시켜 높은 유리전이온도를 갖는 starburst 유도체를 합성한 후 수명이 긴 OLED 전공수송층 소재를 개발하고자 한다. 본 실험에서는 C-C coupling 을 위하여 Suzuki, Heck/Negishi, Kumada 반응을 이용할 것이며, 그 외에도 amination, witting reaction 을 이용하고자 한다. 고순도 화합물을 분리하기 위해서는 recrystallization, chromatography, sublimation, hot filtration 을 이용할 것이다.

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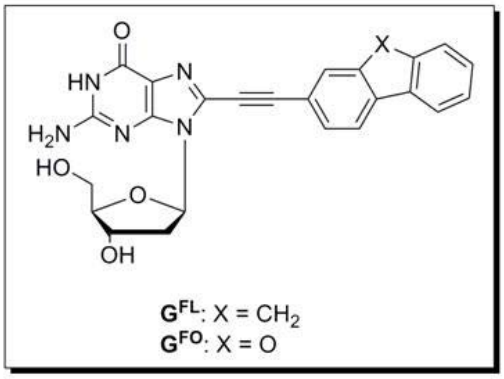
Synthesis and Properties of Fluorescent Oligonucleotides Containing Fluorene- and Fluorenone-Labeled 2'-Deoxyguanosine

김민지 황길태*

경북대학교 화학과

Nucleotides bearing a fluorophore have a wide range of biotechnological applications such as biomarkers for structural studies of nucleic acids, charge generators for DNA electronics, sequencing, and detection of infections and genetic diseases. In particular, we are interested in fluorophore-labeled 2′-deoxyguanosine (G) because it has the lowest oxidation potential among the four nucleotides and hence forms G oxidative products. Although numerous 8-arylethynylated G derivatives have been reported, they may not be applicable to the general use as fluorescent probes.In order to understand the charge transfer process and fluorescent changes in oligonucleotides containing a fluorescent G as a result of duplex formations, we designed fluorene- and fluorenone-labeled G (GFL and GFO) by Sonogashira coupling of 2-ethynylfluorene and 2-ethynylfluorenone with 8-bromo-G derivative, respectively and incorporated it into a central position in the oligonucleotide. Further, we placed the different nucleotides at both the subsequent nucleotide positions of GFL and GFO in order to examine the effects of flanking bases (FBs) on the fluorescence changes. The photophysical properties of GFL and GFO DNAs will be described in detail.



Probes ODN1(N) : 5'-d(TGG ACT **NXN** TCA ATG)-3'
(**X** = $\mathbf{G^{FL}}$ or $\mathbf{G^{FO}}$, **N** = A, C, G, or T)

Targets ODN2(N') : 5'-d(CAT TGA T**N'**T AGT CCA)-3'
ODN3(N') : 5'-d(CAT TGA G**N'**G AGT CCA)-3'
ODN4(N') : 5'-d(CAT TGA C**N'**C AGT CCA)-3'
ODN5(N') : 5'-d(CAT TGA A**N'**A AGT CCA)-3'
(**N'** = A, C, G, or T)

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Development of Macromolecular Therapeutics for the Treatment of Retinal Diseases

유수연 정혜원[1] 김윤경*

한국생명공학연구원 단백체의학연구센터 [1]건국대학교 의학전문대학원/안과

Age-related macular degeneration (AMD) is the deterioration or breakdown of the macular structure in the eye which is a part of the retina responsible for central vision. AMD is the No.1 cause of vision loss and blindness for people over 50 years old in the industrialized world. Of the two types of AMD, the “wet” AMD is characterized by the growth of abnormal blood vessels in the choroid, inducing leakage of blood and fluid to damage the macula. Currently, the most favorable treatment for wet AMD is the intravitreal injection of the anti-vascular endothelial growth factor (VEGF) agents. These drugs can result in regression of the abnormal blood vessels in the retina. However, the current anti-VEGF therapy has limitations such as unwanted side effects, high cost, and inconvenience for the patients during administration. Here, in an effort to develop longer lasting, more effective, cheaper, and less painful treatment for AMD, polyamidoamine (PAMAM) dendrimers of robust size and shape were adopted as drug carriers. Specifically, we synthesized eight fluorescently labeled dendrimers with different biocompatible surface groups in order to systematically compare and find the optimal surface modification that can facilitate the penetration of the intravitreally injected macromolecular drugs into the diseased retinal layer. Interestingly, our preliminary intravetreal injection results showed that the carboxylate-terminated PAMAM dendrimer conjugate has penetrated efficiently into the retinal pigment epithelium (RPE) layer as analyzed by the confocal fluorescence images of the cryosectioned eye of a mouse. We envision that this study would provide valuable information in designing advanced macromolecular therapeutics for the treatment and diagnosis of AMD.

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Naphthalene 과 fluorene 유도체를 갖는 OLED전공수송층 arylamine 합성

송희정 채규윤* 이덕희[1,*] 송미선 박찬용

원광대학교 화학과 [1]원광대학교 생명나노화학과

Naphthalene 과 fluorene 화합물을 도입시켜 높은 유리전이온도를 갖는 starburst 유도체를 합성한 후 수명이 긴 OLED 전공수송층 소재를 개발하고자 한다. 본 실험에서는 triphenylamine 에 NBS 로 선택적 bromination 한 후 fluorenyl boronic acid 와 naphthalenyl boronic acid 를 반응시켜 fluorenyl naphthalenyl amine 을 합성하고자 한다.C-C coupling 을 위하여 Suzuki, Heck/Negishi, Kumada 반응을 이용할 것이며, 그 외에도 amination, witting reaction 을 이용하고자 한다. 고순도 화합물을 분리하기 위해서는 recrystallization, chromatography, sublimation, hot filtration 을 이용할 것이다.

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Improving Tumor Targeting Efficiency of Multivalent Dendritic Ligands for In Vivo SPECT Imaging by Modulating Inner Surface Groups

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한국생명공학연구원 단백체의학연구센터, 한국과학기술원(KAIST) 화학과 [1]한국과학기술원(KAIST) 화학과 [2]한국생명공학연구원 단백체의학연구센터

Dendrimers are made from branched monomers (e.g., AB_2 type) and a central core unit, both of any chemical functionalities, to have a treelike structure. Of many kinds of dendrimers reported to date, polyamidoamine (PAMAM) dendrimers have been widely used for biological applications. Diagnostic nuclear medicine imaging such as single photon emission computed tomography (SPECT) and positron emission tomography (PET) uses radioactive tracers which provide superior image contrast even under microdosing conditions. SPECT imaging agents can be made by labeling the precursor ligand with the radioisotope emitting γ-rays, and usually they have longer half-lives compared to PET agents. In this study, we prepared six ^{125}I-labeled multivalent ligands as new dendrimer-based SPECT tracers for effective tumor diagnosis. Specifically, multiple copies of cyclic RGDfK (c(RGDfK)) peptide, a selective binder at the $\alpha_V\beta_3$ integrin receptor overexpressed in angiogenesis, were attached to the surface of the dendrimer through a long polyethylene glycol (PEG) spacer, as well as tin species (precursor for radiolabeling) and a fluorophore. Here, the remaining bulk of the dendrimer surface was modified to have different functionalities that would vary in overall surface charge, hydrodynamic diameter, and biopermeability. In vitro binding assay at cancer cells using [^{125}I]echistatin as a radioligand and *in vivo* SPECT and optical imaging using mouse tumor models are being carried out to determine the tumor targeting efficiency of our compounds. We anticipate that exquisite tuning of inner surface groups of multivalent RGD ligands for effective tumor targeting may significantly improve the diagnostic sensitivity of SPECT imaging agents.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Benzothiadiazole-centered donor materials for organic photovoltaic cells

전용준 홍종인*

서울대학교 화학부

Since the first report of organic solar cells (OSCs) by Tang, the development of OSCs has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene were used as donor materials for heterojunction solar cells due to good charge transport ability. A benzothiadiazole unit was used as low band gap donor materials due to their broad absorption spectra.To improve performance of heterojunction solar cells, we introduced new low bandgap donor materials, consisting of benzothiadiazole, naphthalene, benzothiophene and thiophene. Details of the synthesis, photophysical, electrochemical and theoretical studies and device data will be presented.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An Efficient Synthetic Method for Propargylamines from Alkyne Carboxylic Acids.

박경호 이선우*

전남대학교 화학과

The decarboxylative multi-component reaction of aldehydes, amines and alkyne carboxylic acids for synthesizing of propargylamines has been developed. The reaction of various substitution of alkyne carboxylic acids were successfully coupled for this reaction. The arylpropiolic acids were synthesized from aryl iodides or aryl bromides with propiolic acid by using efficient palladium catalyzed Sonogashira reaction.

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Pyrene End-Capped Donor Materials based on Benzothiadiazole and Thiophene for Efficient Heterojunction Solar Cells

권종철 홍종인*

서울대학교 화학부

Since the first report of heterojunction solar cells by Tang, the development of heterojunction solar cells has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene, benzothiadiazole, and pyrene were commonly used as organic semiconductors due to good charge transport ability.In this study, we reported new organic donor materials (BP-1 and BP-3), consisting of oligothiophene, benzothiadiazole, and pyrene, as donor materials for heterojunction solar cells. Fabricated heterojunction solar cell devices based on BP-3 exhibited a power conversion efficiency of 3.2%, under simulated AM 1.5 solar irradiation at 100 mWcm-2.

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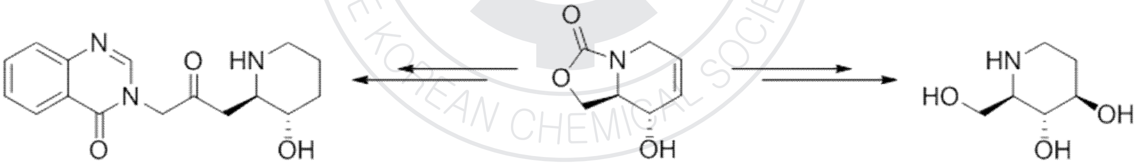
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of (+)-Febrifugine and (D)-Fagomine

정재훈* 하현준 이원구[1]

한국외국어대학교 화학과 [1]서강대학교 화학과

(+)-Febrifugine is a quinazolinone alkaloid isolated Dichroa febrifuga and has antimalarical properties. D-Fagomine was isolated from the seed of buckwheat Fagopyrum esculentum Moech and has antihyperglycemic effect in streptozocin-induced diabetic mice. We synthesized (+)-Febrifugine and D-Fargomine from the common intermediate (8S,8aR)-8-hydroxy-8,8a-dihydro-1H-oxazolo[3,4-a]pyridin-3(5H)-one, which was derived from chiral aziridine.



(+)-Febrifugine

D-Fagomine

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Photo-controllable chloride transporters

김규찬 정규성*

연세대학교 화학과

Azobenzene derivatives have been widely used as photo-responsive functional molecules because of their photochemical isomerization between *cis* and *trans* isomers with light of appropriate wavelength. Herein a series of synthetic molecules based on azobenzene compounds with urea functional groups for anion binding are prepared and their transport abilities of chloride ion across a lipid membrane are systemically optimized. The *trans* isomers negligibly transport chloride ion across a POPC membrane but the corresponding *cis* isomers show much enhanced transporting abilities. In particular, the transport efficiency strongly depends on the nature of substituents at the para position of terminal N- phenyl rings. Details will be presented, including synthesis, ratios of *cis* and *trans* isomers on the PSSs, differences in the binding affinity of two isomers.

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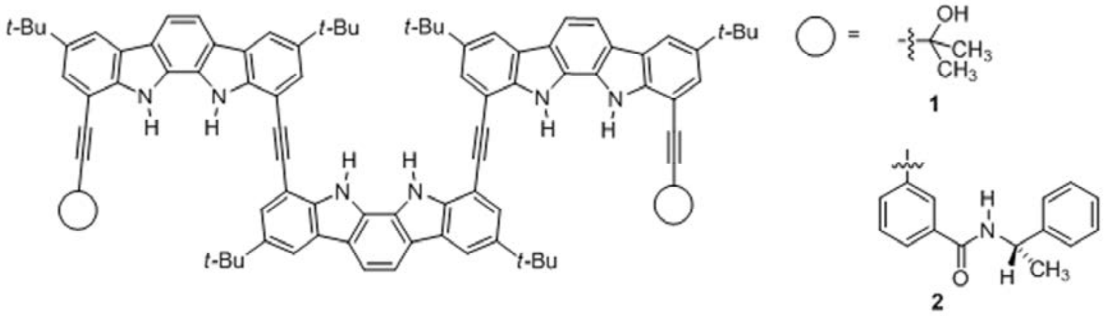
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Induction and Control of the Helical Sense of an Indolocarbazole Trimer by Chiral Moieties

김단아 정규성*

연세대학교 화학과

An achiral indolocarbazole trimer 1 was found to form a 1:1 mixture of two enantiomeric complexes of helical structure. Herein, we prepared a chiral indolocarbazole trimer 2 with (*S*)-1-phenylethylamido units to give two helically folded diastereomers in an unequal ratio. The folding property of 2 was first revealed by circular dichroic (CD) spectroscopy. Compound 2 showed strong CD signals with negative Cotton effects at longer wavelength in nonpolar solvents, suggesting that the *M*-helix form preferentially at least. Upon addition of an anion, CD spectra were inverted giving positive Cotton effects, indicative of reversed helical sense. More evidence for the helical folding of 2 was further obtained ^{1}H NMR spectroscopy and single crystal X-ray structure. Details will be discussed in the presentation.



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장소: 일산KINTEX
발표코드: **ORGN.P-713**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthetic Study of Daphnane Family Natural Products: Formation of 5,7,6-Membered Ring Structure

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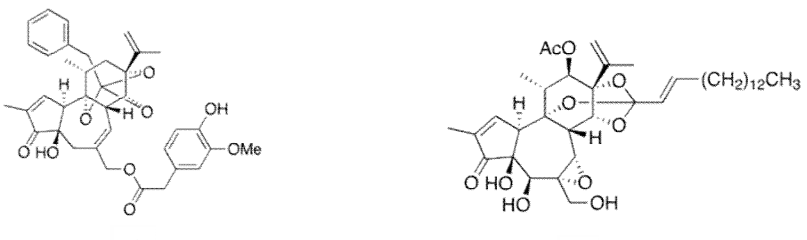
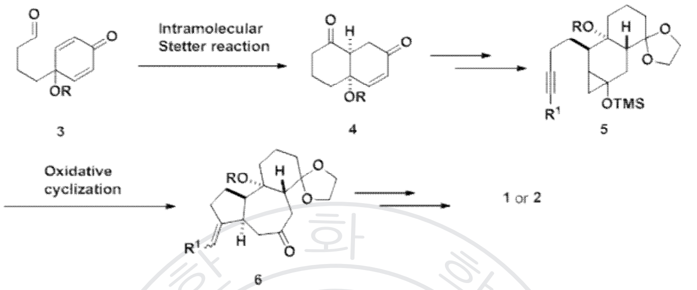
과학기술연합대학원대학교(UST) 생체분자과학 [1]한국과학기술연구원(KIST) 생체과학연구본부 [2]한국과학기술연구원(KIST) 케모인포매틱스연구단 [3]한국과학기술연구원(KIST) 뇌의약연구단

The daphnane family natural products exhibit a broad range of biological activities such as antileukemic, skin irritant, neurotrophic, antihyperglyemic, antifertility and pesticide. Most of the daphnane products constitute 5,7,6-membered ring core structure with quaternary oxygen and orthoester in 7,6-membered ring junction (Figure 1). Due to their biological importance and structural complexities, syntheses of these natural products have been highly attractive to organic chemists as interesting synthetic targets.In our laboratories, we have endeavored to identify an approach that would allow for rapid access to the 5, 7, 6-membered ring core structure. The key feature of our synthesis includes an intramolecular Stetter reaction of dienone 3 followed by oxidative cyclization of the corresponding cyclopropane 5 (Scheme 1). Herein, we report our synthetic approach toward the core ring structure of daphnane-family natural products.



1 **2**

Figure 1. The representative structures of daphnane family natural products: Resiniferatoxin (**1**) and Kirkinine (**2**)



Scheme 1. The proposed synthesis of 5,7,6-membered ring core structure

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of Heterocyclic Molecule for OLEDs

노미정 윤순병 SHAIK BAJI 이상경*

경상대학교 화학과

The heterocycle which has eight membered ring was synthesized. The synthesized compounds were investigated for their optical, thermal and electrochemical properties. The thermal properties of compounds were characterized by TGA and DSC. Electrochemical properties test of compounds were performed on cyclic voltammetry (CV). Hereby reported for the development of synthetic method, special optical character, and electrochemical properties of the synthesized new compound.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Highly Conjugated Oligomers for Organic Thin Film Transistors

SHAIK BAJI 윤순병 노미정 이상경*

경상대학교 화학과

The important requirements for the organic thin film transistor are high charge mobility, on-off ratio greater than 106, thermal stability as well as chemical stability. Here we synthesized more conjugated oligomers. These oligomers have good solubility in organic solvents which can be facilitated by presence of alkyl side chain. The alkyl side in addition to solubility it also helpful in well arranged molecular ordering. These compounds have good thermal stability as well as chemical stability. These compounds have exhibited more absorption values in UV-visible spectra, the presence of more conjugation in the molecule attributed to high λ abs values in UV-visible spectra. Based on these results we can expect OTFTs prepared by using these materials can exhibit high mobility and more on-off ratio.

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Synthesis and TFT Properties of Novel Conjugated Compound for Organic Electronic Materials

윤순병 노미정 SHAIK BAJI 이상경*

경상대학교 화학과

Synthesis and physical properties of the novel p-type Organic thin film transistors (OTFTs) materials containing thiophene, thieno[3,2-b]thiophene and fluorene derivatives were studied. All of the compounds were synthesized by well known reactions, such as Suzuki coupling and Stille coupling and etc. The obtained monomer and polymer were confirmed by FT-IR, 1H-NMR, 13C-NMR spectroscopy and elemental analysis. The synthesized FCTT and PFCTT have moderate solubility in common organic solvents such as chloroform, methylene chloride and THF. The thermal properties of these compounds were characterized by TGA and DSC. Optical and electrochemical properties of the compounds were confirmed by UV-vis and cyclic voltammetry.

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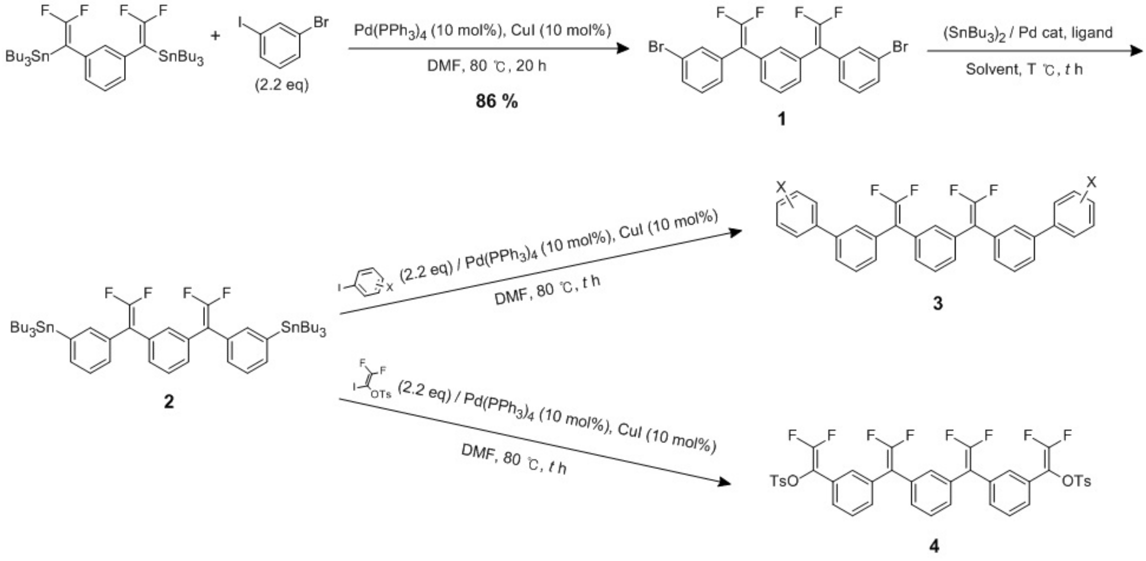
Synthesis and cross-coupling reactions of novel 1,3-bis(1-(3-tributylstannyl)phenyl)-2,2-difluorovinyl)benzene

최수정 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

1,3-Bis(1-(3-tributylstannyl)phenyl)-2,2-difluorovinyl)benzene(2) was prepared in 65% yield from the reaction of 1,3-bis(1-(3-bromophenyl)-2,2-difluorovinyl)benzene(1) with hexabutyldistannane in the presence of Pd cat and ligand. The cross-coupling reaction of 2 with various aryl iodides or 2,2-difluoro-1-iodoethenyl tosylate in the presence of Pd(0) and CuI in DMF afforded the coupled products 3 or 4 in good yields. The scope and limitation will be presented.



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발표코드: **ORGN.P-718**
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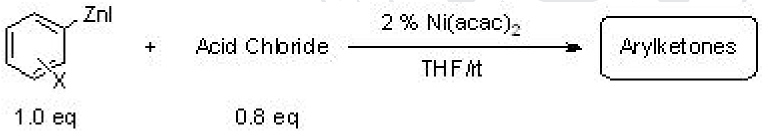
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Versatile Protocol for the Preparation of Highly Hindered Aryl Ketones Using Organozinc Reagents

조현희 김승회*

단국대학교 화학과

A facile synthetic route toward highly hindered aryl ketones has been developed. It has been accomplished by the cross-coupling reaction of organozinc reagents bearing various substituents at the ortho-position with 2,6-disubstituted benzoyl halides. The cross-coupling reactions proceed smoothly under mild conditions to afford the corresponding ketones in moderate to good isolated yields.



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

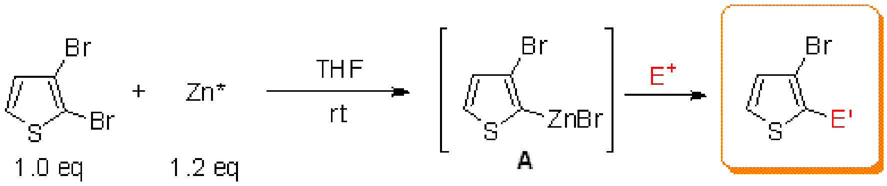
Site-selective mono-oxidative addition of active zinc into carbon?bromine bond of dibrominated-thiophenes: preparation of thienylzinc reagents and their applications

정혜수 김승회* 조현희

단국대학교 화학과

A facile protocol for the preparation of 3-bromo-2-thienylzinc bromide A and 5-bromo-2-thienylzinc bromideB has been developed. It has been successfully accomplished by a site-selective oxidative additionof active zinc into a chemically pseudo-equivalent or equivalent carbon?bromine bond, respectively. Thesubsequent cross-coupling reactions of the organozincs were also successfully carried out under mildconditions providing the corresponding products in moderate to high yields.

Preparation 3-bromo-2-thienylzinc bromide and its coupling reaction



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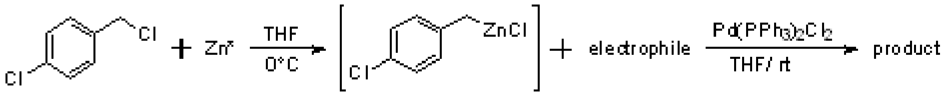
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pyridinyl- and furanyl-methylzinc chloride : direct preparation and coupling reactions

조경환 김승희*

단국대학교 화학과

Benzylic organometal reagents are highly relevant for the synthesis of organic complex molecules, especially for the homologation of organometallics. By utilizing these benzylmetallic reagents, the introduction of a diarylmethane-moiety presented in many natural compounds and biologically active materials has been successfully accomplished. To perform this strategy, a wide range of benzylic metal reagents have been used. Along with the presence of a simple benzylic moiety in many natural materials, a non-functionalized or functionalized heterobenzylic moiety is also found and considered as an important class in biologically active pharmaceutical products. For the synthesis of these active compounds, heterobenzylic halides were used mostly as a coupling partner of the corresponding organometallic reagents in the Stille, Suzuki and Negishi couplings. However, some of the heterobenzylic halides are very unstable in the transition metal-catalyzed coupling reactions. To alleviate this difficulty, heterobenzylic sulfonium salts have also been participated in Pd-catalyzed coupling reactions of organometalllics.



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Highly efficient iron-catalyzed indirect hydration of alkynes in presence of methanesulfonic acid

박정민 윤지희 김재현 이구연*

강원대학교 생명건강공학과

The transition-metal-catalyzed hydration of alkynes is one of the most straightforward approaches for synthesizing compounds with carbon-oxygen bonds. We have demonstrated that the FeCl2 4H2O and methanesulfonic acid systems show high reaction efficiency for the indirect hydration of various alkynes in DCE. The reaction proceeds under mild conditions to produce various ketones from alkynes. A mechanistic study of the reaction intermediates showed that the alkyne was readily converted to the vinylsulfonate corresponding to the addition of MsOH across the C-C triple bonds, which in turn was converted into the ketone in the presence of MsOH. In that procedure, the best results were obtained for the hydration of alkyne in the presence of FeCl2 4H2O (5 mol%) and MsOH (1.1 equiv.) in 1,2-dichloroethane at 60 ℃.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

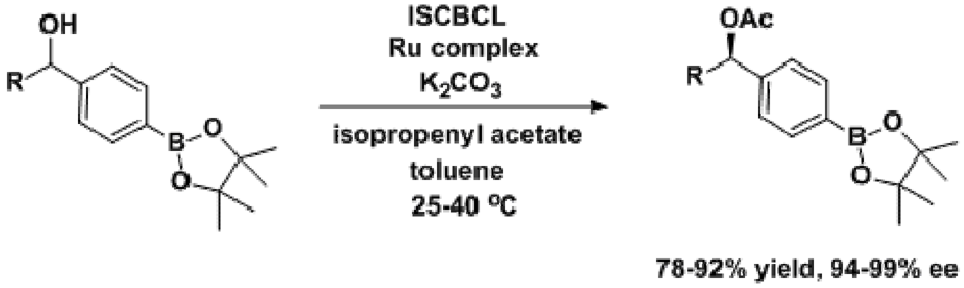
Dynamic Kinetic Resolution of Boron-Containing Alcohols with an Ionic Surfactant-Coated Lipase

조정훈 박재욱* 김만주*

포항공과대학교 화학과

Organoboron compounds are one of the most important reagents for the new carbon-carbon bond formation. Chiral boron-containing compounds are particularly useful in cancer therapy and drug delivery devices. In the meeting, we would like to report a useful procedure based on dynamic kinetic resolution (DKR) for their practical preparation. This process employs an ionic surfactant coated Burkholderia cepacia lipase (ISCBCL)[1] as the resolution catalyst, a Ru complex as the racemization catalyst, and isopropenyl acetate as the acyl donor. The DKR reactions are performed at 25-40°C in toluene and provide good yields and high enantiomeric excesses.[2]

References
1. Kim, H.; Choi, Y. K.; Lee, J.; Lee, E.; Park, J.; Kim, M.-J. Angew. Chem., Int. Ed. 2011, 50, 10944.
2. Kim, C.; Lee, J.; Cho, J.; Oh, Y.; Choi, Y. K.; Choi, E.; Park, J.; Kim, M.-J. J. Org. Chem., DOI: 10.1021/jo3027627



일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN.P-723**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Electroluminescent Properties of New Blue Light-Emitting Diodes Containing Anthracene Derivatives End-Capped with hetero aryl groups.

윤진영 윤승수*

성균관대학교 화학과

A series of blue fluorescent emitters based on 9-naphthylanthracene derivatives were synthesized via Suzuki-cross coupling reaction in moderate yield. Multilayered OLEDs with the structure of ITO (180nm) / NPB (50 nm) / Non-doping Blue Host materials 1-6 (30 nm) / TPBi, (15 nm) / Liq (2 nm) / Al (100nm) has been fabricated to investigate their electroluminescent properties. In particular, the device using compound 3 showed efficient blue electroluminescent properties with a maximum luminous, power, external quantum efficiency and CIE coordinates of 0.71 cd/A, 1.98 lm/W, 1.34 % at 20 mA/cm2 and (x = 0.16, y = 0.20) at 10.0 V, respectively. In addition, a deep blue OLEDs using compound 1 with CIE coordinates (x = 0.15, y = 0.11) at 10.0 V exhibited a maximum luminous, power, external quantum efficiency of 2.12 cd/A, 3.04 lm/W and 1.17 % at 20 mA/cm2, respectively.

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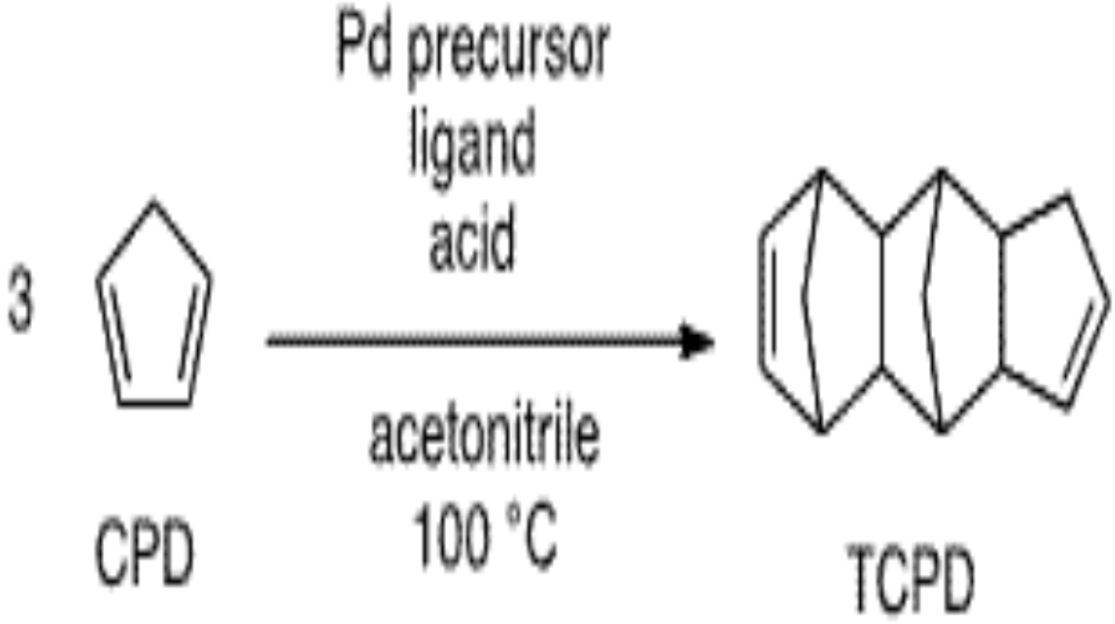
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient and Selective Synthesis of Tricyclopentadiene by Palladium/Acid Catalysts

우명진 박종은 손경선*

충남대학교 화학과

Tetrahydrotricyclopentadiene, which is produced by hydrogenation of tricyclopentadiene (TCPD), is one of the promising high-energy, high-density fuel candidates but the current synthetic method of TCPD is limited by its low yield. To overcome this limitation, we investigated efficient synthetic routes for the TCPD to reachan improved TCPD yield and highselectivity for a single isomer by means of palladium catalysts in acidic conditions. Here we report the effects of Pd precursors, ligands, acids, and the starting materials on the productivity and selectivity in the TCPD synthesis.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-725**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

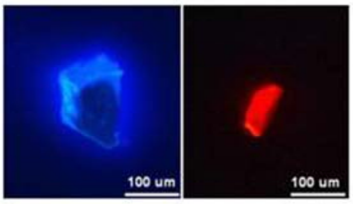
Strongly Luminescent Boron Complexes of 2-(Benzothiazol-2-yl)phenols: Dramatic Substituent Effects

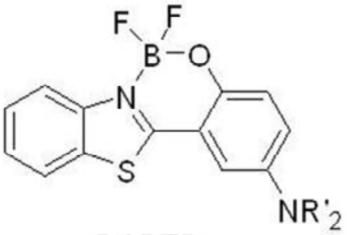
문현수 안교한*

포항공과대학교 화학과

Luminescent organic compounds have received intense interest because they can be applied to photosensitizers, organic light emitting diodes (OLEDs), and so on. Among them, boron complexes of dipyrromethenes (BODIPYs) have been explored for various applications because of their excellent photophysical properties such as high fluorescence quantum yield.[1] However, most of BODIPY dyes show poor emission in the solid state. Therefore, it is important to develop new boron complexes with improved photophysical properties even in the solid state. In the course of our study on the fluorescent probes based on 2-(benzothiazol-2-yl)phenol (BTP), we found that there were impressive substituent effects on their photoluminescence.[2] Boron complexes of the BTP analogues exhibit contrasting emission properties depending on the position of substituents. For instance, BOBTP 1a (R′ = Me) emits blue luminescence (λ_{em} = 430 nm), whereas BOBTP 2a (R′ = Me) emits orange luminescence (λ_{em} = 597 nm).BOBTP 1a, 1b, and 1c show strong luminescence; 1c shows a fluorescence quantum yield close to unity (Φ_F = 0.98 in cyclohexane). Furthermore, BOBTP 1 dyes emit bright luminescence even in the solid state, owing to small spectral overlap as well as little π-π stacking interactions in the solid state.[3] The substituent effects on the photoluminescence can be applied to related boron complexes to modulate and enhance their photoluminescence properties.Reference1. A Loudet, A.; Burgess, K. Chem. Rev. 2007, 107, 4891.2. Santra, M.; Roy, B.; Ahn, K. H. Org. Lett. 2011, 13, 3422.3. Santra, M.; Moon, H.; Park, M.-H.; Lee, T.-W.; Kim, Y. K.; Ahn, K. H. Chem. Eur. J. 2012, 18, 9886.

BOBTP
1a: R' = Me
1b: R' = Et
1c: R' = *n*-Hex





BOBTP
2a: R' = Me

일시: 2013년 4월 17~19일(수~금) 3일간
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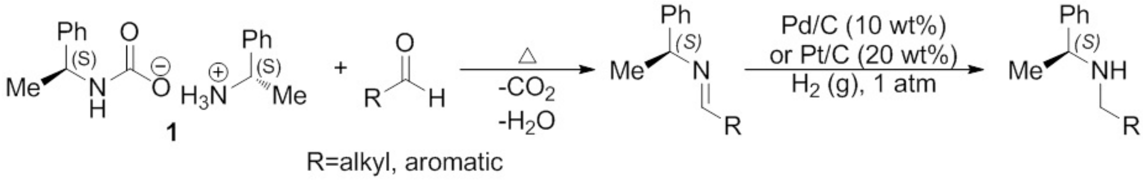
발표코드: **ORGN.P-726**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-Free Reductive Amination of a Solid Amine equivalent with various Aldehydes

강필준 이규명[1] 손세인[2] 이원구* 허남회*

서강대학교 화학과 [1]한국화학연구원 대사증후군치료제연구그룹 [2]서강대학교 화학

Since many amines are liquid at room temperature and have unpleasant odor, there are some difficulties in handling when we use amines as reagents. Therefore, we transformed a liquid amine to a solid form 1 by using supercritical carbon dioxide to provide a carbamate salt. Since the solid amine equivalent is convenient to quantify, reductive amination can be performed between the solid amine equivalent 1 and aldehydes by 1:2 molar ratio. The reductive amination was initiated with the mixture of 1 and an aldehyde to form the corresponding imine without a solvent then the reduction of the imine was catalyzed by Pd/C or Pt/C and completed in one pot under 1 atm of H2 gas. This solvent free reductive amination reaction is environmentally attractive and solid phase amines can find further application in various chemical reactions.



일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-727**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of the Group 4 Organometallic Compounds for ALD

안대준 김현창 이승한[1,*]

경희대학교 응용화학과 [1]경희대학교 응용과학대학 응용화학과

Atomic layer deposition (ALD) has been employed for the deposition of a variety of thin films. However, there are no suitable precursors for group 4 metal oxide thin films utilized in ALD. Thermally stable and highly volatile group 4 organometallic compounds were prepared successfully in good yields using bridged cyclopentadienylethylenemethylamine (CpN) and tetrakisdialkylamido group 4 metals. Especially, CpN-Zr(dimethylamide)$_2$ and CpN-Ti(dimethylamide)$_2$ showed the outstanding thermal stability at high temperature. These precursors can be used effectively in manufacturing the group 4 metal oxide thin films.

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

A highly selective chemosensor for silver ion based on dipodal benzenesulfonohydrazide

고한나 장두옥*

연세대학교 화학과

Silver ion is widely used in the electrical industry, photography / imaging industry, and pharmaceutical industry. However, silver ion has adverse biological effects on human health such as interacting with and displacing essential metal ions like Ca2+ and Zn2+ in bone. We present herein the development a high selective chemosensor of silver ion based on dipodal benzenesulfonohydrazide. The chemosensor is capable of analysed estimation of silver ion with a broad concentration range and is free from the interference from other metal ions.

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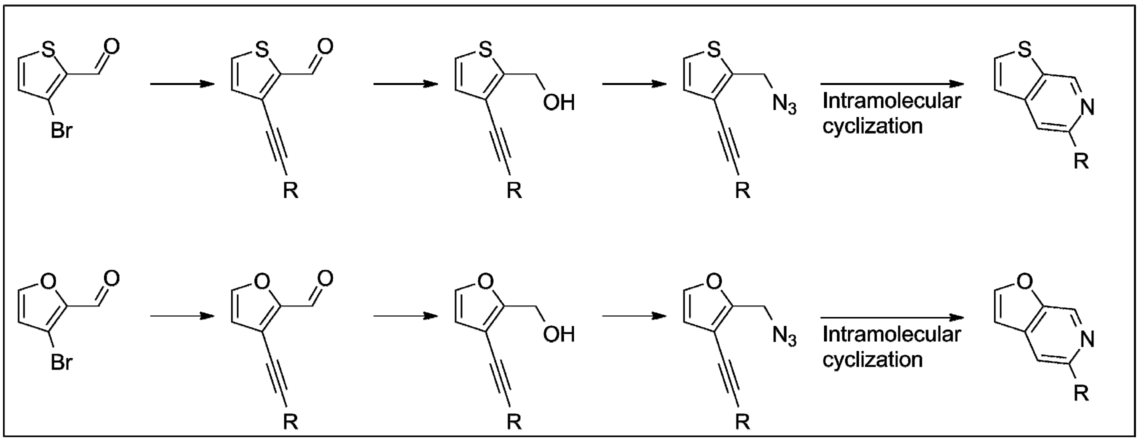
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of variously substituted pyridine-fused ring compounds via Intramolecular Cyclization

이호규 정미진 이원구[*] 하현준[1,*]

서강대학교 화학과 [1]한국외국어대학교 화학과

Thienopyridine and furopyridine are found in various natural products1). Thienopyridine and furopyridine derivatives are the candidates of pharmacologically and biologically active substances. In our previous work, we successfully synthesized substituted azaindoles by intramolecular cyclization reaction of azide and acetylene substituted pyrrole without any catalyst2). By applying similar method, thienopyridine and furopyridine can be synthesized from substituted thiophene and furan.Ref 1) (a) Dzierszinski, F.; Coppin, A.; Mortuaire, M.; Dewally, E.; Slomianny, C.; Ameisen, J.-C.; Debels, F.; Tomavo, S. Antimicrob. Agents. Chemother. 2002, 46, 3197; (b) Kletsas, D.; Li, W.; Han, Z.; Papadopoulos, V. Biochem. Pharmacol. 2004, 67, 1927; (c) Mach, U. R.; Hackling, A. E.; Perachon, S.; Ferry, S.; Wermuth, C. G.; Schwartz, J.-C.; Sokoloff, P.; Stark, H. ChemBioChem 2004, 5, 508; (d) Muscarella, D. E.; O'Brian, K. A.; Lemley, A. T.; Bloom, S. E. Toxicol. Sci. 2003, 74, 66.Ref 2) Hogyu Lee.; Jun Hee Kim.; Won Koo Lee.; Jae-Hoon Jung.; Hyun-Joon Ha. ORGANIC LETTERS, 2012, 14, 3120.


S
O
Br
OH
N_3
Intramolecular cyclization
N
R

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-730**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photoelectrocatalysis to Improve Cycloreversion Quantum Yield of Photochromic Dithienylethene Compounds

이수민 유영민[1,*] 남원우[2,*]

이화여자대학교 바이오융합과학과 [1]한국과학기술연구원(KIST) 의공학연구소 [2]이화여자대학교 화학과

Photochromic dithienylethenes (DTE) compounds undergo reversible interconversion between open and closed forms under alternating photoirradiation, with properties promising for the application for molecular switches. However, photochromic cycloreversion (i.e., ring opening) quantum yields of DTEs are very low, being smaller than those of cyclization (i.e., ring closing) by factors of 10^{-2}-10^{-1}. To improve the cycloreversion quantum yield, we developed a photoelectrocatalytic strategy employing 9-mesityl-10-methylacridinium ion (Acr^+-Mes) as a photoredox catalyst. By using the photoelectrocatalystic method, we accomplished a quantum yield as high as 54%. This value is one order of magnitude improvement relative to the quantum yield (1.6%) obtained under the conventional photochromic method. We further performed mechanistic studies, including nanosecond transient absorption spectroscopy and stopped-flow UV-vis absorption spectroscopy, to elucidate the reaction mechanism of the photoelectrocatalytic cycloreversion. The studies indentified the key steps and their rate constants in the photoelectrocatalytic reaction.

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

Enantioselective Extraction of Amino Acid by Binol Aldehyde with Phenyl Ether Linkage

최미선 김관묵[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과

Amino acid is the most representative chiral material. In particular, D-amino acids are used in food technology and as drug intermediates in Pharmaceuticals. Nevertheless, compared to L-amino acids, D-amino acids are not abundant in nature. Therefore, the synthesis of D-amino acids is an easy and cost-effective way is very important. The previous work in our research group showed that chiral aldehyde, (S)-2-hydroxy-2’-(3-phenyluryl-benzyl)-1,1’-binaphthyl-3-carboxylaldehyde, can convert L-amino acid to D-amino acid based on difference of energy stability between L-form and D-form and this receptor has enantioselective ablility in shuttle process. In this time, we modify a length of ether bond in receptor to make more tight hydrogen bonds between carboxylic acid in amino acid and uryl group in receptor. Then, we monitor its enantioselectivity for amino acid by 1H NMR spectroscopy.

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발표분야: 유기화학

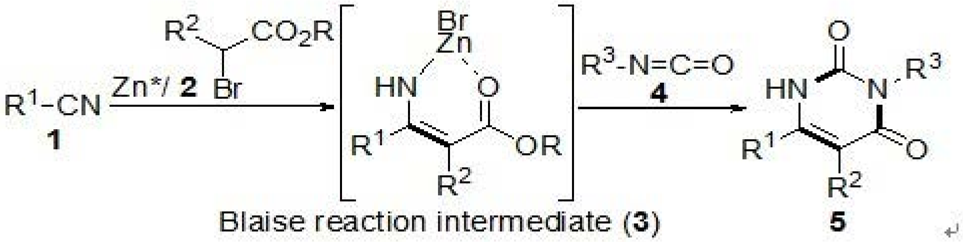
발표종류: 포스터, 발표일시: 수 16:00~19:00

Diversity-Oriented Tandem Synthesis of N-Heterocyclic Compounds using the Blaise Reaction Intermediate

XUAN ZI 전유성[1] 이상기[1,*]

이화여자대학교 화학.나노학과 [1]이화여자대학교 화학/나노과학과

N-Heterocycles are important components in various natural product, bio-molecules, pharmaceuticals. In the course of our ongoing study on tandem use of the Blaise reaction intermediate, we developed an unprecedented tandem one-pot synthesis of pyrimidindione derivatives from nitriles by electrophilic trapping with isocyanates as electrophile in an excellent yield. Moreover, due to consecutive C- and N-nuclephilicities of Blaise reaction intermediate, it allowed us to install different functional groups at C-5 position such as 1-alkyne, NBS, and isocyanate.



Blaise reaction intermediate (3)

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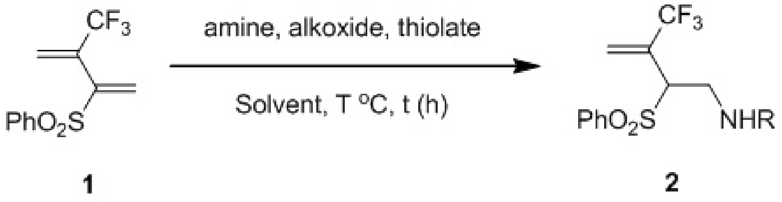
발표코드: **ORGN.P-733**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

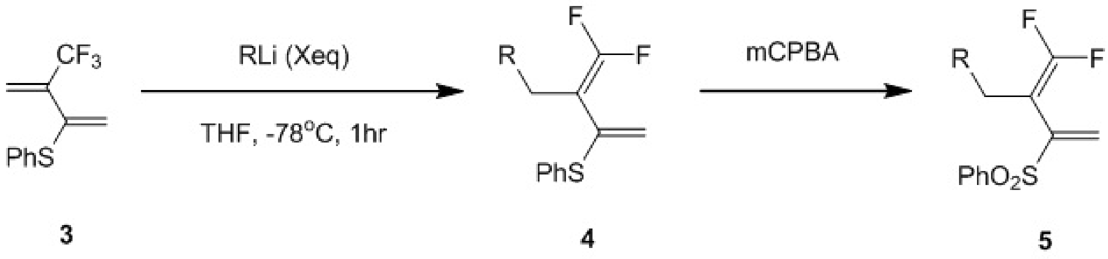
Synthesis of 2-alkylated 1,1-difluoro-3-phenylthio(phenylsulfonyl)-1,3-butadienes and their reactions

김주희 정여진 정인화[1]

연세대학교 화학과 [1]연세대학교 화학및의화학과

2-Trifluormethylated alkenes 2 were obtained in 43-97% yields from the reaction of 2-trifluoromethyl-3-phenylsulfonyl-1,3-butadiene 1 with amine, alkoxide and thiolate reagent. When 2-trifluoromethyl-3-phenylthio-1,3-butadiene 3 was reacted with alkyl-, aryl- and alkynyllithium reagents, however, 1,1-difluoro-3-phenylthio-1,3-butadiene derivatives 4 were obtained in 51-78% yields via allylic defluorination reaction. Oxidation of 4 with mCPBA afforded the corresponding sulfones 5 in high yield.





일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-734**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Tetrahydrothiopheno-calix[4]pyrroles as ion-pair complexants and their cation selectivity

유소은 한인숙[1] 이창희*

강원대학교 화학과 [1]강원대학교 과학교육학부

Calix[4]pyrroles which are fused with tetrahydrothiophene have been synthesized and characterized. The ion binding study of the synthesized hosts displayed very interesting properties. The deep cavity, cation binding pocket which was created by anion binding shows different selectivity depending on the nature of applied cations. For example, the cone conformation resulting upon the pre-complexation with fluoride anion, forms stable ion-pair complex with cesium cation. The cesium cation is thought to be bound to the deep inside the cavity by cation-pi interaction. On the other hand, the mercury(II) ion form stable donor-acceptor complex with the sulfur atom. The ion binding studies confirmed that the synthesized receptors form stable complexes with various metal salts in organic media. The binding affinities and spectroscopic changes upon ion binding will be presented.

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

Total synthesis of 1,12-bis((benzoylamino)methyl)-3,10-perylene quinone as a potential photodynamic therapy (PDT) agent

김범태* 황기준[1] 김효연[2]

전북대학교 생리활성물질연구소, 생리활성소재과학과 [1]전북대학교 화학과 [2]전북대학교 생리활성소재과학과

The perylenequinones have attracted much attention due to their advantages as a photosensitizer. we synthesized novel active perylenequinone compound, 1,12-bis((benzoylamino)methyl)-3,10-perylenequinone, with the amino group at 1- and 12- position of the molecule. The novel perylenequinone core was successfully prepared from the dimerization of the key intermediate, 3-(benzoylamino)methyl-1,2-naphthoquinone. Our synthetic route to the perylenequinone core from commercially available starting material was quiet efficient in terms of relatively short reaction steps (11steps). The evaluate of anticancer activity of the novel perylenequinone is now under progress as selective inhibitory potential against protein kinase C.

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

Semi-synthesis of Hypocrellin B from Phleicrome produced from Cladosporium Phlei

김범태* 황기준[1] 채민선[2]

전북대학교 생리활성물질연구소, 생리활성소재과학과 [1]전북대학교 화학과 [2]전북대학교 생리활성소재과학과

Hypocrellin B is representative in a class of perylenequinones and has a high potential in itself as a photosensitizer in photodynamic therapy (PDT) against diverse cancers, and utilized as an starting material for the further synthetic derivatization for novel lead photosensitizers. These perylenequinones have also been shown to be potent and selective inhibitors of protein kinase C. For these reasons, the sustainable supply of hypocrellin B is crucial, however, it is natural fungal product and its supply-line is actually very limited despite its urgent needs as a raw material. Furthermore, there are several limitations on its total chemical synthesis, such as a large number of reaction steps, low overall yield, expensive costs and difficulty in controlling the stereoselectivity. To overcome these hardships, herein, we study the semi-synthesis of hypocrellin B from other fungal perylenequinone, phleichrome, 4,9-dihydroxy-3,10-perylenequinone. Phleichrome is prepared by extraction from the biomass of the fungus, Cladosporium phlei which is genetically manipulated to alter natural pigment production. We developed an efficient route to prepare hypocrellin B from phleichrome via sequential oxidation and aldol intramolecular cyclization.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper and solvent free, and rapid Sonogashira reaction using heterogeneous Pd/graphine catalyst

김범태* 황기준[1] 박준범[2] 이윤아[3]

전북대학교 생리활성물질연구소, 생리활성소재과학과 [1]전북대학교 화학과 [2]전북대학교 화학교육과 [3]전북대학교 생리활성소재과학과

The Sonogashira cross-coupling reaction of terminal alkynes with aryl or vinyl halides is a powerful method for C(sp)-C(sp2) bond formation. The reaction products are important building blocks for the synthesis of biologically active molecules and synthetic drugs. The development of active catalysts and the efficient reaction conditions for Sonogashira reactions have been investigated in the viewpoint of green chemistry. The use of heterogeneous catalysts in Sonogashira-type reactions could offer advantages in terms of low palladium contamination and even of recycling. Microwave irradiation of organic reaction was found to accelerate a wide variety of transformations and to give good to excellent yields.We have developed a novel heterogeneous Pd/graphine catalysts which is air and moisture stable and even easily prepared. With this catalyst, microwave-assisted Sonogashira reactions were performed under solvent-free condition, and DBU base reaction system increased the yields of the cross coupling reactions. Substrates of substituted aryl halides with electron donating group, such as methoxy and methyl, gave good to excellent yield of cross-coupled products, while the yields decrease as substrates of substituted compounds with electron withdrawing groups, such as nitro and fluorine were adopted.

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Selective fluorescence detection for cysteine in water

임수연 김해조[1]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

Biothiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) are involved in a myraid of vital cellular processes, including redox homeostasis[1] and cellular growth.[2] It serves many cellular functions, including the maintenance of intracellular redox activities, xenobiotic metabolism, intracellular signal transduction, and gene regulation.[3] Although Cys, Hcy and GSH have similar structure, they are associated with different diseases. Therefore, it is important to develop fluorescent probe for detection and discrimination these biothiols. Herein we report rhodamine-based fluorescent probe with enone type of Michael acceptor, which shows selective response for Cys by kinetic discrimination during the cyclization of probe 1 with Cys. When Cys was added, a significant fluorescence response of 1 as well as the color change of 1 was observed so that micromolar concentration of Cys was detectable by the naked eye.Reference[1]. T. P. Dalton, H. G. Shertzer, A. Puga, Annu. Rev. Pharmacol. Toxicol. 1999, 39, 67.[2]. (a) Z. A. Wood, E. Schroeder, J. R. Harris, L. B. Poole, TransBiochem. Sci. 2003, 28, 32. (b) R. Carnel, D. W. Jacobsen, Homocysteine in Health and Disease, Cambridge University Press, UK, 2001.[3]. R. L. Krauth-Siegel, H. Bauer, R. H. Schirmer, Angew. Chem. Int. Ed. 2005, 44, 690.

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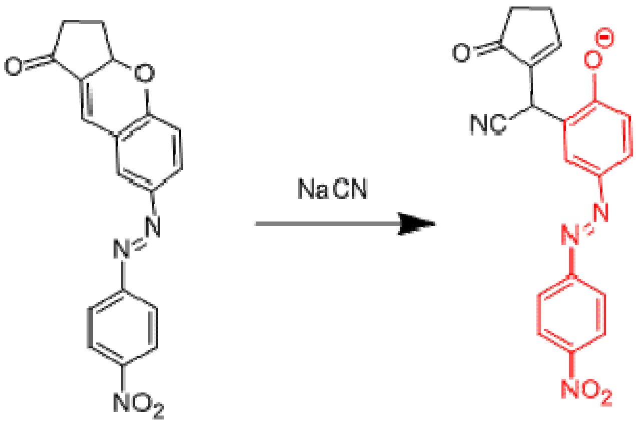
장소: 일산KINTEX
발표코드: **ORGN.P-739**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric Chemodosimeter for Cyanide Based on an Azo Dye

홍금희 김해조[1]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

The cyanide ion is one of the most toxic anions and damages to organism by absorption through the lungs, gastrointestinal tract, and skin and can lead to death [1]. The cyanide ion inactivates the process of cellular respiration by interacting heme unit in the active site of cytochrome-a_3 [2]. In the environment, cyanide ions are widely distributed and effect human being. We therefore report a designed probe (1) for cyanide that was prepared through the Baylis-Hillman Condensation reaction and applied to a Michael acceptor type of probe for cyanide. The probe (1) exhibited a highly selective and colorimetric response to cyanide ions over other anions through 1,4-addition of cyanide to α,β - unsaturated ketone in the probe. Cyanide ion was added, dramatic colour change of 1 was observable by the naked eye [3].Scheme 1. The reaction of 1 with cyanide.References1. Baskin, S. I.; Brewer, T. G. *In Medical Aspects of Chemical and Biological Warfare*; Sidell, F., Takafuji, E. T., Franz, D. R., Eds.; TMM Publications: Washington, DC, 1997; pp 271?286. 2. Kellin, D. *Proc. R. Soc. London, Ser. B.* 1929, *104*, 2063. (a) Hong, K.-H.; Kim, H.-J. *Supramol. Chem*. 2013, *25*, 24. (b) Park, S.; Hong, K.-H.; Hong, J.-I.; Kim, H.-J. *Sens. Actuators, B.* 2012, *174*, 140.



1
colorless

1-CN
Red

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
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Imidazolium salt-functinalized ionic CNT-supported Ru-carbene/palladium nanoparticles for recyclable tandem metathesis/hydrogenation in ionic liquid

신주연 이상기*

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Tandem catalytic processes allow several transformations in a one-pot operation, negating the need for handling and isolating intermediates. One class of reaction that has come to prominence in tandem reactions is the olefin metathesis reaction. Grubbs and co-workers developed tandem metathesis-hydrogenation with the Grubbs's 1stor 2nd-generation Ru complexes and also numerous other tandem processes have also been developed by combining Ru-catalyzed metathesis with hydrogenations, Claisen rearrangements, Diels-Alder reactions, etc. However, all these reported metathesis-based tandem transformations involve homogeneous catalysis. The use of supported catalysts that enable recovery and reuse could make the tandem catalysis more sustainable. We previously reported that palladium nanoparticles (Pd NPs) supported on IM-f-MWCNTs showed high reactivity and recyclability in an ionic liquid and found that Ru-carbene complexes supported on IM-f-MWCNTs also showed excellent catalytic activity and recyclability for ring closing metathesis (RCM). Based on these observations, two different catalysts, a Ru-carbene complex and palladium nanoparticles, are immobilized onto the same imidazolium salt-functionalized ionic CNTs. The supported dual-function catalysts showed excellent catalytic activity in tandem metathesis/hydrogenation in an ionic liquid, and can be recovered and reused four times.

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Synthesis of Phenanthrenes via In(III)-Catalyzed 6-*Exo-Dig* Cycloisomerization

조현경 김상희[1,*]

서울대학교 약학과 [1]서울대학교 약학대학/약학과

Phenanthrenes have versatile physicochemical properties and present in a lot of natural products and synthetic compounds. Therefore, many scientists tried to synthesize phenanthrenes efficiently by various synthetic routes. Among the diverse methods, intramolecular hydroarylation has been concerned because it makes easier to create polysubstituted phenathrenes. In this reason, base or metal catalyzed cyclizations has been reported in many journals. Especially we envisioned metal mediated cyclization using o-alkynylbiaryl generating both 6-*endo-dig* product and 5-*exo-dig* product competitively. Thus, we developed Indium(III) catalyzed system that favored only 6-*exo-dig* selective product of o-propargylbiaryls. Intramolecular cyclization of o-propargylbiaryls possibly offers 6-*exo-dig* and 7-*endo-dig* products. However electrochemical properties and entropy would promote the 6-*exo-dig* product preferably. The reaction with InCl3 induced desired product in high yields and showed extremely improved selectivity. We identified intermediate and confirmed mechanistic hypothesis that the product was formed via intramolecular hydroarylation and subsequent double bond migration. Furthermore, we obtained various highly substituted phenanthrenes through this method efficiently. This synthetic protocols could be an alternative path for synthesizing phenathrenes consequently.

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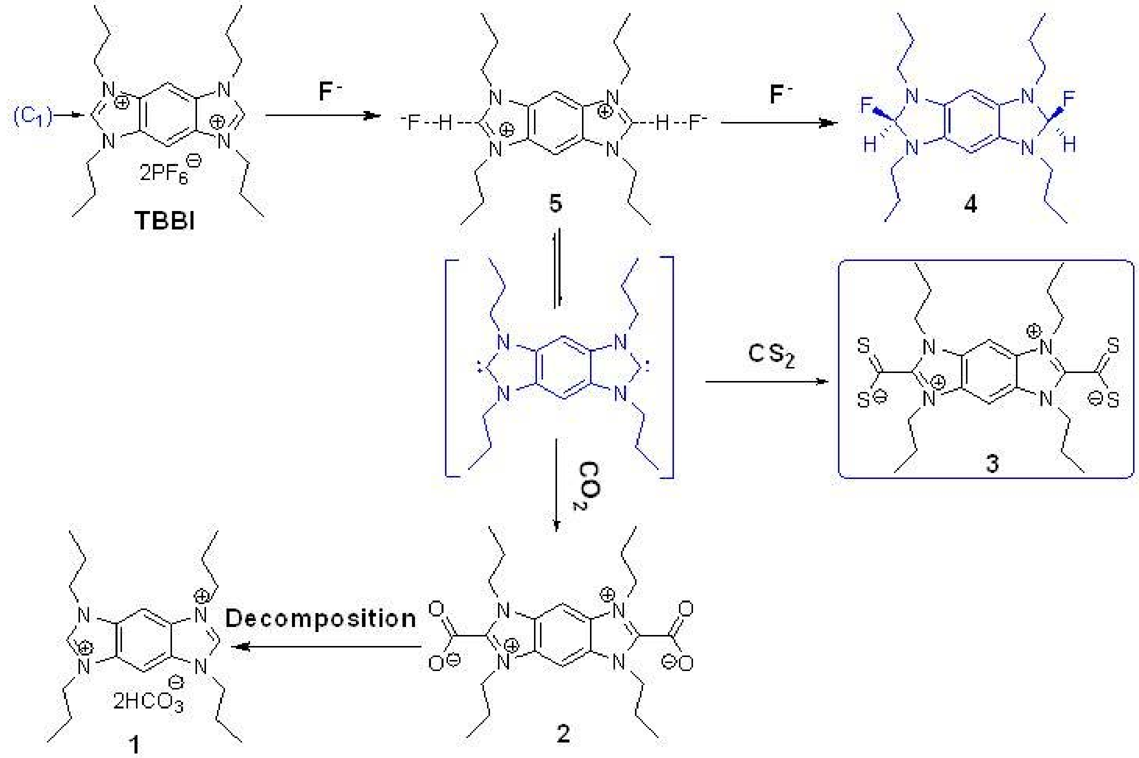
Imidazolium-based Fluorescent Chemosensor for CO_2

이민지 문종훈[1] 윤주영[2,*]

이화여자대학교 화학나노과학과 [1]성균관대학교 화학과 [2]이화여자대학교 화학-나노과학과

Carbon dioxide is a known greenhouse gas and linked to global climate change. As such, monitoring CO_2 levels in the atmosphere and aquatic environments is therefore an urgent and important task. Although there are many common methods for CO_2 detection, these methods are generally expensive and rely on bulky instrumentation. In contrast, optical CO_2 gas sensors based on fluorescence changes are attractive due to their simple and inexpensive construction, high sensitivity, rapid sensing capabilities, and ability to operate at ambient temperature. So it is great important for development fluorescent and colorimetric chemosensor for CO_2 with simplicity operation and the high limit of detection. In general, N-heterocyclic carbenes (NHCs) can be obtained by deprotonating the corresponding imidazolium salt with strong bases. The resulting species are capable of activating CO_2 to form imidazolium carboxylates. However, known systems for generating NHCs require dry and air-free conditions, and lack the features needed to be useful as CO_2 sensors. Thus, we launched a search for an NHC system that would allow the requisite chemistry to be carried out under less forcing conditions. Finally, we have found that the strong $(C\text{-}H)^+$??X^- hydrogen bonds between the salts of the imidazolium cation and anions allow us to activate the imidazolium group for CO_2 capture and sensing.To use this system, we synthesized three imidazolium derivatives and we can present a new strategy that provides a direct, reaction-based approach to the detection of CO_2.


(C1)
2PF6⊖
TBBI
F⁻
F⁻
5
4
CS2
3
CO2
Decomposition
2HCO3⊖
1
2

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

New Pyrene Derivatives as Fluorescent Receptors for Anions

김재미 이민지 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학-나노과학과

Anions play a major role in diverse fields of the environment. Therefore anion sensors have been interesting research subjects for many years. Biologically, detecting anions is highly important for systematic process.We synthesized and characterized two pyrene based compounds. Since these two pyrene derivatives contain hydroxyl group, they can effectively detect fluoride and cyanide anions. These hydroxyl groups can catch highly electronegative anions and then show change of fluorescent wavelength and intensity. Compound 1 is made up of two pyrene groups and each pyrene group has hydroxyl group and compound 2 is formed of one pyrene group and two near hydroxyl group. Compound 1 can selectively detect fluoride, cyanide anions among several anions. However 2 shows selectivity for fluoride, cyanide and acetate anions. And the change of color can be easily identified in visually.According to the use of polar solvent, the changes of fluorescent in presence of anions are different. When these reactions are detected under addition of ethanol or water, the intensity of fluoride more decreased than cyanide or acetate. Consequently, we can suppose the effect of solvation also.

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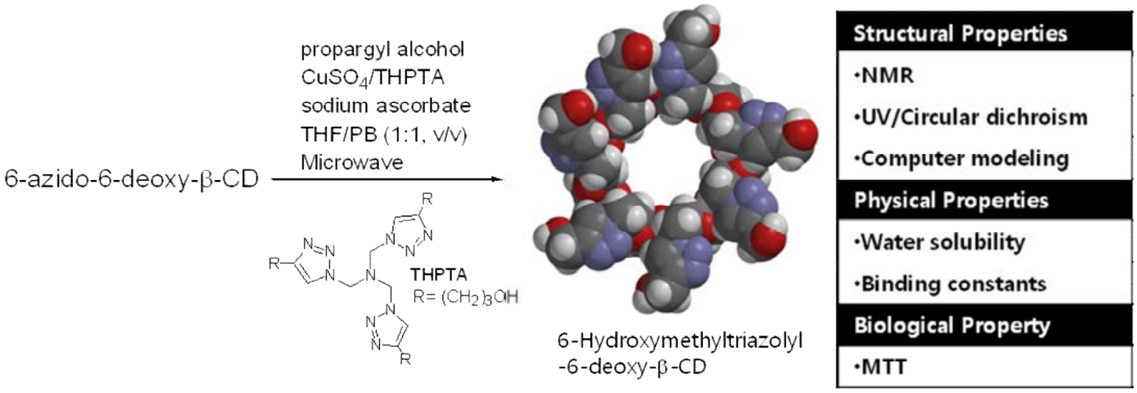
Copper(I)-Catalyzed Azide-Alkyne Cycloaddition of 6-Azido-6-Deoxy-α-Cyclodextrin & Structural/Physical Property Investigation of 6-Hydroxymethyltriazolyl-6-deoxy-β-Cyclodextrin Investigation

송정은 **Le Thi Hoa**[1] 임춘우[1,*] 김태우[1,*]

경희대학교 동서의과학과 [1]경희대학교 동서의학대학원

In a microwave and ligand-assisted cyclodextrin click cluster synthesis, we observed the cooperative perfunctionalization. MALDI-MS data and partial fluorescein labeling via the one-pot/stepwise methods confirmed the occurrence of cooperative perfunctionalization: the fully triazole-functionalized cyclodextrin click cluster became the major product with limited alkyne equivalents. Under our optimized reaction condition, we synthesized 6-Hydroxymethyltriazolyl-6-deoxy-β-Cyclodextrin and its structural, physical, and biological properties were investigated by a variety of methods, including NMR, UV/vis. & circular dichroism spectroscopy, computer modeling, turbidity testing, Ka measurements, and the MTT assay. The experimental results suggest that 6-Hydroxymethyltriazolyl-6-deoxy-β-Cyclodextrin is structurally well-defined, highly water-soluble, and has low cytotoxicity.



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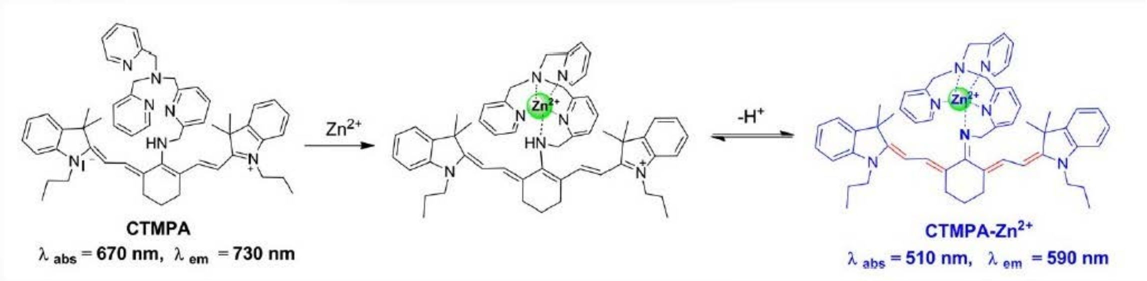
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

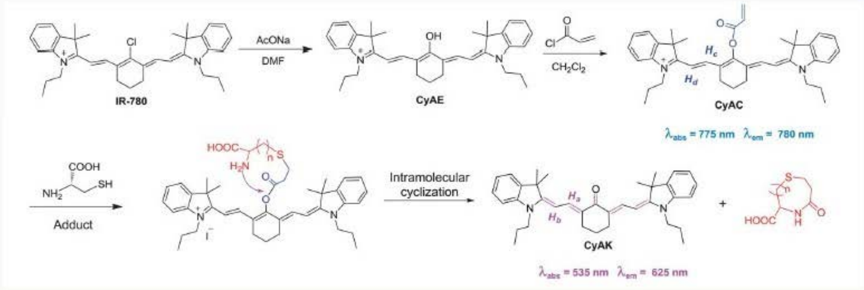
New Cyanine-based New IR probe

<u>Hu Ying</u> 신인재[1] 윤주영

이화여자대학교 화학-나노과학과 [1]연세대학교 화학과

The highly sensitive and selective, cyanine-based Zn2+ fluorescent sensor CTMPA was designed, prepared and utilized to monitor endogenous zinc ions in live cells and organisms. Upon addition of Zn2+ to solutions of CTMPA, an observable blue to light red color change occurs that can be monitored by using UV-vis spectroscopy, The association of the probe with Zn2+ leads to shortening of the conjugated, p-electron system in the cyanine dye, the phenomenon likely responsible for the large hypsochromic shift observed in emission spectra. The effort has demonstrated that a strategy, which relies on changes in the p-electron conjugation length of cyanine molecules promoted by guest coordination, has great potential for the creation of cyanine-based probes. We also developed a highly selective ratiometric near-infrared cyanine-based probe CyAC for cysteine (Cys) over homocysteine (Hcy) and glutathione (GSH). Upon the addition of Cys to the solution of CyAC, remarkable shifts in the spectra of CyAC can be monitored (from 770 nm to 515 nm in absorption spectra and from 780 nm to 570 nm in emission spectra). This paradigm by modulation of the polymethine p-electron system in the cyanine dye provides a promising methodology for the design of ratiometric cyanine-based sensors.


CTMPA
λ abs = 670 nm, λ em = 730 nm
Zn2+
-H+
CTMPA-Zn2+
λ abs = 510 nm, λ em = 590 nm


IR-780
AcONa
DMF
CyAE
CH2Cl2
CyAC
λabs = 775 nm λem = 780 nm
Adduct
Intramolecular cyclization
CyAK
λabs = 535 nm λem = 625 nm

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Ionic Liquid-Tagged Ru-Carbene Complex for Sustainable Olefin Metathesis

정다정 신주연[1] 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

Ru-carbene complexes became one of the most privileged catalysts for the olefin metathesis. To overcome their limitations associated with recovery and reuse of the expensive catalysts, different kinds of strategies, mostly based on “release-return” mechanism, have been investigated. However, the concomitant decomposition of active Ru-Catalysts could not be avoided decreasing catalyst recyclability. In oder to address this problem, we attempted to immobilize the Hoveyda-type Ru-carbene complex through anchoring the ionic liquid moiety onto the Ru-metal.

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Iridium-catalyzed Allylic Amination Reaction: Regiospecific&Stereospecific Synthesis of α,β-Unsaturated γ-Amino Esters

이준희 전현지[1] 이상기[2,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학/나노과학과

The synthesis of densely functionalized molecules in an efficient and straightforward manner represents an ongoing challenge in organic chemistry. Of particular interest are catalytic methods that allow access to useful three-dimensional structural motifs in a chemoselective, regioselective, and stereoselective fashion from readily available starting materials. Due to not only their polyfunctionality for further manipulations, but also their abundance in bioactive natural and nonnatural products, the α,β-unsaturated γ-amino acid derivatives has attracted significant interest in the synthetic community. Several catalytic methods for their selective construction have been developed with limited success. In fact, the classical Wittig-type olefination of N-protected α-amino aldehydes, which requires multi-step synthetic procedures, is still one of the most reliable synthetic methods for α,β-unsaturated γ-amino acid derivatives. Despite these advances, step-economic methods for obtaining catalytic enantioselective access to α,β-unsaturated γ-amino esters have not been fully delineated and remain to be developed. In the context of our research program directed toward the extensions of transition-metal-catalyzed allylic amination reaction for the preparation of synthetically useful structural motifs, we envisioned that the allylic amination of electronically biased allylic electrophiles possessing an alkyl, aryl, or heteroaryl substituent and anelectron withdrawing group, such as an ester functionality, at C1 and C3, respectively, would provide ready access to α,β-unsaturated γ-amino acid derivatives. This presentation will deal with the full details of this novel reaction.

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Highly Sensitive and Selective Fluorescent Sensor for Au^{3+}

이혜연 이민지[1] 신승훈[2] 신인재[3,*] 윤주영[4,*]

이화여자대학교 화학나노과학 [1]이화여자대학교 화학나노과학과 [2]한양대학교 화학과 [3]연세대학교 화학과 [4]이화여자대학교 화학-나노과학과

Gold ion are known to activate carbon-carbon multiple bonds, especially alkynes, toward nucleophilic addition. A variety of organic transformations using gold ions have been investigated owing to the characteristic alkynophilicity of the gold ion. Despite the interesting properties, gold ions are known to tightly bind enzymes or DNA, leading to cytotoxicity and damage to the liver, kidneys and the peripheral nervous system. Thus, it is very importance to develop gold ion sensors for monitoring of gold ions in environmental and biological samples. As conventional fluorescent dyes, 4-Amino-1,8-naphthalimides derivatives have advantages for developing fluorescent sensors, such as strong absorption and emission in the visible region etc. In addition, surfactant has benefits for many utilizations since it can offer a special phase or microenvironment, such as a micelle, distinct from the bulk solution. These new microenvironments could share their virtues with small fluorescent sensor molecules and lead to elevation to large-amplituded performance such as enhanced sensitivity. Herein, we report a novel 4-amino-1,8-maphthalimide-derived ratiometric fluorescent chemosensor which is highly selective and sensitive for a gold(Ⅲ) ion. In our target molecule, the fluorophore was linked to proparylamine which acts as receptor of the target species. The target molecule showed an excellent selectivity toward the gold(Ⅲ) ion in emission spectra. This sensor exhibited some enhanced sensitivity and desirable spectral changes in a surfactant induced microenvironmental condition. Furthermore, The probe was successfully applied to bioimaging of gold(Ⅲ) ion in live cells and differentiated adipocytes. We also report the new gold(Ⅲ) ion sensor based on 1H-naphth[2,3-d]imidazole derivatives.

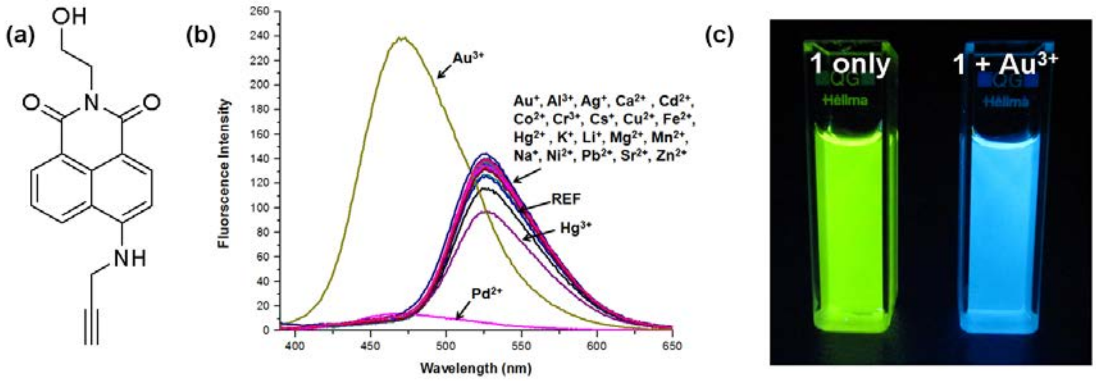

Figure 1. **(a)** Structure of Compound **1** **(b)** Fluorescent changes of **1** (20 μM) upon the addition of various metal ions (5 equiv.) in EtOH-PBS buffer (pH 7.4) (4 : 96 v/v) (λ_{ex}=364 nm) **(c)** Fluorescence picture of **1** (20 μM) (left), **1** with addition of 5 eq. of Au$^{3+.}$ (right side).

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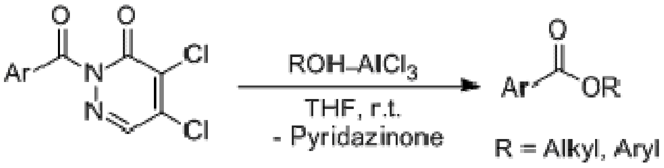
Esterification of 2-Acyl(or aroyl)pyridazin-3(2*H*)-ones with ROH-$AlCl_3$ salt under Ambient Conditions

김보람 성기현 김점종[1] 윤용진

경상대학교 화학과 [1]한국전자통신연구원 IT부품산업기술연구부

Esterification of alcohols is the most fundamental and important reactions in organic synthesis. Many processes are reported for esterification. In esterification, alkoxide and protonated alcohol use generally. However preparing alkoxide ion and the protonation of alcohol is very limited. When the protonated alcohol is use, the dehydration product such as corresponding alkenes are commoly formed. Therefore significant academic efforts are underway to make convenient method for alkoxide or alkoxide equivalent without the hydration under acidic condition. Our research motivation is the generation of alkoxides or alkoxide equivalent using Lewis acids with alcohols.

Herein, we attempt to synthesize the esters using (ROH-$AlCl_3$) adduct and 2-acyl-4,5-dichloropyridazin-3(2*H*)-one system in THF at room temperature.



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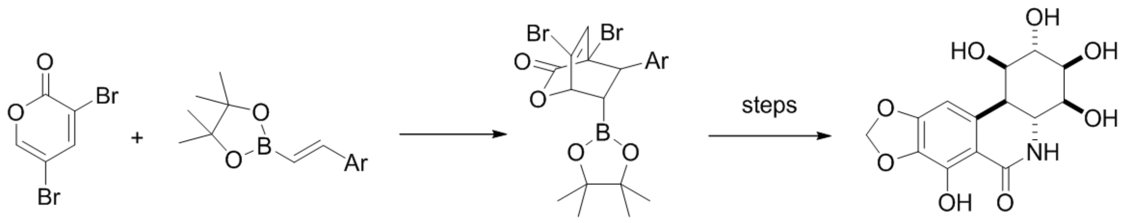
장소: 일산KINTEX
발표코드: **ORGN.P-750**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Use of β-boronyl styrene in the cycloaddition reaction with 3,5-dibromo-2-pyrone for the total synthesis of (±)-pancratistatin

조현규 조천규*

한양대학교 화학과

Pancratistatin is a natural compound that was initially extracted from Spider Lily a Hawaiian native plant that belongs to the family of Amaryllidaceae. It has been shown to have potent anti-cancer activities and selectively induce apoptosis in several human cancer cell lines. The promising biological activity and natural paucity has made pancratistatin an interesting target for total synthesis. Ever since the first total synthesis reported by Danishefsky and coworkers in 1989, many research groups around the world have presented novel strategies and routes to this natural compound. A few years ago, we have reported the first total synthesis of trans-dihydronarciclasine, very close congener of pancratistatin, by utilizing Diels-Alder reaction of 3,5-dibromo-2-pyrone. Recently, we have successfully executed the total synthesis of pancratistatin by utilizing the same strategy. During the synthesis, we have learned β-boronyl stryrene can undergo cycloaddition reaction with 3,5-dibromo-2-pyrone and the boronate group of the cycloadduct can be readily converted into hydroxyl group. Presented herein would be our new approach to (±)-pancratistatin.



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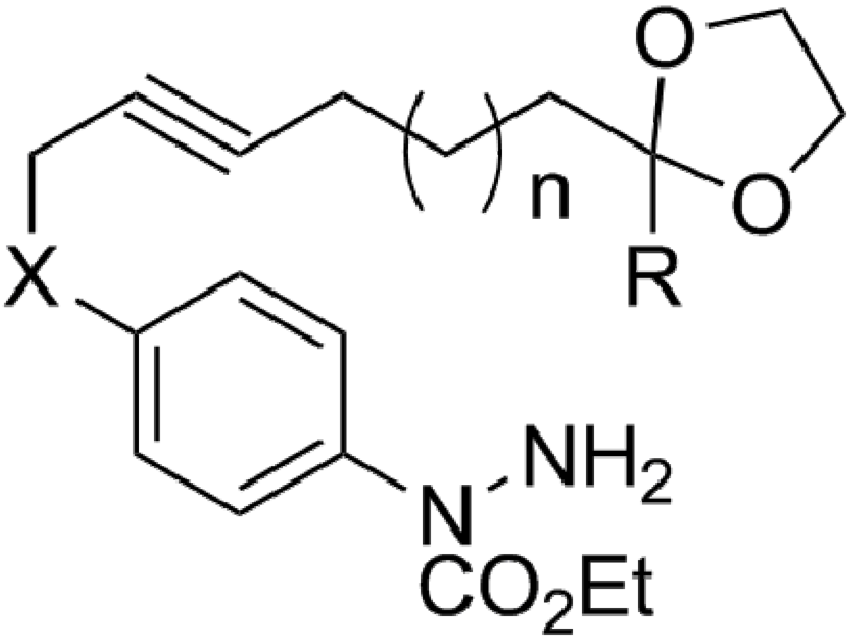
Intramolecular Fischer indolization coupled with cycloisomerization of alkyne tethered aryl hydrazide

박준 조천규*

한양대학교 화학과

We have previously reported that the Fischer indolization can be combined with an aromatic [3,3]-sigmatropic rearrangement reaction toward the synthesis of tricyclic benzo[cd]indoles. In this reaction sequence, aryl hydrazide with a carbonyl function attached to the para-position of the aryl ring undergoes a Fischer indolization reaction to give indole. Owing to the C-C double bond deliberately embedded in the tether, an aromatic [3,3]-sigmatropic rearrangement reaction is engaged to proceed to generate new C-C bond at C4 position, affording tricyclic benzo[cd]indoles. As a continued study, aryl hydrazides bearing a carbon-carbon triple bond in the tether were prepared and subjected to the similar tandem process, in hopes that the initially formed indolophane intermediate would undergo cycloisomerization reaction to give tetracyclic indolo-chromene. The ring strain embraced in the loop of indolophane inoculated by the intramolecular Fischer indolization would empower the ensuing cycloisomerization that normally requires high reaction temperature or a metal catalyst. Ozonolysis or equivalent reaction would provide the carbonyl function, a handle for further manipulation. These potential synthetic utilities prompted us to study the tandem reaction of aryl hydrazide with alkyne tether. Presented would be the progress in this line of chemistry.


O
O
n
R
X
NH2
N
CO2Et

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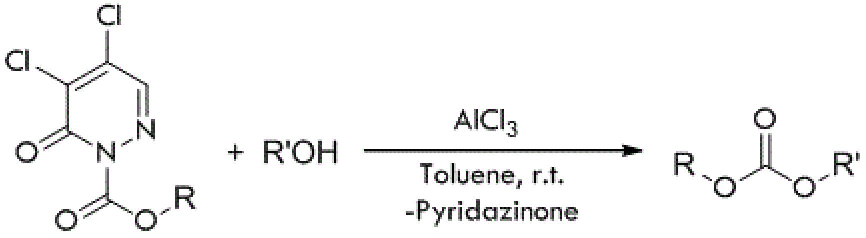
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Simple Synthesis of Organic Carbonates Using Activated Alcohols with 2-Alkoxycarbonyl-4,5-dichloropyridazin-3(2*H*)-ones

성기현 김보람 김점종[1] 윤용진[*]

경상대학교 화학과 [1]한국전자통신연구원 IT부품산업기술연구부

Organic carbonates are very important compound as the synthetic intermediates, solvents of Li-ion battery, fuel additive, reaction solvent and reagents. Carbonate derivatives were synthesized using toxic and/or gaseous carbonyl source such as phosgene, CO_2 and CO. These have also some drawbacks such as use of specific additives and side reactions. Inspired by recent other report of the conversion of *N*-phenylcarbamate to unsymmetric urea, we investigated to develop facile synthesis of carbonates. Herein, we present a convenient method of symmetric and unsymmetric carbonates using ($ROH-AlCl_3$) adducts with 2-alkoxycarbonyl-4,5-dichloropyridazin-3(2*H*)-ones.



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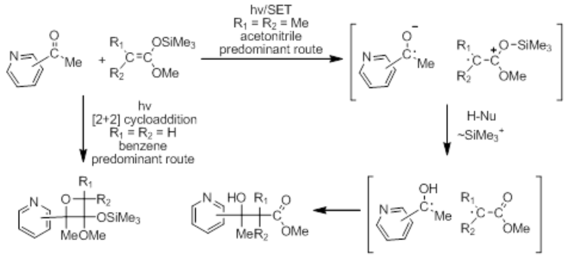
Photoreactions of Acetylpyridines with Silyl Ketene Acetals: SET vs [2+2]-Cycloaddition Pathways

조대원* 윤웅찬[1]

영남대학교 화학과 [1]부산대학교 화학과

Photoreactions of silyl ketene acetals with 2-, 3-, 4-acetylpyridines have been explored. The results of this study show that the acetylpyridines react with the electron rich, dimethyl substituted silyl ketene acetal via single electron transfer (SET)-induced excited state pathways to produce high yields of beta-hydroxyesters. In contrast, photochemical reactions of the acetylpyridines with electron deficient, nonmethyl-tethered silyl ketene acetal mainly lead to the formation of oxetanes arising by excited state [2+2] cycloaddition. In addition, solvent polarity is found to have a noticeable influence on the relative efficiencies of the competing SET- vs. [2+2]- excited state reaction pathways. However, pyridine moiety is not involved in photochemical reaction pathways. Finally, the results of this effort demonstrate that SET-induced photochemical reactions between acetylpyridines and electon rich, silyl ketene acetals represent a useful methodology to bring about beta-hydroxyester forming Claisen/ Mukaiyama condensation reactions under mild conditions.


hν/SET
R1 = R2 = Me
acetonitrile
predominant route
hν
[2+2] cycloaddition
R1 = R2 = H
benzene
predominant route
H-Nu
~SiMe3+
OSiMe3
OMe
Me
O-SiMe3
OH
HO
MeOMe
MeR2

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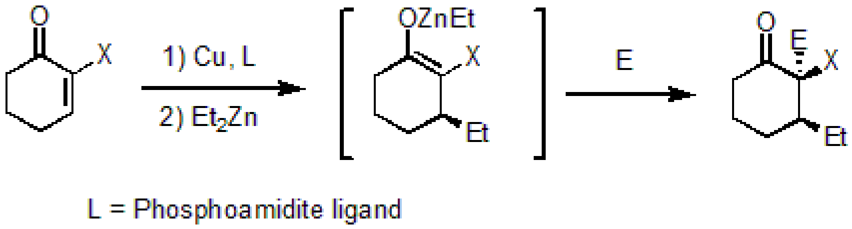
Tandem Asymmetric Cu-Catalyzed Conjugate Addition - Electrophilic Trapping

고영옥 이상기[1,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학/나노과학과

The great advance has been achieved in the two decades in the field of enantioselective Cu-catalyzed conjugate additions of organometallic reagents to Michael acceptors.[1] Especially, Cu-catalyzed conjugated additions of dialkylzinc reagents to cyclic or acyclic enones have been reported high enantioselectivities and yields with chiral phosphoramidate ligands. However, the reactivity and tendency for cyclic enones bearing an electron-withdrawing group at α-position has narrowly studied. As part of a research program on the development of tandem reactions, we investigated the tandem Cu-catalyzed asymmetric conjugate addition-electrophilic trapping reactions of organozinc reagents to α,β-unsaturated cyclic dicarbonyl compounds. In this tandem sequence, two-stereogenic centers including a quaternary stereocenter could be generated. Various kinds of chiral phosphoamidate ligands have been designed, synthesized, and investigated their catalytic activity for this tandem reaction.References: [1] T. Jerphagnon, M. G.Pizzuti, A. J. Minnaard, B. L. Feringa. Chem. Soc. Rev., 2009, 38, 1039?1075.



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Kinetic and Dynamic Kinetic Resolution of Sterically Bulky Propargyl Alcohols

오연옥 박재욱* 김만주*

포항공과대학교 화학과

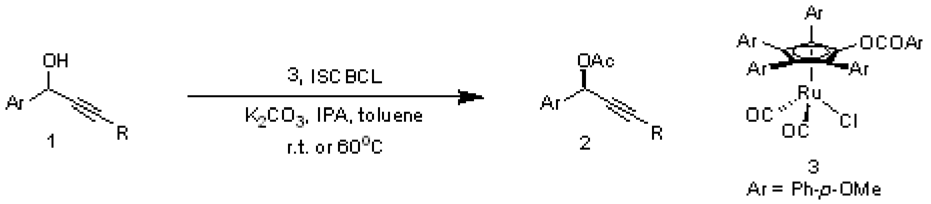
Most lipases are poorly active or enantioselective toward secondary alcohols which have two sterically bulky substituents at the hydroxymethine center. We found that an ionic-surfactant-coated *Burkholderia cepacia* lipase(ISCBCL) displayed good activity and high enantioselectivity toward those sterically demanding secondary alcohols.[1]

In the meeting, we would like to present the results from the ISCBCL-catalyzed kinetic and dynamic kinetic resolution of alpha-chiral propargyl alcohols with two bulky substituents at alpha- and gamma-positions.[2]The ISCBCL-catalyzed kinetic resolution of 1 provided good yields and excellent enantiomeric excesses (up to 99 %). The corresponding dynamic kinetic resolution of 1 by the combination of ISCBCL and a ruthenium complex 3 (as the racemization catalyst) in the presence of isopropenyl acetate (as the acyl donor) also gave similarly good results.

References

1. Kim, H.; Choi, Y. K.; Lee, J.; Lee, E.; Park, J.; Kim, M.-J. *Angew. Chem. Int. Ed.* 2011, *50*, 10944-10948.

2. Kim, C.; Lee, J.; Cho, J.; Oh, Y.; Choi, Y. K.; Choi, E.; Park, J.; Kim, M.-J. *J. Org. Chem.* DOI: 10.1021/jo3027627



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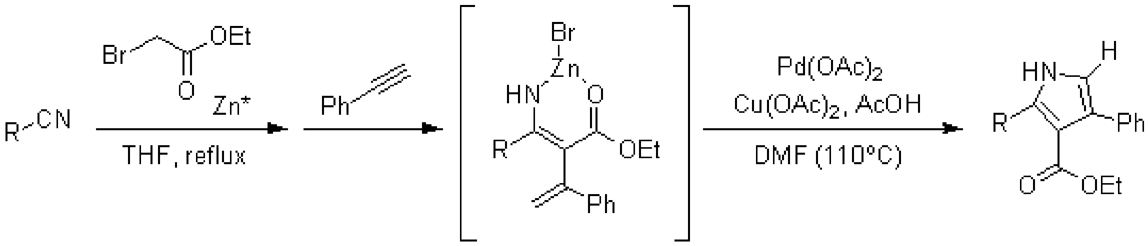
One-pot synthesis of pyrroles via tandem Blaise/vinylation/palladium-catalyzed intramolecular C-N bond formation.

최서영 김주현 이상기*

이화여자대학교 화학/나노과학과

Pyrrole is one of the most ubiquitous chemical motifs thathave been found in many natural molecules, phamarcheuticals, catalysts, and advanced materials. A number of classical methods including Paal, Paal-Knorr, and Hantzsch syntheses are known for synthesizing pyrrole derivatives, albeit many of them require multistep reactions. As part of our ongoing recent study on the development of tandem reactions by using the Blaise reaction intermediate, we investigated one-pot synthesis of polysubstituted pyrroles from the readily available nitriles through the regioselective vinylation, followed by Pd-catalyzed intramolecular heterocyclization of the Blaise reaction intermediate. The reaction of the Blaise intermediates with 1-alkynes produces α-vinylated β-enaminoesters via C-nucleophilic reaction. Combination of tandem vinylation and palladium-catalyzed Wacker-type oxidative N-C bond formation of the Blaise reaction intermediates affords the polysubstituted pyrroles.



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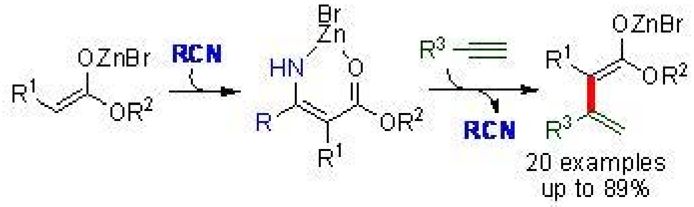
Nitrile-Mediated Tandem Intermolecular Addition of Unstabilized Enolates to 1-Alkynes

김주현 이상기*

이화여자대학교 화학/나노과학과

The intermolecular addition of enolates to non-activated C-C multiple bonds is a synthetically important reaction for C-C bond formation. During last decades, significant advances have been made in the addition of enolate nucleophiles to unactivated alkenes. In contrast, the intermolecular additions of enolate nucleophiles to alkynes have been largely unexplored. Moreover, due to the acid-base reactions of enolate with acidic acetylenic Csp-H, the addition of unstabilized enolates nucleophile to 1-alkynes is inherently difficult to achieve, and remained as a formidable challenge. As part of our ongoing recent study on the development of tandem reaction by using the Blaise reaction intermediate, we developed a conceptually distinctive nitrile-mediated tandem regioselective addition of unstabilized ester zinc enolates (Reformatsky reagents) to 1-alkynes and 1,3-enynes.



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Donor-Acceptor Conjugated Polymer Based on Alkoxysubstituted-MBI for High Performance Organic Photovoltaics

김남희 신경아 송수희 진영읍[1] 서홍석*

부산대학교 화학과 [1]부경대학교 공업화학과

Polymer solar cells (PSCs) have received increasing attention because of the potential for fabrication of light-weight, large area, and flexible light-harvesting devices through low-cost solution processing. Considerable progress has been made in this area, as evidenced by the improvement of the power conversion efficiencies (PCEs) of PSCs from around 1% to more than 9% over the past decade. PSCs usually adopt a bulk-heterojunction (BHJ) structure, where a phase-separated blend of donor and acceptor materials are used as the active layer. In most cases, fullerene derivatives, such as [6,6]-phenyl-C61-butyric acid methyl ester (PC61BM) or [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM), are used as acceptors, and conjugated polymers are used as donors.4,5 Because most of the solar energy is harvested by donor polymers, extensive research efforts have been devoted to developing small band gap conjugated polymers for PSCs. It is well recognized that both the band gaps and energy levels of donor polymers should be optimized simultaneously to obtain high PCEs. we design and synthesize three D?A alternating copolymers with thiophene and bithiophene as the donor unit and 4,7-dibromo-5,6-dioctyloxy-2,2-dimethyl-2H-indene as the acceptor unit. The above result demonstrates that the absorption and electrochemical properties can be improved by fine-tuning the conjugated polymer structure. The best solar cell performance obtained has a layered structure of ITO / PEDOT:PSS / PTDOMBI:PC71BM(1:4) / Al. Under white light illumination (AM 1.5 G, 100 mW/cm2), the obtained Jsc is 4.03 mA/cm2, Voc is 0.58 V, FF is 32%, and PCE is 0.76%. Study to improve the solar cell architecture and PCE is underway.

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Organic Sensitizers Based on 3,6-Disubstituted Carbazole and Quinacridone for Highly Efficient Dye-sensitized Solar Cells

양동욱 홍종인*

서울대학교 화학부

Solar energy is expected to be the most renewable alternative energy source. Dye-sensitized Solar Cells (DSCs) are attracting attention because of their relatively low cost of manufacturing, easy fabrication and comparatively high power conversion efficiency than other kinds of solar cells. As a key factor in highly efficient DSCs, dyes should possess several properties: Optimum absorption overlap with the solar spectrum for efficient light harvesting, appropriate HOMO and LUMO energy levels for efficient electron injection and regeneration, and hydrophobicity for minimizing charge recombination. In this respect, we have developed bulky organic dyes of a D-D-pi-A structure to reduce the molecular aggregation and enhance the blocking effect, thereby improving the Voc[1]. In this presentation, we report several organic dyes based on a 3,6-disubstituted carbazole moiety as an electron donating unit and a quinacridone pi-spacer as an electron transferring unit for efficient DSCs. Quinacridone, an electron-deficient unit employed as the pi-spacer, is not commonly used in DSCs but exhibited outstanding long-term stability when used with ionic-liquid electrolytes.[2] Not only photophysical and electrochemical properties of the dyes but photovoltaic performance of the DSC devices were systematically investigated. Details will be discussed in the presentation.Reference[1] Chem. Asian. J., 2012, 7, 343.[2] J. Mater. Chem., 2012, 22, 24356.

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Synthesis and Properties of Conjugated Polymers Based on Cyclopentadithiophene and Phenanthrothiadiazole Moiety

김남희 신경아 송수희 진영읍[1] 서홍석[*]

부산대학교 화학과 [1]부경대학교 공업화학과

Organic photovoltaics have attracted substantial attention due to their potential to provide an alternative renewable energy with low-cost, light weight and flexibility.A new acceptor unit, phenanthro[9,10-c][1,2,5]thiadiazole, was synthesized. New donor-acceptor conjugated polymers, PCPDTPTp and PCPDTPTm, were synthesized by Stille polymerization. This novel phenanthro[9,10-c][1,2,5]thiadiazole with electron deficient thiadiazole group can improve planarity of the compound. The solid films show absorption bands with maximum peaks at 450, 550 nm, respectively. Under white light illumination (AM1.5G, 100 mW/cm2), polymer:PCBM layers showed PCE of 1.80, 1.00%, respectively.

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Photovoltaic property and Characterization of Polymers Based on Phenanthrothiadiazole Moiety

김남희 신경아 송수희 진영읍[1] 서홍석[*]

부산대학교 화학과 [1]부경대학교 공업화학과

Finding an alternative source of renewable energy is recently an active research area. One of them is Organic photovoltaics with bulk heterojunction architecture due to its low-cost manufacturing and industrial and scientific interest. A new acceptor with phenanthro[9,10-c][1,2,5]thiadiazole unit was synthesized of conjugated polymers PCPDTDTPT and PCDTPT. The spectra of the solid films show absorption bands with maximum peaks at 492, 394 nmand the absorption onets at 620 and 519nm, corresponding to band gaps of 2.00 and 2.39eV. The devices with PCPDTDTPT:PC71BM with Tiox layer showed a Voc of 0.77V, a Jsc of 4.71 mA/cm2, and a FF of 0.36, giving a powewr conversion efficiency of 1.24%.

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Molecular modulated cysteine-selective fluorescent probe

정효성 강철훈[1] 김종승*

고려대학교 화학과 [1]경희대학교 동서의학대학원

We have demonstrated a selective molecular recognition of Cys over other structurally and functionally similar amino acids, Hcy and GSH, by its fluorescence turn-on through a Michael-type reaction. This can be achieved under physiological conditions by utilizing a comparatively lower pKa value of Cys to generate a stronger nucleophile, and by modifying hosts in such a way that the larger nucleophile experiences a higher steric factor to reach the electrophilic center. These points are evidenced from the lowest reaction rate constant (highest energy barrier) for GSH in the second-order reaction and supported by the highest interaction energy (calc.) for GSH. This probe detects Cys in aqueous solutions with a detection limit of $10^{?7}$ M. Moreover, the probe was successfully applied to the fluorescence imaging of intracellular Cys in HepG2 cells.

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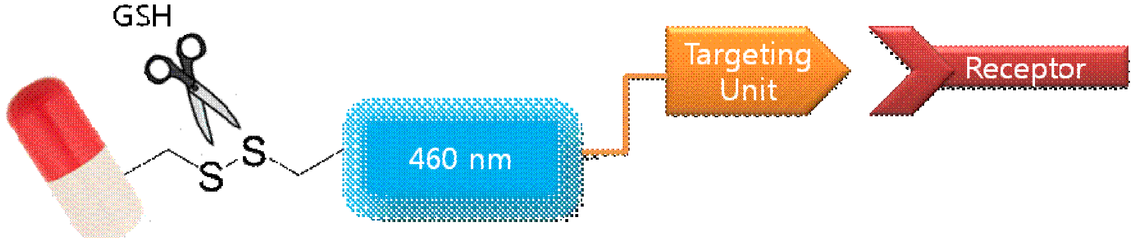
Asialoglycoprotein Receptor Mediated Camptothecin Prodrug for Visualization of Drug Delivery in Hepatocyte Cancer Cells

동방선 김종승*

고려대학교 화학과

Our research group developed a drug delivery system probe which enables us to visualize successful release of anti-cancer drug upon the stimulation by intracellular GSH. Through such system, the amount of drugs released by GSH, its intracellular pathway & subcelluar distribution status, and its resulting efficacy can be visually tracked down. The probe described here specifically targets hepatocyte cells by using terminal galactose as the radar to detect asialoglycol protein receptor which is expressed relatively abundantly in liver cells. Disulfide bond, which can be cleaved by thiols, links the anti-cancer drug Camptothecin and the fluorescence Naphthalimmide because it uses intracellular GSH as the driving force for the drug release. GSH is a type of thiol which is reported to exist more in cancer cells compared to normal cells, by a thousand fold, thereby ensuring the probe to be effectively reduced specifically in the designated cells. Therefore, the probe that initially emits blue fluorescence at 470 nm changes to a yellow fluorescence at 570nm after the probe is internalized in the cancer cell and cleaved by the intracellular GSH, enabling the visualization of the amount of the release of the camptothecin drug and its subcellular location. Furthermore, we tend to manipulate the drug’s pathway in order to investigate its efficacy as a drug depending on its final destination. We believe that such data will pave the way in investigating not only targeting cancer cells, but also in enhancing the accuracy in targeting its subcellular destination once it has been internalized. Such information is expected to contribute to researching drug release process & its kinetics and pave the way in practical application of early diagnosis of cancer.



Blue Fluorescence of the hepatocyte targeting DDS probe prior to drug release by intracellular GSH

Change in fluorescence to yellow green, indicating successful drug release by intracellular GSH

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1,8-Naphthalimide based DTTA Derivative: a Copper ion triggered Bimodal Contrast Agent for cellular imaging

장주희 김종승*

고려대학교 화학과

Magnetic resonance imaging (MRI) is an important imaging in diagnostic medicine. It provides high-quality three-dimensional images of tissue and anatomical resolution without use of injurious ionizing radiation. Gadolinium-based chelates are the most commonly used MRI contrast agents because the chelated Gd3+ metal ion enhanced MR signal by decreasing the longitudinal relaxation time (T1). As a result, T1-weighted MR image is brighter. We developed metal ions induced MR/Fluorescence signal enhanced bimodal imaging agent by taking of 1,8-naphthalimide framework with appended DTTA as Gd3+ chelating site. MR signal was enhanced in presence of biologically relevant target metal ions and fluorescence signal also altered. This dual modulated CA can be used as cationic sensor which is a new biocompatible detector for biologically relevant metal ions to detect them in a noninvasive manner.

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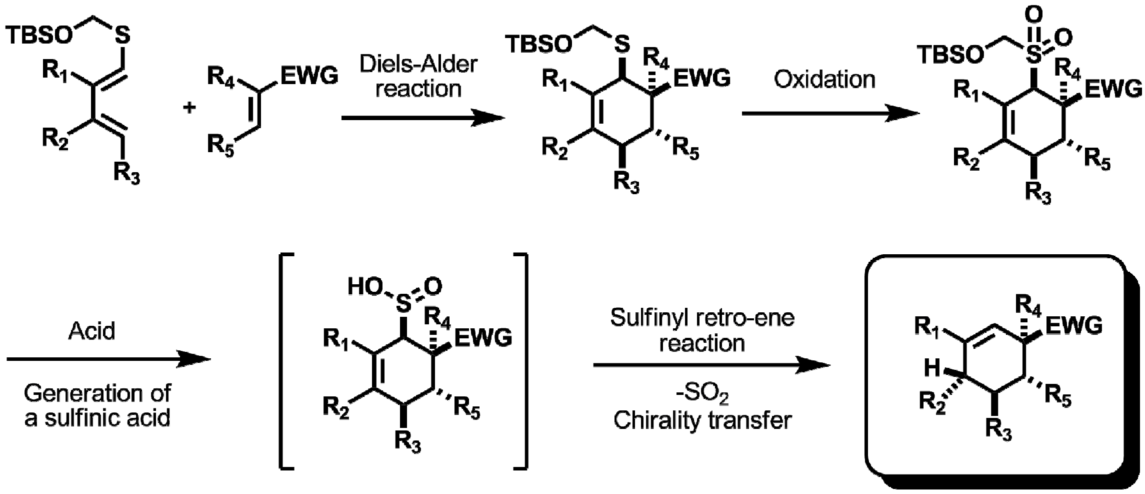
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Highly Substituted Cyclohexenes via Traceless Diels-Alder and Sulfinyl Retro-ene Tandem Reaction

최진 박호윤 이철범*

서울대학교 화학부

The Diels-Alder reaction has provided the foundation for some of the most impressive achievements in the area of cyclohexene derivative synthesis. Among various categories of the Diels-Alder reaction, the tandem reaction provides additional diversity to the Diels-Alder adduct. Our laboratory has been interested in sulfinyl retro-ene reaction that can be performed in tandem with the Diels-Alder reaction as a new post-modification sequence and developed a protocol for the synthesis highly substituted cyclohexenes. We have synthesized, designed and used (tert-Butyl)dimethylsilyloxymethyl (TBSOM) substituted dienes as a new diene for the Diels-Alder reaction. Using this new diene, the Diels-Alder reaction has been performed in thermal or Lewis acid catalyzed reaction conditions. The Diels-Alder adduct then can be oxidized and treated with an acidic reagent, whereby a sulfinic acid group is generated and undergoes a retro-ene reaction to give a series of cyclohexene core obtained via the reductive transposition. The reaction described here represents significant expansion of the scope of the Diels-Alder reaction. The details of our studies will be shown in this poster.


TBSO
S
R_1
R_2
R_3
+
R_4
EWG
R_5
Diels-Alder reaction
TBSO
S
R_4
EWG
R_1
R_2
R_5
R_3
Oxidation
O
TBSO
S
O
R_4
EWG
R_1
R_2
R_5
R_3
Acid
Generation of a sulfinic acid
HO
S
O
R_4
EWG
R_1
R_2
R_5
R_3
Sulfinyl retro-ene reaction
$-SO_2$
Chirality transfer
R_4
EWG
R_1
H
R_2
R_5
R_3

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Synthesis, Properties, and Photovoltaic Performances of Donor-Acceptor Copolymers Having Indenoindene and Benzimidazole Units

신경아 김남희 송수희 진영읍[1] 서홍석[*]

부산대학교 화학과 [1]부경대학교 공업화학과

Driven by the urgent need for a renewable energy supply, polymer photovoltaic technologies have been developed extensively in recent years. Bulk-heterojunction (BHJ) polymer solar cells (PSCs) have attracted tremendous attention due to their their advantages of having low cost and easy fabrication, being lightweight, and having the capability to fabricate flexible large-area devices. Recently, benzothiadiazole (BT) unit have attracted great interest for use in polymer molecule organic solar cells. In MBI, the sulfur at 2-position of BT unit was replaced with dialkyl substituted carbon, while keeping the 1,2-quinoid form, to improve the solubility of the polymers. A series of new semiconducting polymers with 2,2-dimethyl-2H-benzimidazole, 2,7-dihydroindeno[2,1-a]indene and thiophene (or bithiophene) units was synthesized using Stille and Suzuki polymerization to generate PININEDTMBIs (or PININEBBTMBIs). The absorption spectra of PININEDTMBI with thiophene units exhibit two maximum peaks at about 418 and 637 nm in solution. The solutions of PININEBBTMBI show two absorption peaks at about 438 and 634 nm which is red-shifted about 20 nm as compared to PININEDTMBI caused by the introduction of bithiophene units. In case of the most efficient polymer PININEBBTMBI, the device annealed at 100 oC for 10 min demonstrated a VOC of 0.78 V, a JSC of 6.66 mA/cm2, and a FF of 0.41, leading to the power conversion efficiency of 2.11%, under white light illumination (AM 1.5 G, 100 mW/cm2)

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Synthesis of the pyrrolo[3,2-b]pyrrole-based conjugated polymers and HOMO level tuning for high VOC photovoltaic cell

신경아 김남희 송수희 진영읍[1] 서홍석*

부산대학교 화학과 [1]부경대학교 공업화학과

Polymer-based organic photovoltaics (OPVs) have stimulated broad interest due to their potential advantages such as facile fabrication, low cost, lightweight, and flexibility. Much of the focus has been on the development of polymer-based OSCs which have seen a dramatic rise in efficiency over the last decade, and the encouraging power conversion efficiency (PCE) over 8% has been achieved from bulk heterojunction (BHJ). A new accepter unit, pyrrolo[3,2-b]pyrrole-2,5-dione, was prepared and utilized for the synthesis of the conjugated polymer containing electron donor?acceptor pair for OPVs. Pyrrolo[3,2-b]pyrrole-2,5-dione unit, regioisomer of the known pyrrolo[3,4-c]pyrrole-1,4-dione, is originated from the structure of stable synthetic pigment. The new conjugated polymer with pyrrolo[3,2-b]pyrrole-2,5-dione, thiophene and carbazole was synthesized using Suzuki polymerization to generate P1. The solid thin film of P1 shows absorption band with maximum peaks at 374 and 548 nm, and the absorption onset at 679 nm, corresponding to band gap of 1.83 eV. The field-effect hole mobility of P1 is 2.2×10?5 cm2/Vs. The device based on the polymer:PCBM (1:2) blend without thermal treatment showed a VOC of 0.82 V, a JSC of 6.28 mA/cm2, and an FF of 0.39, giving a PCE of 2.00%.

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Synthesis of phenathrothiadiazole-based small molecules as donor materials for organic photovoltaics

신경아 김남희 송수희 진영읍[1] 서홍석[*]

부산대학교 화학과 [1]부경대학교 공업화학과

In recent years, conjugated polymers have generated a large amount of interest as potential replacements. It is generally understood that organic photovoltaics (OPVs) have several major advantages over their inorganic counterparts, including the ability to fabricate lightweight flexible devices, the opportunity to make large area devices using low-cost solution-based techniques, and the variety of optical and electronic properties that can be attained through chemical synthesis. A common theme in the design of new donor is the incorporation of fused heterocycles into the materials' backbone. A new accepter with phenanthro[9,10-c][1,2,5]thiadiazole unit was synthesized and utilized for the synthesis of the small molecules for OPV devices. Lowering of the LUMO level through modification of the acceptor component in these D-A copolymers will enable improved light-harvesting characteristics, and adding fused aromatics should lead to a higher degree of crystallinity in the eventual oligomers, which could provide superior charge-transport properties. The HOMO?LUMO energy bandgaps of this material shows 1.81 eV for PBDTPT.

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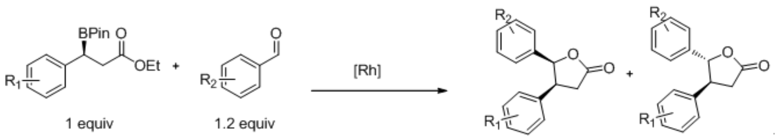
Rhodium-Catalyzed 1,2-Addition of Functionalized Boronates to Aldehydes.Asymmetric Synthesis of γ-Butyrolactones.

ZHANGCHANGWAN 윤재숙

성균관대학교 화학과

The Rh-catalyzed 1,2-addition and 1,4-addition of boronates to aldehydes, enones and imines, has spawned a major area of research. The 1,2-addition reaction has enjoyed significant development. However, the most of these reactions are limited to the use of sp^2-carbon boron derivatives(aryl- or alkenylboronic acids, esters or organotrifluoroborate salts). Recently, Aggarwal and co-workers reported rhodium-catalyzed 1,2-addition of secondary and tertiary alkyl trifluoroborate salts to aldehydes in the presence of [$\{RhCl(cod)\}_2$] in good yield and with retention of stereochemistry. Herein, we applied functionalized secondary organoboronic esters having sp^3 C-B bond to the rhodium catalyzed addition. We can synthesize enantioenriched γ-butyrolactones with high enantioselectivity.



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Synthesis of 3,4-Dihydroisoquinolin-1-ones by *in situ* Friedel-Crafts-type cyclization of *N*-Boc-carbamates via isocyanate intermediates

박희민 김상희[1,*]

서울대학교 약학대학 약학과 [1]서울대학교 약학대학/약학과

Dihydroisoquinolin-1-ones are extremely useful synthetic intermediates for the synthesis of various natural product scaffolds and biologically active compounds. Historically, the classic Bischler-Napieralski reaction was used for construction of dihydroisoquinolin-1-ones but the reaction has some problems, such as requirement of harsh conditions and low regioselectivity. Here in, we present development of the *in situ* Friedel-Crafts-type cyclization of *N*-Boc-carbamates as a versatile alternative to the original Bischler-Napieralski reaction for synthesizing dihydroisoquinolin-1-ones. The notable features of the reaction are that it involves the use of TF_2O and 2-chloropyridine, and *in situ* generated isocyanates are likely to be key intermediates, which is the possible cause of the high regioselectivity. Moreover, the method could be extended to substrates with less nucleophilic aryl moieties by the addition of acid additives and requires milder reaction condition than previous methods. Consequently, this method allowed the synthesis of various substituted isoquinolin-1-ones and related heterocycle-fused ring systems in good yields and with high regioselectivities.

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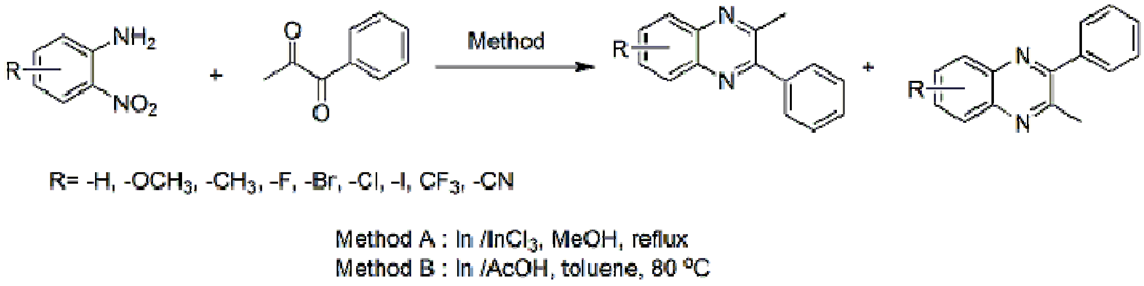
Synthesis of quinoxalines from o-nitroanilines via indium-mediated heterocyclizations (Ⅰ)

이근수 고아라 이병민[1] 김병효*

광운대학교 화학과 [1]한국화학연구원 신화학연구단

The quinoxaline derivatives are found in a number of drugs or drug candidates with various biological activities, such as anti-inflammatory, anti-viral, anti-bacterial, anti-biotic, and kinase inhibitor. Additionally, they are potential building blocks for the synthesis of organic semiconductors and electroluminescent materials. Indium metal is sable in water and toxicity observed for other metals are little known for indium. Because the first ionization potential of indium is as low as that of lithium or sodium, it is easy to act as a SET agent.In continuation of our efforts for developing for the the heterocycle synthesis, 2-methyl-3-phenylquinoxalines and 3-methyl-2-phenylquinoxalines were synthesized from o-nitroanilines with 1-phenyl-1,2-propanedione using indium/indium(Ⅲ) chloride or indium/AcOH in reasonable yields (61-98%). The ratio of regioisomers was confirmed by the NMR titration.



R= -H, -OCH$_3$, -CH$_3$, -F, -Br, -Cl, -I, CF$_3$, -CN

Method A : In /InCl$_3$, MeOH, reflux
Method B : In /AcOH, toluene, 80 °C

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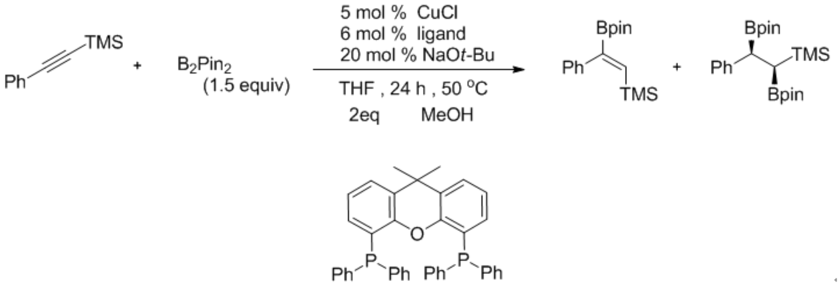
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper(I)-Catalyzed Boron Addition to Silylated Internal Alkynes.

채영미 윤재숙

성균관대학교 화학과

The boration of alkyne is a useful method for the preparation of alkenylboron compounds, Cu-catalyzed boration of internal alkynes using diboron reagents in the presence of alcohol, generates formally mono-hydroborated alkenylboron compounds with excellent regioselectivity. While the double addition reactions was highly efficient for aryl-substituted alkynylsilanes and silylacetylene, only monoborylation observed alkyl-substituted alkynylsilanes to yield (Z)-(β-borylvinyl)silanes under the developed catalytic conditions. A range of alkyl-substituted substrates were examined and the results will be presented.



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A proficient solution-phase synthesis of a natural piper amide-like compound library without chromatographic purification

장주림 김상희*

서울대학교 약학대학/약학과

Natural piper amides are known to exhibit broad biological activities including anti-inflammatory, antifungal, and antitumor activities. The structure of natural piper amides is characterized by the α,β-unsaturated amide scaffold appeared in many active compounds and pharmaceuticals. We were interested in this moiety and planned to develop a proficient solution-phase synthesis of a natural piper amide-like compound library. The β-phosphono amide was synthesized from β-phosphono-N-hydroxysuccinimidyl ester and subsequent Horner-Wadsworth-Emmons (HWE) type olefination with aldehydes generated the desired α,β-unsaturated amides. Girard's reagent T was used to make excess reactants into water-soluble byproducts in each step enabling to be removed by simple aqueous work-up purification only. This methods provided three points of diversity in aldehydes, amines, and the α-position of the amide and we synthesized totally 237 α,β-unsaturated amide compounds with high yield and purity. Several compounds of this library exhibited nanomolar to micromolar range of EC50 values toward recombinant bombesin receptor subtype-3 (BRS-3) known to be bound to GPCR receptor and related with obesity. We believe that this efficient solution-phase synthesis of natural piper amide-like compound library would be useful tools for further generation of chemical library and drug discovery.

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Asymmetric Synthesis of Hygroline and Pseudohygroline from Chiral Aziridine-2-carboxylate

이재덕 하현준 이원구[1]

한국외국어대학교 화학과 [1]서강대학교 화학과

1-Methyl-(2R) and (2S)-acetyl methyl pyrrolidin-5-ones were prepared from (3R) and (3S)-aziridin-2-yl-propanoate through methylative aziridine ring opening reaction with cyanide nucleophile followed by reductive cyclization. Methylation and the subsequent selective reductions afforded the asymmetric synthesis of hygroline and pseudohygroline which are pyrrolidine alkaloid natural products isolated from *Carallia brachiata* with potent biological and pharmacological activities.

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Simple Fluorescent Chemosensors for Polynitroaromatics:One Step Synthesis

이은비 조동규*

인하대학교 화학과

A simple fluorescent chemosensor was used to identify electron-deficient aromatic explosives in semi-aqueous media, by employing hydrophobic interactions and induced conformational strains. Despite being a simple molecule, fluorescent chemosensor 4 can detect < 2 ppb of TNT in a semi-aqueous solution. Furthermore, this chemosensor can be easily obtained via a single reaction using readily available starting materials.

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Synthesis of 4-Phenylquinolines and (5Z,11Z)-6,12-Diphenyldibenzo[b,f][1,5]diazocines derivatives under Microwave Irradiation

이용균 김아영 이언진 정대일 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Quinoline family have antiseptic, antipyretic, and antiperiodic properties. They are also used as catalyst, corrosion inhibitor, preservative, and as solvent for resins and terpenes. Quinolines are well known not only for their significant biological activities but also for their formation of conjugated molecules and polymers that combine enhanced electronic, optoelectronic, or nonlinear optical properties with excellent mechanical properties. Recently, much attention has focused on microwave assisted organic reaction in the absence of solvent. We report Synthesis of 4-phenylquinolines and (5Z,11Z)-6,12-diphenyldibenzo[b,f][1,5]diazocines under microwave irradiation.

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A Study on the Synthesis of Dihydroquinazolinones from Anthranilamide and Aldehydes by cyanuric chloride

정대일* 양정우 이도훈 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Quinazolinone is an exciting motif as regards its pharmacological importance and is a building block for about 150 naturally occurring alkaloids. They have been studied as an effective anticonvulsant, anti-inflammatory, analgesic and cyclooxygenase-2 (COX-2) inhibitor. 2-substituted-2,3-dihydro-4(1H)-quinazolinones are class of heterocycles which exhibit biological and pharmaceutical activity as antitumor, diuretic, and herbicidal agents. Recently, the synthesis of 2-substituted-2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids has been described and their catalystfree synthesis in ionic liquids or 2,2,2-trifluoroethanol has also been reported. We now report reactions of anthranilamide and aldehydes with cyanuric chloride(or 1,3-acetonedicaboxylic acid) as a catalyst.

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Synthetic Study of Thienopyridine Antiplatelet Drugs

정대일* 김수완 김인식[1] 송주현 한정태[2]

동아대학교 화학과 [1]동아대병원 산업의학과 [2]영동대학교 뷰티케어과

Clopidogrel and prasugrel are thienopyridine prodrugs that inhibit adenosine-5'-diphosphate(ADP)-mediated platelet aggregation in vivo. These compounds are converted to thiol-containing active metabolites through a corresponding thiolactams. The 2 compounds differ in their metabolic pathway to their active metabolites in humans.We tried the synthesis of thienopyridine metabolite like clopidogrel and prasugrel

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A Study on the Reaction of 2,3-Butanedionemonoxime and Aromatic Vicinal Diamines

최순규 권연근 김성태 정대일 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Micro-assisted heating under controlled condition has been proven as an invaluable technology for organic synthesis and their application in several cases has lead to acceleration of reaction, improvement of yield and selectivities. Especially, quinoxaline is very important structure in antibiotics like echinomycin, levomycin and actinoleutin. Moreover, it is basic structure in organic semiconductor, anion receptor, and DNA cleavage reagent. Generally, we have known combination of 1,2-diamines and α-diketones and 1,4-addition of 1,2-diamines and diazenylbutenes for synthetic method of Quinoxalines. We now report our reactions of 2,3-butanedionemonoxime instead of using α-diketone with various of aromatic vicinal diamines under microwave irradiation.

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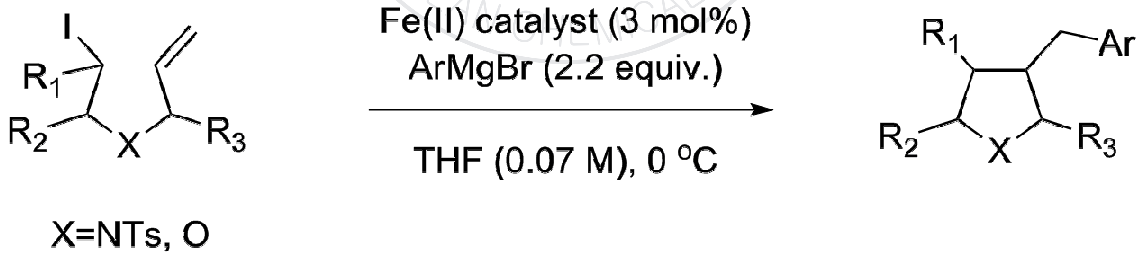
Iron(II)-catalyzed Tandem Radical Cyclization and Cross-coupling Reactions of Alkyl Halide with Aryl Grignard Reagent

김재곤 서진원[1] 백종화[1] 강은주[1]

경희대학교 화학과 [1]경희대학교 응용화학과

The radical reactions of alkyl halide have been well-known as carbon-carbon bond formation reactions. In despite of Fe-Grignard complex is one of the most efficient initiator for Fe catalyzed radical reaction, Grignard reagent is used only to activate Fe catalyst. Herein, we reported Fe catalyzed atom-economical tandem reaction of alkene-iodide in the present of equimolar aryl Grignard reagent. Aryl Grignard reagent is used to generate Fe-Grignard complex and the counter aryl anion is used in the further cross-coupling, thereby affording the tandem cyclization/cross-coupling radical reaction.



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Regioselective nucleophilic cyclization of allenes and dienes catalyzed by Fe(lll) and Cu(I) catalysts.

신예호 황준영[1] 김재형[1] 강은주[2]

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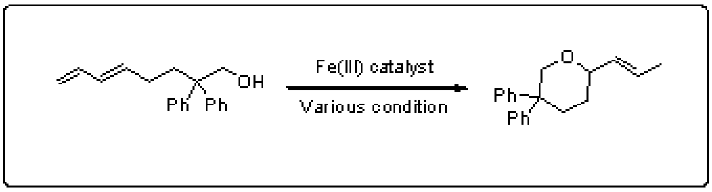
The development of efficient synthetic methodologies for C-C, C-O, or C-,N bond formation is of fundamental interest to modern organic chemists. The use of transition metals as catalysts to induce new C-C, C-O, or C-N bond formation. We research functionalization 1,3-diene amides or 1,3-diene alcohols and cyclized compounds containing O or N heteroatom by non-toxic, inexpensive, easy to handle Fe(lll) catalysts. It is worthy to investigate the cheaper and more easily available eco-friendly catalyst as unsaturated C-C bond activators toward nucleophilic attack. In our research aiming to develop green catalytic reactions, the nucleophilic cyclization reactions of 1,3-diene were catalyzed by Fe(III) to afford the corresponding heterocycle compound.


OH
Ph
Ph
Fe(III) catalyst
Various condition
O
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Ph

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Brønsted acid Catalyzed Tandem Flavan Synthesis with Phenols and Aryl Allenes

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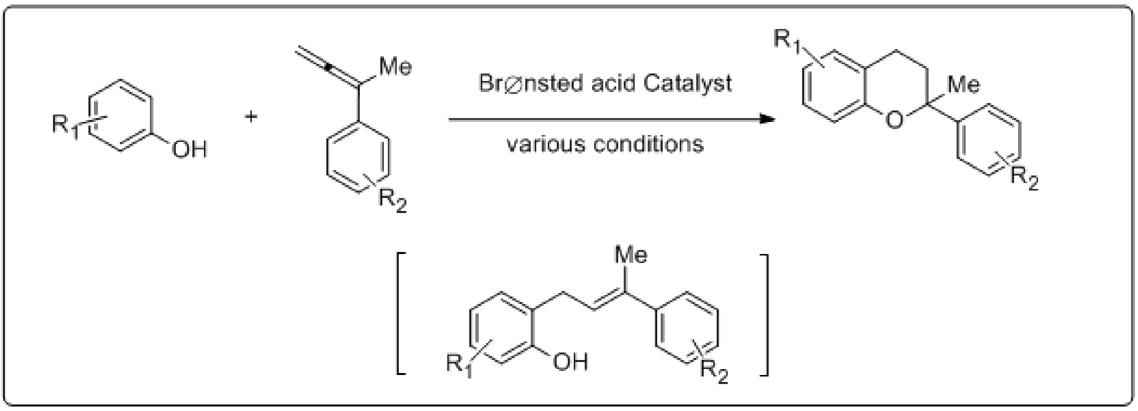
An efficient synthesis of functionalized flavans from commercially available phenols and easily available aryl allene derivatives is reported, which are important skeletons in biological and pharmaceutical fields. The synthesis involves a brønsted acid catalyzed intermolecular hydroarylation and intramolecular hydroalkoxylation reactions. This one-pot synthesis showed a high regioselectivity in both hydroarylation reacting at the terminal position of allenes and hydroalkoxylation forming 6-membered furan derivatives.



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Synthesis of energetic plasticizers from dinitrovaleric acid

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젬-다이나이트로를 에너지기로 도입하고 반대편에는 비극성 화합물인 선형 혹은 가지친 알킬기를 도입하여 기존의 에너지화 가소제의 극성을 낮추는 것을 연구의 목적으로 하여 합성을 진행하였다. 상업적으로 구할 수 있는 원료인 1,1-dinitroethane 을 출발물질로 하고 butyl, hexyl, heptyl, 2-ethylhexyl 등의 아크릴 reagent 로부터 Micheal addition 반응을 하여 합성하였다. 또 다른 합성방법으로는 dinitrovaleric acid 를 출발물질로 하고 알콜로부터의 esterification 반응도 진행하였다. 현재 두가지 반응 생성물의 열적 특성과 점도 특성 등을 비교분석 중이다.본화합물을 복합화약 조성의 가소제로 적용할 경우, 기존의 에너지화 가소제보다 극성을 낮추어 분자화약의 형상변형으로부터 오는 민감도를 낮출 수 있고, 비활성 가소제보다는 성능이 높아 둔감도와 성능을 동시에 향상시킬 수 있을 것으로 기대된다.

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Synthesis of New Donor-Acceptor OLED Electronic Materials Based on Phenothiazine and Quinoline

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경성대학교 화학과

Dono-acceptor (D-A) molecules have recently attracted considerable attention as electroluminescent multifunctional materuals for organic light-emitting diodes (OLEDs). D/A units could allow the control of the HOMO/LUMO levels and the emission color of the D-A molecule. EL colors including blue, green, yellow, and red have been achieved from OLEDs based on D-A molecules. in this study, the synthesis of new donor-acceptor molecules based on conjugated triphenylquinoline and phenothiazine via the Friedlander condensation and Suzuki coupling reaction have been described.

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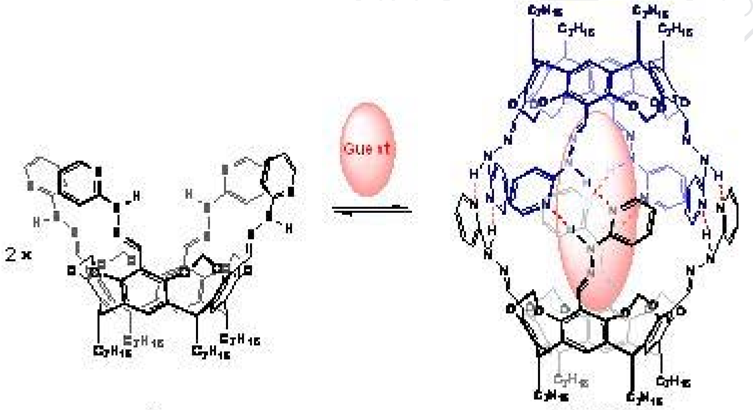
Molecular capsule controllable by pH switching

<u>박주완</u> 박연실 백경수

숭실대학교 화학과

A new self-assembled molecular capsule was developed by the introduction of four aminopyridine moieties on the upper rim of a imino-cavitand based on resorcin[4]arene. Cavitand 1 having four aminopyridine moieties self-assembles into molecular capsule 1_2 through the eight intermolecular amine N-H···pyridine hydrogen bonds when suitable guests are present in noncompeting solvent. Molecular capsule 1_2 encapsulates various neutral molecules to form complexes G@1_2 which could be dynamically controlled using pH switching. The synthesis and characteristics of molecular capsule 1_2 will be presented.



1

Guest@1_2

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Multigram synthesis using a continuous flow reactor

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Multigram synthesis can make the target product rapidly, easily and it is useful to the industry. Also continuous flow reactor has the attractive merit of using, rather than a conventional reactor, which is better control of reaction conditions, improved safety, and portability. And best of all, it is very usefully can make the targeted amount of the specific product at steady state. In this research, we used the photooxygenation on particularly being designed the continuous flow reactor, that has the pored tubing tube to well offer oxygen and can sufficiently get the light. So specially being designed reactor has high efficiency of photooxygenatoin gas-liquid reaction. Through this reactor, Rose oxide and Ascaridole are obtained from (-)-beta-cirtonellol and alpha-terpiene. The photochemical oxidation of (-)-beta-cirtonellol is used to produce (-)-rose oxide as an elemental substance in the perfume industry, and also ascaridole is mainly used as an anthelminitic drug.

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Palladium chemistry in the switchable gas conditions in microreactor

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Transition metal-catalyzed coupling reactions are powerful tool for C-C bond formation. In particular, palladium chemistry known as heck and suzuki reactions is widely use in a number of syntheses. Recently, biaryl derivatives synthesis via one-pot tandem Pd-catalyzed boron-Heck and Suzuki reaction was reported. The previous studies, however, had an inconvenient process such as changing the gas condition. Herein, our new approach to change the gas atmosphere is easy by using the switchable gas system in microreactor. This suggested that we could simply change the different atmosphere, and the synthesis process is more convenient and efficient in good yield. Furthermore, we can handle stably at high temperature and accelerate the reaction rate.

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Chemical analysis based on IR thermal camera using Microfluidic systems

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Microfluidic systems have recently attracted much interest for various research and applications of chemistry field by mixing, separating and handling different components at micro-scale. As a proof of concept, this paper presents a droplet-based microfluidic platform for miniaturized combinatorial synthesis. Using hydrophilic surface of Lab on a chip(LOC) for generation of oil-in-water droplets. It has excellent chemical compatibility, high throughput generation of a few ?m droplets and high visibility. Furthermore, This platform has dimensional scaling benefits that have enabled controlled and rapid mixing of fluids in the droplet reactors. in addition, droplet-based systems also will be used to directly analysis of heat of reaction during flow process. The final application of these research has shown that using a thermal imaging camera to measure the heat of reaction as a visible that accompanies a chemical reaction. The heat of reaction is expected to be able to quickly and easily identify compared to conventional chemical analysis using this method.

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Supramolecular Control of 1-D and 2-D Self-assemblies based on Copillar[5]arene

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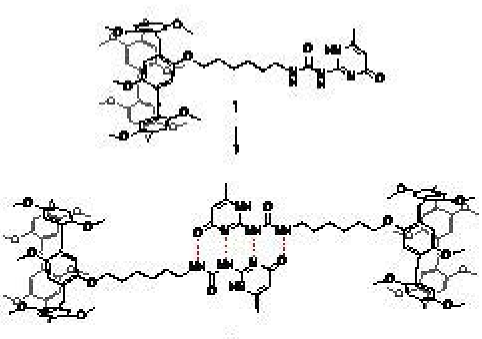
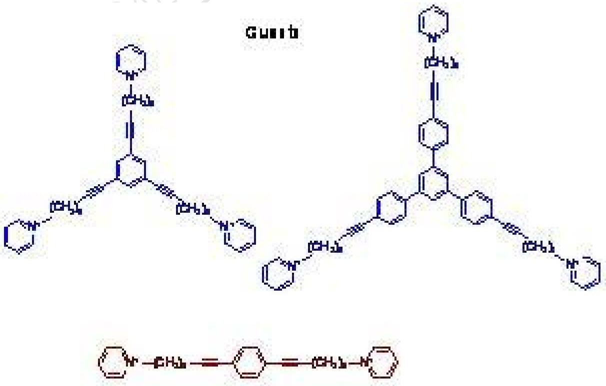
숭실대학교 화학과

Copillar[5]arene 1 mono-substituted with ureido-4[1H]-pyrimidone itself forms stable dimer 1_2 by quadruple hydrogen bonds, and the dimer 1_2 can self-assemble into supramolecular structures through cation-π interactions when tri-cationic and/or di-cationic bridging guests are present. 1-D and 2-D supramolecular self-assemblies could be controlled in their size and shape according to the sequence of the addition of copillar[5]arene 1 and the cationic bridging guests. The synthesis and characteristics of these self-assembled supramolecular structures will be presented.



1_2



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Novel Cadmium Ion Colorimetric Chemosensor through imine Hydrolysis

심남연 윤희상 남계춘

전남대학교 화학과

Recently there has been a lot of interest in the design, synthesis and evaluation of colorimetric sensors that selectively complex metal ions because of their potential analytical applications in many fields, for example, chemistry, medicine, biology and the environment. In particular, Cd2+ is the environmentally important metal ions due to their detrimental effects on human health. Chronic cadmium exposure can cause renal dysfunction and increased incidence of certain forms of cancer. Accordingly, considerable attention has been devoted to the development of colorimetric chemosensor for the detection of Cd2+ with sufficient selectivity. Colour changes that can be detected by the naked eye are widely used as signals for events owing to the inexpensive equipment required or no equipment at all. In pursuit of a selective Cd2+ ion chemosensor, an imine derivatives were synthesized, and its cation binding properties were investigated by 1H NMR, UV-vis spectroscopy, color changes, and X-ray structural analysis.

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Toward new helical structures in unnatural peptides

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연세대학교 화학과

The natural peptides (α-peptide) have been shown to adopt a helical conformation defined by C=O(i)→ N-H(i + 3) (“12-helix”) and C=O(i)→ N-H (i + 4)(“α-helix”). The unnatural peptides have also been observed to adopt a helical conformation defined C=O (i) → N-H(i + 3) (12-helix). Here, we designed chimera α/β-peptides backbone to observe α-helix ((i)→ (i + 4)) structure. A number of studies of the former have been already accomplished, but little research has been achieved until now. In this work, we synthesized the Dimethyl trans-2-aminocyclopentanecarboxylic acid (dm-ACPC) by using reductive amination. First, we synthesized starting material, methyl 4,4-dimethyl-2-oxocyclopentane carboxylate, for dm-ACPC using Dieckmann cyclization and microwave-assisted Wolff rearrangement of cyclic 2-diazo-1,3-diketones. In addition, we synthesized several chimera oligomers that contain α/β unit by using canonical synthetic method and peptide coupling strategies.

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Study on the conformational behavior of depsipeptides containing unnatural residues

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Within the past decade, the folding properties of several types of foldamers with unnatural backbones have been explored. At this point, We will discuss a new helical secondary structures of depsipeptides. Depsipeptides containing one or more ester bonds in addition to the amide bonds have emerged as an important source of biomedical compounds. In this study, We incorporated unnatural residues into a depsipeptide, then studied on the conformational behavior of depsipeptides.

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Structural Characterization of 1:1 α/β-Peptides containing 8-aminocyclooct-4-enecarboxylic acid

이우형 권선미 **Ilia A. Guzei[1]** 강필재 최수혁* 최문근

연세대학교 화학과 [1]Department of Chemistry, Univeristy of Wisconsin-Madison

The research of oligomers that contain alternative α- and β-amino acid residues is a fascinating topic to explore synthetic foldamers that adopt helical secondary structures. These foldamers that show such conformational propensities as helix, sheet, and turns play pivotal roles in living systems. What is more, the conformationally restricted β-amino acid residues give the outstanding ability to maintain conformational stability with hydrogen bonding interaction, including the intrinsic attributes of β-amino acid residues like willingness to form well-defined secondary structure as few as four residues, the richer possible derivatives than α-amino acid, and superior stability toward enzymatic degradation. In addition, the foldamers with heterogeneous backbones have the several advantages. The alternating α/β-peptides can display distinct helical folding patterns with respect to the direction of carbonyl groups. One is a backward orientation of the carbonyl bonds that have the aligned direction of macrodipole with α-helix, and the other is an alternating orientation of the carbonyl bonds that have the reduced overall macrodipole. A number of studies of the former have already been accomplished, including accounts of interconverting helical formations between 11-Helix and 14/15-Helix. On the other hand, little research of the latter was achieved until now. Accordingly, we have focused on the topic of the study of the alternating α/β-peptides that promote distinct helical folding like the latter. In this work, we have prepared β-lactam that is a precursor to restricted β-amino acid residues by using [2+2] cycloaddition with chlorosulfonyl isocyanate (CSI) and 1,5-cyclooctadiene. We also synthesized a series of α/β-peptides in a 1:1 alternating pattern by using canonical synthetic method and peptide coupling strategies. Furthermore, we have studied structural information of our foldamers with respect to helicity with 1D NMR, 2D NMR, X-ray crystallography, and circular dichroism spectroscopy.

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Fluorescent Off-On Chemosensor for Anions with Antraquinone Based on Triphenylphosphine

윤희상 심남연 남계춘

전남대학교 화학과

Design and development of artificial molecular systems for sensing anions in biologically relevant conditions is a challenging task in supramolecular chemistry. In particular, sensing anion has attracted increasing interest in the molecular recognition community because of its pivotal importance in many areas of biological and chemical sciences. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, the development of reliable sensors for F- is needed for environment and human health care. Colorimetric chemosensors can be effectively used as a tool to analyze and clarify such roles of charged chemical species in living system as well as to measure the amount of ions. Among anion receptors, colorimetric chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition.

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Glucose-Neopentyl Glycol (GNG) Amphiphiles for Membrane Protein Crystallization

조경호 채필석*

한양대학교 생명나노공학과

Membrane proteins carry out various functions such as signal transduction, material transfer and cell-cell recognition across lipid barriers. Our understanding of membrane protein structure and function, however, is significantly hampered by the difficulties associated with handling these bio-macromolecules. Amphipathic agents, called detergents, are used inevitably for membrane protein manipulation and play pivotal roles in determining the success of protein structure analysis. Here we introduce Glucose-Neopentyl Glycol (GNG) amphiphiles designed for this purpose. This class of agents displayed favorable behaviors toward membrane protein solubilization and stabilization. More importantly, a GNG agent was successfully used in the structure determination of a sodium-pumping pyrophosphatase. These results indicate that the GNG agents could be promising as tools for membrane protein study.

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The Design and Synthesis of Hydroxylbenzyl Borondipyrromethene (BODIPY) Derivatives

김철용 이정태*

한림대학교 화학과

BODIPY is a well-known fluorescent dye and has recently been studied as a solar cell. Usually fluorescent dyes do not have a lot of difference between λ_{ab} and λ_{em}, give that, BODIPY has relatively a large stokes-shift between λ_{ab} and λ_{em}. Furthermore, it has narrow emission bandwidths and high molar absorption coefficients. The introduction of various functional groups, especially water solubilizing moeities, to the bodipycore could change its physical chemical charateristics. Here we report the design, synthesis and characterization of the hydroxylbenzyl BODIPY dyes suitable for in vivo imaging in physiological condition.

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Light-Driven Molecular Shuttle based on Calix[4]arene

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고려대학교 화학과

Supramolecular systems that can be converted from one state to another by an external stimulus (such as chemical, optical, electrical, and mechanical on the nanometer scale) are of utmost interest in the fields of molecular memories, binary logic computing and molecular machines. Molecular switches that are capable of the controlled release or capture of guest species have potential applications in triggering chemical or biochemical reactions and for transporting species across membranes. Therefore development of reversible switches that can undergo repeated release-and-recapture cycles are significantly important. Molecular switching can be controlled by chemical, optical, thermal or electrical stimuli, however, light is especially useful because it works rapidly, remotely, reversibly and can be controlled precisely in space and in time. Calixarenes are flexible macrocyclic compounds and useful building blocks for the construction of relatively rigid cation receptors and carriers with desired properties. From last few years our research focused on the design and development of calix[4]arene based receptors for different analytes. The present work focus on the design, synthesis and evaluation of light driven molecular shuttle based on calix[4]arene appended with two different azacrowns. The molecular shuttle involves the metal ion translocation by a sole light stimulus, without protonation or any other chemical modification of the molecule. The calix[4]arene shuttle bear two different photoactive centers which are excitable at two different wavelengths, in order to fully control the back and forth movement of the cation. Upon irradiation of a photoactive center of calix[4]arene shuttle at specific wavelength, a positive charge would be developed in the vicinity of a bound cation which then push the bounded cation towards the other site. The same will happens when molecular shuttle exited at different wavelength. Therefore, we present here a light-driven molecular shuttle based oncalix[4]arene.

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Dual-Color Imaging of Mitochondria and Lysosomes using Two-Photon Fluorescent Probes

김형중 김환명*

아주대학교 에너지시스템학부

Mitochondria and lysosomes are found in almost every eukaryotic cell. Mitochondria provide energy of the cells, while lysosomes are used to digest food or break down the cells when it dies. These two organelles play crucial roles in autophagy. Autophagy plays critical roles in many physiological and pathological processes. Old, damaged, or surplus mitochondria are the major targets for autophagy. An attractive approach to detect this function in deep inside the tissue is through the use of two-photon microscopy (TPM). Herein, we report that a pair of two-photon (TP) fluorescent probes for lysosome and mitochondria, which emit TPEF in the short (BLT-blue) and long wavelength regions (FMT-green). These probes emit strong TP excited fluorescence in the different spectral ranges and can simultaneously detect the activities of lysosome and mitochondria in live cells and tissues for a long period time by TPM with minimum interference.

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

Design of Ratiometric Two-Photon Fluorescent Probes for Bioimaging Applications

이효원 김환명*

아주대학교 에너지시스템학부

Two-photon microscopy (TPM) has become essential to the study of physiology, neurobiology, embryology and tissue engineering, because of the capability of the molecular imaging deep inside living tissues. A variety of two-photon turn-on probes has been developed to date for make the most use of TPM. Their turn-on responses, however, can vary depending on the imaging conditions such as probe concentration and incident laser power, making it unsuitable for quantitative detection. Therefore, ratiometric imaging with suitable probes are an essential tool for quantitative detection of various biological phenomena in living cells and tissues. Herein, we present the design, synthesis, photophysical properties, and TPM imaging application of ratiometric two-photon fluorescent probes that can detect intracellular thiols and enzyme activities through the use of TPM.

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

Design of Two-Photon fluorescent Probe for Amyloid-β Plaques in Living Mice

허철호 김형중 김환명*

아주대학교 에너지시스템학부

Alzheimer's disease (AD) is an age related neurodegenerative disorder with cognitive impairment and chronic dementia. The pathogenesis of AD is associated with beta amyloid (Aβ) containing amyloid plaques and neurofibrillary tangles in specific brain region. Direct detection of Aβ plaques is emerging as a key challenge for elucidating fundamental aspects and early diagnosis of AD. An attractive approach for the in vivo imaging of Aβ plaques is the use of two-photon microscopy (TPM). TPM has the advantages of increased penetration depth (> 500 μm), localized excitation, and prolonged observation time. However, there has been no report on the development of two-photon (TP) fluorescent probe that is applicable for in vivo imaging for Aβ plaques by TPM. Herein, we have designed a TP fluorescent probe (SAD1) that shows a significant TP action cross section (170 GM), high sensitivity and selectivity for Aβ plaques, and pH insensitivity in the biologically relevant range. SAD1 readily enters the brain through the blood brain barrier (BBB) and can direct three dimensions (3D) monitor the individual Aβ plaque in living transgenic mice brain at more than 380 μm depths with minimum background emission and photo-bleaching artifacts.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of 3-substituted isoindolinones via radical addition to C=N bond in the presence of Lewis acid

ZHANGLIANJIN 장두옥*

연세대학교 화학과

The important and widespread use of 3-substituted isoindolinone skeleton in many drugs, of natural and synthetic origin, has led to interest in its synthesis. Much effort has been focused toward preparing 3-substituted isoindolinones. However, there remained considerable scope for improvement of the reaction conditions such as a more suitable catalyst, commercially available starting materials, simple reaction steps, and obtaining higher yields. We investigated an effective synthetic route to afford 3-substituted isoindolinones. Treatment of benzoyl hydrazones derived from methyl 2-formyl benzoate derivatives with diphenylsilane, alkyl iodide, Et_3B in the presence of Lewis acid gave the corresponding 3-substituted isoindolinones in high yields.

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

The on/off fluorescence switching of rhodamine 6G derivative

장우식 김기백 손문수 장승현*

대구대학교 화학과

The on/off fluorescence switching of these chemosensors was based on structure change of the rhodamine moiety between spirocyclic and open/close ring forms. Thus Structure changed rhodamine 6G derivative is displayed strong fluorescence. These synthesized compounds were confirmed by FT-IR, H-NMR, FAB-Mass measurement. And selectivity(Fe^{3+} > Al^{3+} > Sn^{2+}) of Metal appeared in the fluorescence spectrum measurement.

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

Synthesis of recognition and fluorescence properties new kinds of bis-pyrene compounds

손문수 김기백 장우식 장승현*

대구대학교 화학과

In this research, we have studied the molecular recognition about various metals and the character of fluorescence including pyrene by synthesized new host material. The structures of all reaction products were identified by ^{1}H-NMR,GC-Ms,FAB-Ms,FT-IR. We synthesized new host compounds containing bis-pyrene (C1 and C2). Compound1 was synthesized from 2,2'-oxybis(ethylamine and 1-pyrene carboxaldehyde(C1), Compound2 was synthesized from 1,2'-bis(2-aminoethoxy)ethane and 1-pyrene-carboxaldehyde(C2). New host compounds had a sensitive recognition fluorescent properties against various metals.

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

Synthesis and Recognition properties of new Crown Ethers containing fluorene moiety.

김기백 손문수 장우식 장승현*

대구대학교 화학과

New kinds of crown ethers containing fluorene compounds were synthesized by fluorene and crown ethers functionalized. They are in the ratio of 1 : 1 respectively imine was synthesized by the reaction. Compound 1 was synthesized from 9H-fluorene-2-carbaldehyde and 4'-aminobenzo-15-crown-5. Compound 2 was synthesized from 9H-fluorene-2-carbaldehyde and 4'-aminobenzo-18-crown-6. Synthesis, fluorescence properties will be discussed. The structure of compound 1 and compound 2 were characterized by ^{1}H NMR, UV-Vis and IR spectroscopy. We will also present some recent recognition results of fluorescent properties of the crown ethers.

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

Structural Characterization of 11/9-Helical 1:1 α/β-Peptides by Racemic Crystallography

이미혜 심지현 강필재 **Ilia A. Guzei**[1] 최문근 최수혁*

연세대학교 화학과 [1]Department of Chemistry, Universty of Wisconsin-Madison

Foldamers are any polymers that have specific conformations in three-dimensional space. Among these polymers, peptide foldamers can form stable secondary structures like biopolymers (proteins and RNA) by variable intramolecular interactions including hydrogen bonds. In this work, we designed and synthesized 1:1 α/β-peptides that consists of D-Alanine and (1R, 2S)-2-aminocyclohexanecarboxilyc acid (cis-ACHC) and studied their conformation with various methods.In general, it is widely known that the racemic compounds more rapidly crystallize than their enantiopure compounds because the racemates can achieve centrosymmetric arrangements. So, we additionally synthesized the opposite chiral α/β-peptides and obtained the cystals from their racemic mixtures. These crystal structures adopted centrosymmetric arrangements and obviously showed that α/β-peptides form 11/9-helices. In addition, these α/β-peptides also have a tendency to form 11/9-helical conformation in solution state according to the study by using IR, NMR and CD spectroscopy.

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

Using Iminium/Copper catalysis, Synthesis of α,β-Disubstituted Aldehydes

이화정 장혜영[1,*] 정원지[2]

아주대학교 응용화학과 [1]아주대학교 화학과 [2]아주대학교 에너지시스템학부

The combination of a chiral amine catalyst and a copper complex induces α,β-disubstituted aldehyde syntheses from unsaturated aldehydes. Highly optically active α,β-disubstituted aldehydes were synthesized with good yields in tandem reaction using iminium/copper catalysis. The β-substitution of aldehydes occurred by iminium-catalyzed diethylmalonate Michael addition to α,β-unsaturated aldehydes, followed by copper-assisted 2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO) addition at the aldehyde α-position. The cyclization of α,β-Disubstituted Aldehydes has been tested and analysis by crystallography.

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

Organic Base-mediated acetylene carboxylation using carbone dioxide

임유나 지미란 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Recentyl the use of carbon dioxide (CO2) as a C1 building block for chemical synthesis has attracted much interest because of its abundance, cost-efficiency, nontoxicity, and high potential as a renewable source. As a CO2 adsorption reagent, 1,5,7-triazabicyclo[4,4,0]dec-5-ene(TBD) has been utilized. In this study, the organic base(TBD)-mediated carboxylation of acetylene derivatives under conditions that are free of transition metals, inorganic salts, and organometallic reagents has been reported. 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, CO2 fixation to acetylene occurs under environmentally benign and free of metal species conditions

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Selective Detection of Mitochondrial Copper in Liver Cells with a Novel Fluorescent Probe

이윤학 강철훈[1,*] 김종승[*]

고려대학교 화학과 [1]경희대학교 동서의학대학원

Nature has originated sophisticated machinery to control the activities of essential trace elements, which contain enzymes, cofactors with catalytic functions, and structural support elements in human beings. Among these elements, copper is the third most abundant essential trace element in a variety of biological process and can be generally found as Cu2+ in living environment. However, unbalanced uptake of copper homeostasis can cause many human diseases, especially liver disease with long-term exposure. Thus, developments of sensitive techniques for the detection of Cu2+ from pollutants are very important to prevent poisoning in environmental and biological fields. Here, we present the design, synthesis and evaluation of a novel fluorescent probe for imaging labile copper level in liver mitochondria. This probe consists of naphthalimide with a copper chelator to provide a selective and sensitive fluorescence quenching with copper. Further, it is a multifunctional probe that incorporates a single galactose moiety as hepatocyte targeting unit, and a triphenylphosphonium ion as mitochondria-specific targeting unit. The ability to recognize real-time copper fluxes in living cells offers potentially opportunities to monitor copper in biological systems.

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

Conformational analysis of 1:1 α/β peptides contanning 2-aminocyclooctane

권선미 이우형 최수혁*

연세대학교 화학과

Proteins called as polymers play a very important roles in living system. For example, catalysis, specific binding, directed flow electrons. In general, proteins have specific compact conformations and they are composed of amino acids connected by peptide bonding. We synthesized the unnatural polymers. Unnatural polymers are called as foldamer. Foldamers adopt a specific compact conformation and form stable secondary structure by intramolecular interaction including hydrogen bonds. These foldamers can form well-difined secondary structure such as helices, sheets. In this work, we synthesized the 1:1 α/β-peptides contanning 2-aminocyclooctane. The conformational behaviors of the oligomers were analyzed by NMR, 2D, CD spectroscopy.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and conformational analysis of unnatural peptides containing cis-4-Aminopiperidine-3-carboxylic acid

심지현 이미혜 최수혁*

연세대학교 화학과

Foldamers are unnatural peptide oligomers that adopt compact, specific and predictable shapes. Unnatural peptide oligomers with a strong tendency to adopt specific and predictable conformations in solution have been the subject of extensive investigation in recent years. we prepared cis-4-Aminopiperidine-3-carboxylic acid(cis-APiC) in enatiomerically pure form and synthesized a number of peptide oligomers containing cis-APiC. The conformational behaviors of the oligomers were analyzed by various methods.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric synthesis of cyclic γ-amino acids with five-membered ring constraint

정윤식 강필재 최수혁* 최문근 정낙철[1]

연세대학교 화학과 [1]고려대학교 화학과

Synthesis and studies of unnatural amino acids have been of interest to chemists for decades. Since γ-amino acids play an important role in nervous system, they have intrigued many scientists following Seebach and Hanessian’s studies. Moreover, γ-amino acids are the key of treatment of disease related to neuro-system such as Parkinson's disease and Alzheimer's disease. To synthesize cyclic gamma amino acid stereoselectively, Methyl 2-(2-oxocyclopentyl) acetate and 1-phenylethylamime(PEA) were used as starting materials and sodium triacetoxy borohydride was used as reducing agent.The structurally-restricted and stable products were obtained in two ways; 1)Direct reductive amination, 2)Indirect reductive amination in two steps (imine preparation followed by reductive amination).The other starting material was tested to compare with non-protecting reactant. Diverse solvents, acids and different temperature conditions have also been tested.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A new synthetic method towards trans-3,4-dihydroxy-2-alkylpyrrolidines

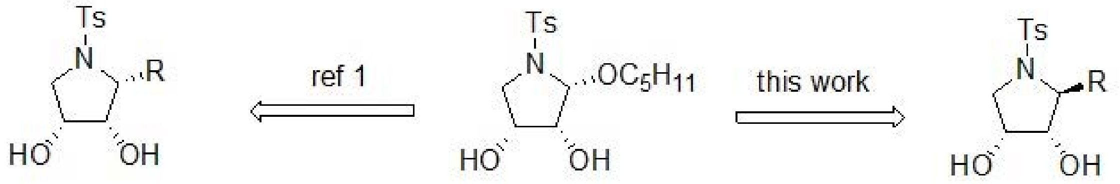
강소영 김동길 이영호*

포항공과대학교 화학과

We recently developed a new synthetic strategy towards cis-3,4-dihydroxy-2-alkylpyrrolidines which exploits the stereodefined cyclic N,O-acetals. In the course of our efforts to extend the scope of the reaction, we recently developed a synthetic pathway towards diastereomeric trans-3,4-dihydroxy-2-alkylpyrrolidines. Notably, the protective group on the hydroxyl groups played a critical role. Application of the method in the synthesis of alkaloid natural products will be also introduced.

Referecne

1. Kim, H.; Lim, W.; Im, D.; Kim, D.; Rhee, Y. H. *Angew. Chem. Int., Ed.* 2012, *51*, 12055.



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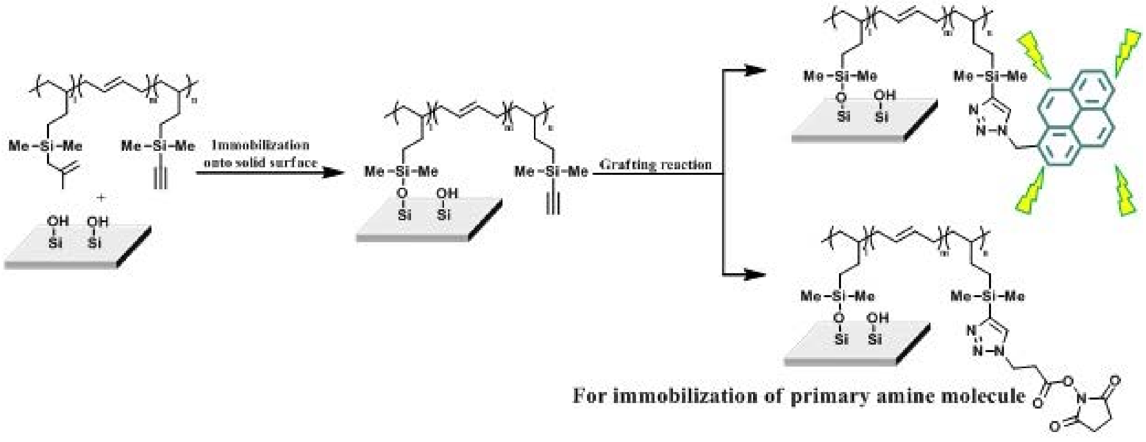
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Immobilization of Dual-Functionalized Polybutadiene onto Solid Surface for Functional Hybrid Materials

김민석 박정우 전철호*

연세대학교 화학과

In this research, we describe fabrication of highly robust organic-inorganic hybrid material that can be modified to various functional groups by catalytic grafting reaction. Although, we developed immobilization of functionalized monomer onto solid surface, we found the low immobilization efficiency. To improve this problem, we used polymer, which could be functionalized. For this purpose, we chose polybutadiene, which has many vinyl groups that can be transformed into various functional groups. Polybutadiene can be transformed into both methallysilyl, and silylacetylene group-impregnated polymer. To measure immobilization efficiency, a calibration curve was made by immobilizing. Using this calibration curve, we measure the grafting efficiency onto solid surface.



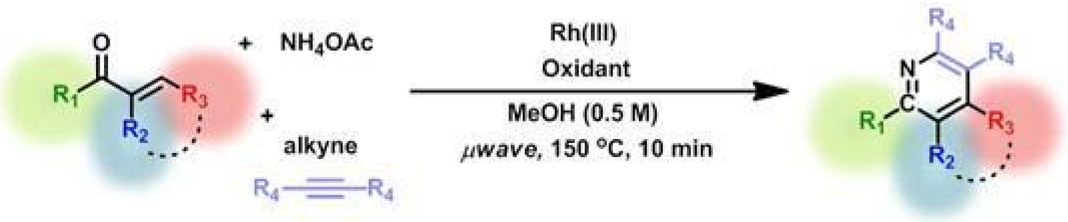
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-814**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-pot synthesis of *N*-heterocyclic compounds *via* Rh (III)-promoted *N*-annulation reaction under Microwave irradiation

이혜정 심용균 박정우 전철호*

연세대학교 화학과

Rh (III)-catalyzed organic reaction *via* cleavage of sp^2 C-H bond is efficient method to synthsize *N*-heterocyclic compounds. Especially, this protocol through one-pot three component coupling reaction of a,b-enone, NH_4OAc and alkyne under microwave irradiation is one of important methods for the synthesis of *N*-heterocyclic compounds such as pyridines and isoquinolines, and so on. This reaction shows that the steric effect depending on the substituent-size or-position of a,b-enone influences on *N*-annulation reaction. This protocol is a novel method for the preparation of *N*-heterocyclic compounds having advantages of easy handling, atom-economic and time-economic through Rh (III)-promoted *N*-annulation reaction under microwave irradiation.



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장소: 일산KINTEX
발표코드: **ORGN.P-815**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Bronsted acid Catalyzed Enantioselective Reduction of Imines: Alternative way for Pictet-Spengler reactions.

김경희 천철홍*

고려대학교 화학과

Asymmetric Bronsted acid catalysis has been widely used in asymmetric transformations during the last decade. Among the transformations developed with chiral Bronsted acids, intramolecular Friedel-Crafts reaction, known as Pictet-Spengler reaction, has received a lot attention due to easy formation of nitrogen-containing polycyclic systems. However, the lower reactivity of Bronsted acid has limited the use of this reaction to highly reactive heteroaromatic compounds, such as indoles and pyrroles. In order to expand the scope of Bronsted acid catalyzed Pictet-Spengler reaction to simple arene uncleophiles, we have developed an alternative synthetic method: Bischler-Napieralski reaction followed by enantioselective reduction of imines. Herein we will present our progress in this field.

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

A Practical Method for Synthesis of Both (R)- and (S)-3,3'-Diaryl BINOL Derivatives via Diastereomeric resolution of rac-BINOL Boronic Acid with a Chiral Ligand

이춘영 천철홍*

고려대학교 화학과

(R)- and (S)-3,3'-diaryl substituted BINOL derivatives via diastereomeric resolution of rac-BINOL with a chiral ligand, which is first example without using hydroxy group, followed by Suzuki coupling reaction. It could reduced synthetic route of enantiopure BINOL derivatives from commercially used rac-BINOL beacause diasteromeric resolution process was performed in the intermediate stage. In the 4 kinds of PIDA boronate, we tried, PIDA and OBn-PIDA were effective to seperate each enaniomer using silica column chromatography.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyglycerol-Dendronized Fluorophores

양시경 **Steven Zimmerman**[1]

전남대학교 화학교육과 [1]Department of Chemistry, University of Illinois at Urbana-Champaign, USA

Fluorophores are powerful tools for studying biological processes, especially those that are bright, photostable, water-soluble, and biocompatible. We designed and synthesized a series of perylenediimides (PDIs) encapsulated in polyglycerol dendrons which confer high water-solubility on the PDIs while retaining their excellent fluorescent properties in aqueous media. This strategy was also employed for solubilizing and protecting a ring-fused boron-dipyrromethene (BODIPY), which was rendered water-soluble by covalent linkage to a biocompatible polyglycerol dendrimer. This probe exhibited excellent brightness and photostability. The most notable feature is the long-lasting emission with a strikingly low level of blinking in single-molecule experiments even in the absence of anti-fading agents such as Trolox. These interesting properties greatly simplify use of the fluorophore in single-molecule fluorescence imaging.

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발표분야: 유기화학
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Development of Two-photon Probes for Thiols in Mitochondria

subhankar 안교한*

포항공과대학교 화학과

Thiols are involved in the redox processes in biological systems. Biological thiols such as glutathione (GSH), cysteine (Cys), homocysteine (Hcy), and hydrogen sulfide (H2S) play crucial roles in a variety of physiological and pathological processes.[1] Imbalance in the thiol concentrations causes severe health problems. To monitor the functions and concentrations of thiols, selective and organelle specific thiol detection using two-photon fluorescent probes is very important.[2]Herein, a new donar-acceptor type two-photon fluorescent probe for thiols has been developed based upon thiol mediated reduction of an aryl sulfonazide (Sulfo-Az) to the aryl sulfonamide (Sulfo-NH2).[3] Sulfo-Az has almost no fluorescence, but upon reduction to Sulfo-NH2 it shows strong fluorescence enhancement in aqueous media. The reactivity of Sulfo-Az depends upon the reduction potential of the corresponding thiols as well as their biological concentrations. Due to higher concentration of GSH (1-15 mM) in cellular matrices, Sulfo-Az is most reactive towards GSH in the biological system. Moreover Sulfo-Az shows selective fluorescent enhancement towards only thiols compared to other amino acids or other reducing anions.After confirming the reactivity of Sufo-Az towards thiols, we elaborated the thiol probe into a mitochondria targeting probe by attaching triphenylphosphonium ligand to Sulfo-Az. This Sulfo-Az (Mito) has been successfully applied to image the mitochondrial thiols in HeLa cells using two-photon microscopy (TPM).References1 Wood, Z. A.; Schroder, E.; Harris, J. R.; Poole, L. B. Trends Biochem. Sci. 2003, 28, 32.2 Lim, C. S.; Masanta, G.; Kim, J.H.; Han, J. H.; Kim, H. M.; Cho, B. R. J. Am. Chem. Soc. 2011, 133, 111323 Ahn, K. H. and co-workers, unpublished work

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-819**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and evaluation of novel lipoic acid-dopamine and dopamine derivative as cholinesterase inhibitors with selectivity towrads butyrylcholinesterase

김재관 이승환[1] 임용배[2] 김범철[3] 장미[1] 박정호[4]

한밭대학교 생유기화학실험실 [1]한밭대학교 응용화학과 [2]한밭대학교 응용화학 [3]한밭대학교 생명공학과 [4]한밭대학교 응용화학생명공학부

Alzheimer’s disease (AD) is a progressive neurodegenerative disorder of brain and the most common form of age related dementia that begins with memory loss and progresses to include severe cognitive impairment. we are aiming for finding and developing inhibitor of acetylcholinesterase (AChE) which is popularly know as treatment of AD and butyrylcholinesterase (BuChE) found in AD patient's brain. We synthesized (R)-Lipoic acid-dopamine and Lipoic acid-Dopamine derivative compounds and evaluated the inhibition activity against AChE and BuChE.

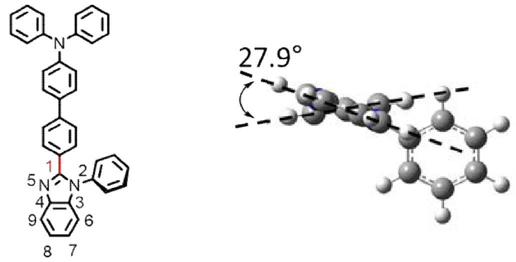
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-820**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient deep-blue-emitting triphenylamine-linked benzimidazole derivatives in nondoped fluorescent organic light-emitting diodes

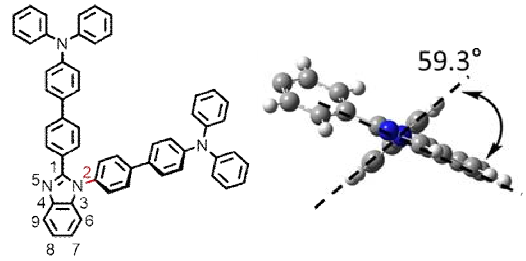
정성진 김성현* 홍종인*

서울대학교 화학부

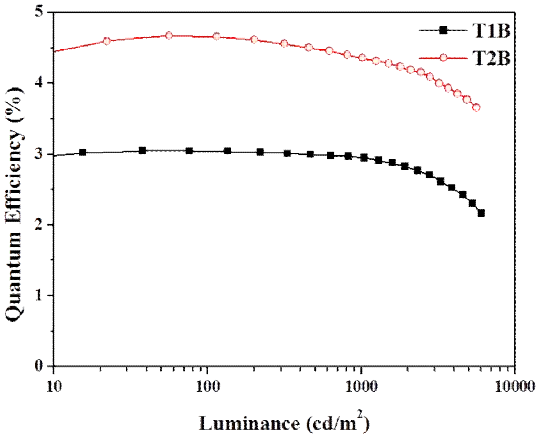
Deep-blue fluorescent organic light-emitting diodes (FLOLEDs) possessing high efficiency and pure Commission Internationale de l'Eclairage (CIE) chromaticity coordinates are a prerequisite for full-color displays and lighting devices. Nonetheless, because of the wide bandgap of blue emitters, only a few examples of high-performance blue FLOLEDs have been reported, in contrast to red and green FLOLEDs. A nondoped system has an advantage in that it has a simple device structure that employs only a single emitting material without using a complicated host?dopant codeposition process. Two triphenylamine-substituted benzimidazole derivatives were designed and synthesized for use as efficient deep-blue emitters in nondoped FLOLEDs. Nondoped FLOLED devices fabricated using 4′,4″-(1H-benzo[d]imidazole-1,2-diyl)bis(N,N-diphenylbiphenyl-4-amine) (T2B) as a blue emitter exhibited an external quantum efficiency of 4.67% with CIE coordinates of (0.15, 0.08).


27.9°
N
1
2
3
4
5
6
7
8
9
N
N

T1B


59.3°
N
N
1
2
3
4
5
6
7
8
9
N
N

T2B


T1B
T2B
Quantum Efficiency (%)
0
1
2
3
4
5
10
100
1000
10000
Luminance (cd/m^2)

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-821**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic enantio- and diastereoselective Michael addition reactions of α-cyanoketones to nitroalkenes

우샛별 김대영*

순천향대학교 화학과

The catalytic enantioselective and diastereoselective Michael addition reactions promoted by chiral bifunctional organocatalysts are described. The treatment of α-cyanoketones with nitroalkenes under mild reaction conditions afforded the corresponding γ-nitro α-cyanoketones with excellent diastereoselectivities (up to syn/anti >99/1) and excellent enantioselectivities (up to 99% ee).

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장소: 일산KINTEX
발표코드: **ORGN.P-822**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective synthesis of tetrahydroquinolines via chiral primary amine catalyzed tandem 1,5-hydride transfer/ring closure reaction

강영구 김미현 김대영*

순천향대학교 화학과

The development of C-H bonds functionalization has become an area of intense interest in synthetic organic chemistry because such reactions offer new strategies for the synthesis of complex organic targets. Lewis or Bronsted acids-mediated activation of unreactive C-H bond was recently reported. Herein, we report enantioselective intramolecular 1,5-hydride transfer/ring closure reaction using chiral primary amine catalysts. This redox reaction cascade allows for the efficient formation of ring-fused tetrahydroquinolines in high enantioselectivities (up to 94% ee).

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-823**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic enantioselective decarboxylative conjugate addition of benzoylacetic acids to enones

임영조 김세령 김대영*

순천향대학교 화학과

The Michael addition reaction is one of the most important and powerful methods for formation of C-C bonds in organic synthesis. Recently, the catalytic enantioselective decarboxylative reactions of β-ketoacids such as the Michael addition to nitroalkenes in the presence of chiral Ni(II) complexes and aldol-type reactions with trifluoromethyl ketones and isatins using organocatalysts were reported. However, the catalytic enantioselective decarboxylative Michael addition of β-ketoacids to α,β-unsaturated ketones has not been reported so far. Herein, we report a highly efficient catalytic enantioselective decarboxylative Michael addition reaction of benzoylacetic acids to α,β-unsaturated ketones using a cinchonidine-derived chiral primary amine organocatalyst. The desired 1,5-diketones were obtained in good to high yields, and excellent enantioselectivities were observed.

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발표코드: **ORGN.P-824**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly enantioselective Friedel-Crafts alkylation reaction catalyzed by chiral organocatalysts : synthesis of modified chiral chromanes

이현아 김대영*

순천향대학교 화학과

Modified chiral chromanes are important structural motifs in organic synthesis and have been found as core structural elements that have shown potent biological and pharmaceutical activities. Therefore, the development of highly efficient asymmetric synthetic methods to access these compounds is particularly appealing. Herein, we present the synthesis and preliminary biological evaluation of various modified chromanes via a tertiary amine-thiourea-catalyzed highly enantioselective Friedel-Crafts alkylation reaction of naphthols with β,γ-unsaturated α-ketoesters. The desired chromane derivatives were obtained good yields, excellent diastereoselectivities, and excellent enantioselectivities.

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장소: 일산KINTEX
발표코드: **ORGN.P-825**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective conjugate addition of of 2-hydroxy-1,4-naphthoquinone to β,γ-unsaturated-α-ketoesters catalyzed by binaphthyl-derived organocatalyst

이지현 김대영*

순천향대학교 화학과

Naphthoquinone derivatives have attracted much attention due to the broad scope of their biological activities. There are a few reported examples of the catalytic enantioselective Michael reaction of 2-hydroxy-1,4-naphthoquinone with β,γ-unsaturated-α-ketoesters. In this presentation we wish to report enantioselective conjugate addition reaction of 2-hydroxy-1,4-naphthoquinone with β,γ-unsaturated-α-ketoesters. The process was promoted by bifunctional organocatalyst that is binaphthyl scaffold with H-bonding motif and afforded the chiral adducts in high yields and excellentenantioselectivities under mild conditions.

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-826**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric synthesis of 3-hydroxy oxindoles via decarboxylative addition of β-keto acids to isatins

서창원 장철우 최건웅 김대영*

순천향대학교 화학과

The highly enantioselective decarboxylative addition of β-keto acids to isatins catalyzed by bifunctional organocatalysts have been developed, allowing facile synthesis of biologically important 3-hydroxy oxindoles in good yields and excellent enantioselectivities. The method represents a valuable approach of utilizing β-keto acids as synthetic equivalents of aryl/alkyl methyl ketone enolates.

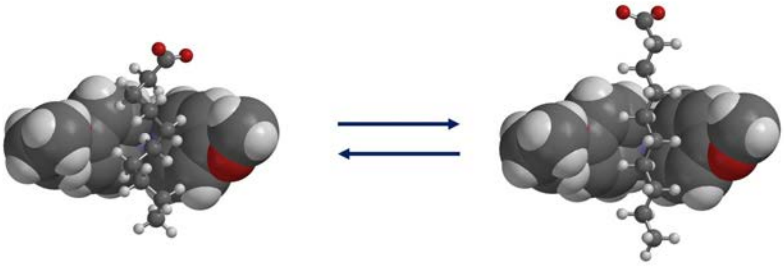
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-827**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dynamic Helical Coiling of Alkyl Chain induced by Self-assembled Macrocycles

송영란 임춘우[1,*] 김태우[1,*]

경희대학교 동서의과학과 [1]경희대학교 동서의학대학원

The poster describes a helical coiling of fatty acid induced by inclusion in the truncated cavity of macrocyclic host. Helical coiling or folding is one of the most fascinating subjects in chemistry, since, in nature, it has been found in an interactive fashion and regarded as a unique structural change induced by noncovalent interaction. For example, helical coiling of alkyl group of fatty acid is relatively unfavorable in thermodynamic process, compared to anti-conformation, which are observed in the preformed micelles in aqueous solution as well as a pure liquid phase. However, at the molecular level (below critical micelle concentration), fatty acids exist as random coiling structures in an aqueous solution, with alternating anti and gauche conformations. Our research was inspired from dynamic conformational aspect of alkyl group in aqueous solution. Macrocyclic host induces helical coiling of fatty acids at the molecular level and fatty acid helical coiling in the cavity fluctuates in time. Dynamic helical coiling of alkyl group in the cavity of macrocycle host has been investigated by a difference in helical coiling degree of two fatty acids. This result features dynamic nature of molecular recognition as well as helical conformation induced by host-guest interaction. CH - ? attraction as well as hydrophobic interaction might contribute to dynamic helical coiling of fatty acid in the aromatic environment of macrocycle host.



일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN.P-828**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

A simple Strategy for the Construction of Combinatoroal Cyclic and Bicyclic Peptoids.

이지훈 임현석* **Amanda M. Meyer[1]**

포항공과대학교 화학과 [1]Indiana University

We describe a simple method that allows for rapid and easy sequence determination of cyclic peptoids. The key idea in our strategy is a post-screening “ring-opening” of "Hit" cyclic and bicyclic peptoids identified from a high-throughput screen, result in the corresponding linear peptoids, which can be sequenced by tandem mass spectrometry. Thus, there is no need for encoding.

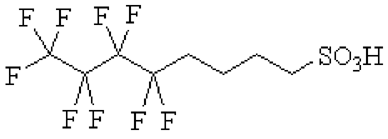
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-829**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and properties of new PFOS alternatives

Vijay kumar **B.Prem kumar 고요한 신동수***

창원대학교 화학과

Perfluorooctanesulfonic acid (PFOS) 1, having a C8-fluorocarbon chain is the key ingredient in many stain repellents and also proven to be toxic towards health and environment due to its non-biodegradability. Three partially perfluoroalkyliodides were simultaneously coupled to phenyl-vinylsulfonate in presence of Zn/CuI in ionic liquid [BMIM]Cl as well as in formamide to obtain phenylperfluoroalkylsulfonate. Various salts of each sulfonic acid series were synthesized (some in gram scale) from corresponding phenylsulfonates by hydrolysis.



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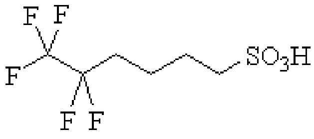

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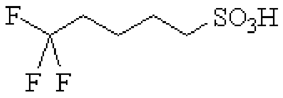


4

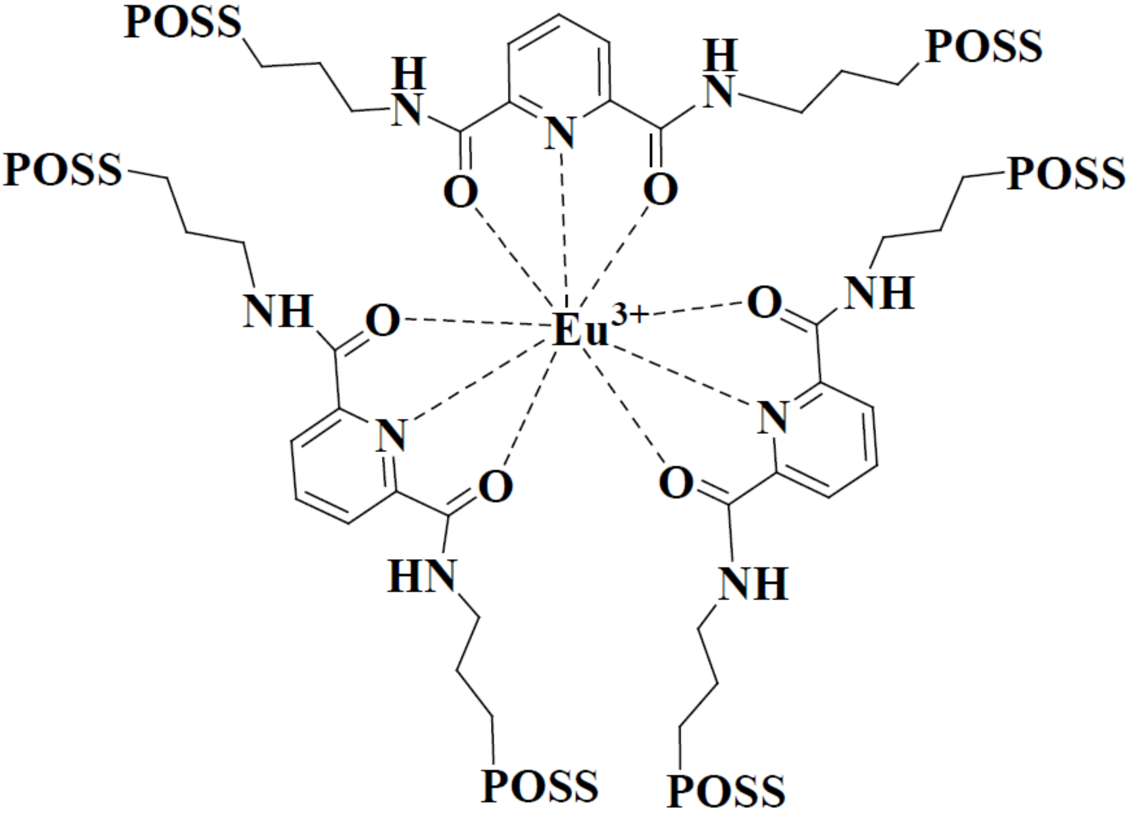
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-830**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of PDC-POSS-based hybrid fluorescent material

B.Prem kumar Vijay kumar S.J. Hashavardhan 신동수*

창원대학교 화학과

In this study, we chose the 2,6-pyridinedicarboxylic acid chloride (PDC) as the original ligand to construct bridge molecule with POSS amine, which afterward binded with Eu3+ to obtain the binary lanthanide organic?inorganic hybrid material Eu-PDC-POSS. The complex 1 showed efficient fluorescent activity when subjected to different excitation wavelengths like 254 nm, 288nm, 393 nm and 464nm.


POSS
H
N
N
H
N
POSS
POSS
O
O
POSS
NH
O
Eu^{3+}
O
NH
N
N
O
O
HN
NH
POSS
POSS

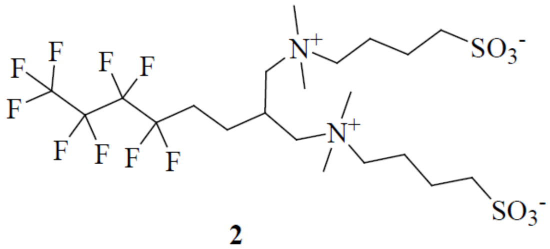
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-831**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of gemini sulfobetaine surfactants

B.Prem kumar Vijay kumar S.J. Hashavardhan 신동수*

창원대학교 화학과

A series of surface active gemini sulfo-propane betaines and sulfo-butane betaines were synthesized with high yields by the reaction of an appropriate N,N-dimethyl alkylamine with an excess of 1,3-propane sultone and 1,4-butane sultone. Gemini zwitterionic surfactants, which contain one hydrophobic which is connected to two hydrophilic groups with positively and negatively charged head groups, are interesting molecules because of their many unique properties.



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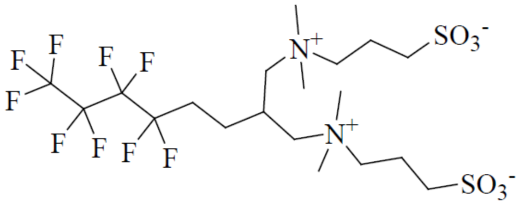


1

일시: 2013년 4월 17~19일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN.P-832**

발표분야: 유기화학

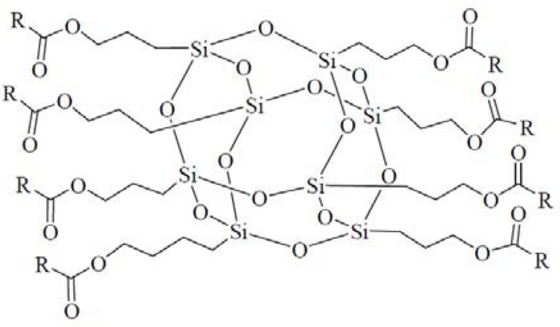
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of POSS derived inorganic/organic hybrid insulating oils

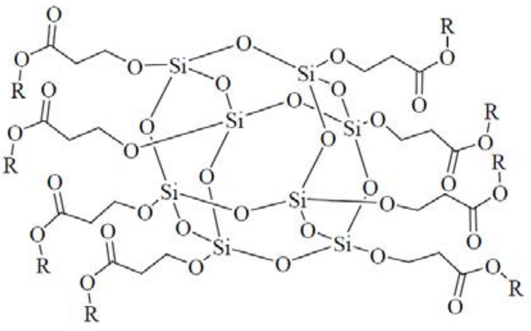
<u>S.J. Hashavardhan</u> B.Prem kumar Vijay kumar 신동수*

창원대학교 화학과

Biodegradable oils show the importance of biodegradability and nontoxicity. Polyhedral oligomericsilsesquioxanes (POSS), having a rigid and durable cage structure, is known for its stability even at higher temperatures and expected to show good flow ability at lower temperature when attached to certain ester moieties. Herein, we described the synthesis of esters of octahydroxy-POSS derivative and acyloxysilyl POSS towards thevarious biodegradable insulating oils.



I



II

일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-833**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Control of Regioselectivity in the Gold-catalyzed Formal Enyne Cross Metathesis

전정호 신선웅 신승훈*

한양대학교 화학과

We recently reported Au(I)-catalyzed intermolecular reaction between acceptor-substituted alkynes and alkenes leading to formal enyne metathesis products. While Grubbs' on Ru-carbene-based system produces 1,3-dienes as a mixture of E/Z isomers, the Au(I) catalyst gave the products in a perfectly stereo-controlled fashion via dyotropic rearrangement mechanism and thus could serve as a complementary method. The remaining issue in this formal enyne metathesis is a control of regioselectivity. Gratifyingly, the terminal olefins including gaseous alkenes (propene) and haloalkenes turned out to give the formal cross metathesis products with an excellent regioselectivity.

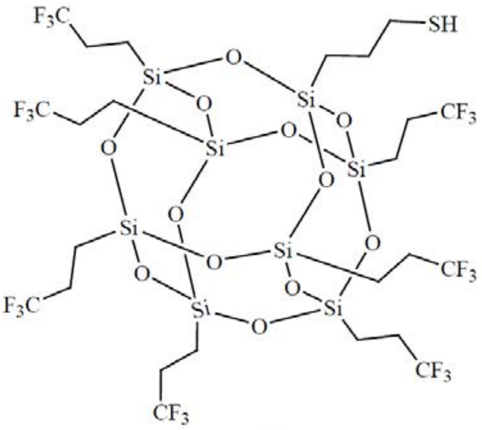
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-834**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of fluoro-POSS-sulfonicacid

S.J. Hashavardhan B.Prem kumar Vijay kumar 김영은 신동수*

창원대학교 화학과

Polyhedral oligomericsilsesquioxanes (POSS) in the form of sulfonic acid derivatives and various alkyl groups were synthesized using POSS-triol with 3-chloropropyltrichlorosilane to form POSS caged monochloride. This chloride was converted to sulfonic acid by various synthetic routes. Our main purpose was to reuse the POSS-sulfonic acid after the reaction by different method.



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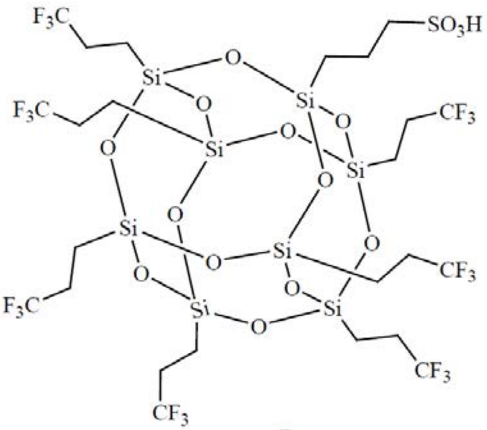


B

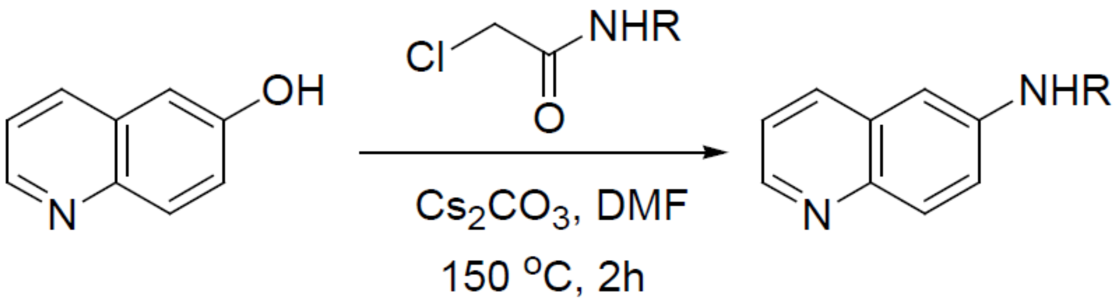
일시: 2013년 4월 17~19일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-835**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Practical one-pot synthesis of N-substituted 6-aminoquinolins from 6-hydroxylquinolin by smiles rearrangement

xieyongsheng 신동수*

창원대학교 화학과

A series of N-substituted 6-aminoquinolins as potent acetylcholinesterase inhibitors were easily prepared in moderate to good yields by a practical one-pot tandem C-N coupling reaction of O-alkylation/Smiles rearrangement/hydrolysis between 6-hydroxylquinolin and N-substituted 2-chloroacetamides.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold Catalyzed Intermolecular Coupling of Acceptor-Substituted Alkynes with Allyl Ethers

전정호 안준현 신승훈*

한양대학교 화학과

Au(I) catalyzed tandem reaction comprised of initial intramolecular alkoxy addition and the following 3,3-sigmatropic rearrangement occurs with exceptional efficiency unlike thermal Claisen rearrangement. However, the intermolecular reaction has not been reported presumably because of a lack of nucleophilicity of allyl ethers, although such process would not require synthesis of elaborate starting materials and tend to increase the molecular complexity more rapidly and thus allow more diverse applications. Herein we present our recent results on the intermolecular alkoxyaddition-Claisen rearrangement employing acceptor-substituted alkynes, such as propiolates and sulfonyl acetylenes. This process occurs efficiently despite competing pathways such as hydration and allyl fragmentation. The absence of cross-over products indicated that both 1,3- and 3,3-rearrangement occurs in a concerted fashion.

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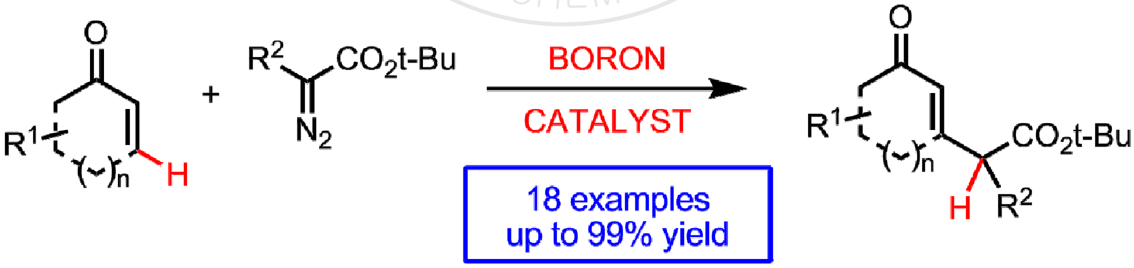
Catalytic Carbon Insertion into the *β*-Vinyl C-H Bond of Cyclic Enones with Alkyl Diazoacetates

이성일 황금숙[1,*] 류도현[*]

성균관대학교 화학과 [1]한국기초과학지원연구원 통합대사체연구그룹

The selective functionalization of the C-H bond is one of the most progressive and challenging topics in current organic chemistry. *β*-Substituted enones are versatile intermediates in the synthesis of biologically active molecules and pharmaceuticals.The first example of boron Lewis acid catalyzed C_{sp2}-H functionalization of cyclic enones was achieved using diazoacetates. The insertion of the carbon atom of diazoacetates utilizes BF_3?Et_2O or a newly designed oxazaborolidinium ion as a catalyst to afford *β*-functionalized cyclic enones from simple cyclic enones in a single step and high yields. The reaction mechanism was investigated with deuterium labeled 2-cyclohexen-1-one.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a facile synthetic method for 4-quinazolinones via aerobic oxidation in DMSO

김라연 천철홍*

고려대학교 화학과

Quinazolinones are common building blocks in biologically and pharmacologically important compounds, natural products, and materials science. Consequently, great efforts have been made to develop efficient methods for the synthesis of these important building blocks. However, the methods previously developed have some limitations, such as the need to use stoichiometric or superstoichiometric amounts of reagents, production of waste, expensive separation process, and harsh reaction conditions. Thus, it is desired to develop more efficient methods for the preparation of quinazolinones. Herein, we would like to present our recent development for the efficient synthesis of quinazolinones via aerobic oxidation in DMSO without any need of bases and metal co-oxidants.

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Convergent synthesis of PAMAM dendrimers using click chemistry of azide-functionalised PAMAM dendrons

<u>윤성희</u> 최인화 이재욱

동아대학교 화학과

Azide functionalized PAMAM dendrons containing an azidopropylamine focal point were synthesized by the divergent method and applied for the construction of symmetric PAMAM-like dendrimers containing 1,2,3-triazole rings as connectors via stitching with two different multi-terminal alkynes. The stitching method was based on the click chemistry protocol, i.e., the copper-catalyzed cycloaddition reaction between an alkyne and an azide.

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Synthetic Study of Donor-Acceptor Dyads Containing Pyromellitic Diimide, Naphthalene Diimide, and Perylene Diimide Connected by Aryl and Alkyl Spacers

김성식 **T. Majima[1]**

전북대학교 화학과 [1]Osaka University

Synthetic investigation of several donor-acceptor dyads containing pyromellitic diimide, naphthalene diimide, and perylene diimide is described. Aryl and alkyl groups were introduced as spacers for the synthesis of target molecules. Three dianhydrides such as pyromellitic dianhydride, naphthalene dianhydride, and perylene dianhydride were used to prepare intermediates. Two different types of reactions, which include 1:1 reactions and 1:1:1 reactions, ware compared. N-Boc protecting group was also introduced to get intermediates. Two different types of final intermediates were synthesized to get the target molecules. The spectroscopic properties of the dyads are also described.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

수소결합에 의해 자기조립되는 Dipeptide Liquid Crystal 합성과 구조분석

최한라 이명훈[1,*]

전북대학교 고분자 나노 공학과 [1]전북대학교 고분자나노공학과

생체모방(biomimetic) 재료는 생체모방 기술을 이용해 자연 물질이 가지는 독특한 성질과 구조를 모방 한 것으로 최근 들어 많은 연구가 진행 되는 있는 분야 중 하나로 항공기, 의료, 자동차 등 다양한 분야로 응용이 되고 있다. 많은 연구가 진행되고 있는 생체모방 재료는 자연 물질을 구성 요소로 하는 재료, 자기조립 하는 자연 물질을 응용한 재료, 자연 물질과 세라믹 또는 고분자가 결합된 재료, 분자 단위의 생체 물질을 합성한 재료로 크게 4 가지로 나눌 수 있다. 생체모방 재료 중 하나인 자기조립 되는 자연 물질을 응용한 재료는 수소 결합과 친수-소수성 분자력, π-π 간 상호작용, 금속-리간드 결합에 의해 만들어 진다. 본 연구실에서는 단백질과 구조가 비슷하고 수소결합을 하는 dipeptide liquid crystal 을 합성하였다. Dipeptide liquid crystal 은 두 개의 아미노산이 축합 반응에 의해 합성된 dipeptide 와 methyl 3,4,5-trihyroxybenzoate 를 알킬화와 가수분해 시켜 methyl 3,4,5-tris(n-dodecan-1yloxy) benzoic acid 를 에스터화 시켜 합성하였다. 합성한 dipeptide liquid crystal 은 H1-NMR 을 이용해 구조 확인을 하였다. 그리고 dipeptide liquid crystal 이 용매 증발 자기조립법과 이중용매 계면 자기 조립법, 이외의 다른 자기조립 방법을 사용하여 dipeptide 부분 끼리 수소결합에 의해 자기 조립이 되었을 때 어떠한 구조를 갖는지에 대해 논의를 하고자 한다.

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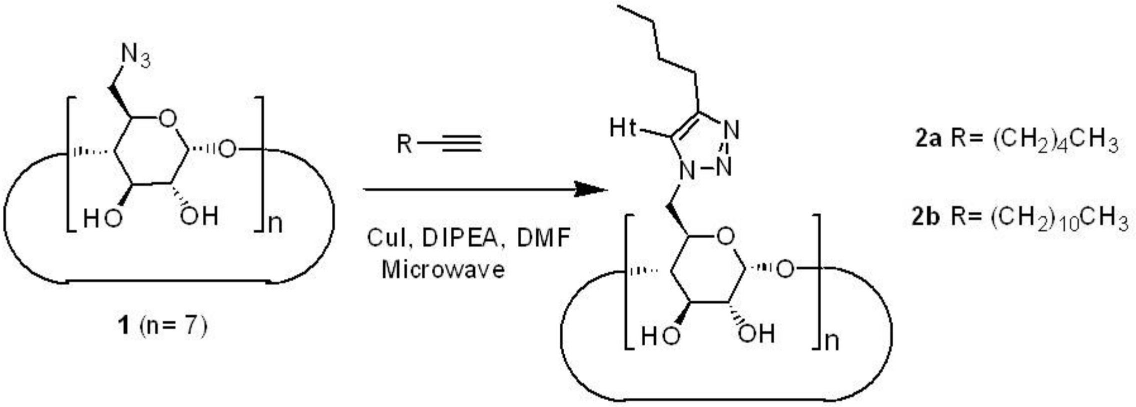
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and charaterization of beta-cyclodextrin derivatives with different length of hydrophobic tail.

천지현 **Le Thi Hoa**[1] 임춘우[1,*] 김태우[1,*]

경희대학교 동서의과학과 [1]경희대학교 동서의학대학원

Amphiphilic cyclodextrin has drawn interesting attention on the fabrication of self assembled nanomaterials on an interface or in an aqueous solution. Vesicle or micelle is one of examples in self assebled structures of amphiphilic material and employed as a multi-functional platform for research of targetted drug delivery system.Our research is based on the construction of multi-functional platform via synthetic and host-guest chemistry. Synthetic scheme is mainly achieved using click reactions on the primary face of cyclodextrin. We have charaterized cyclodextrin derivatives by way of 1D-, 2D-NMR and Mass spectrometry. We present the recent progress on assembly of amphphilic cyclodextrin.



1 (n= 7)

2a R= $(CH_2)_4CH_3$

2b R= $(CH_2)_{10}CH_3$

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

Synthesis of Dendronized Linear Polymers between Polystyrene with Side-Chain Azide and the Propargyl Functionalized Dendrons

윤성희 최인화 한승철 이재욱*

동아대학교 화학과

Our strategy for the synthesis of dendritic polymers utilized the Cu(I)-catalyzed Huisgen [2 + 3] dipolar cycloaddition reaction between an organic azide and a terminal alkyne. To apply the click chemistry concept in the construction of the dendronized linear polymers, we synthesized the polystyrene having pendent azides which was reacted with the propargyl functionalized dendrons (PAMAM and Frechet-type polyether dendrons) to provide the dendritic polymers. The dendritic polymers were characterized by 1H-NMR spectroscopy, IR spectroscopy, and GPC analysis.

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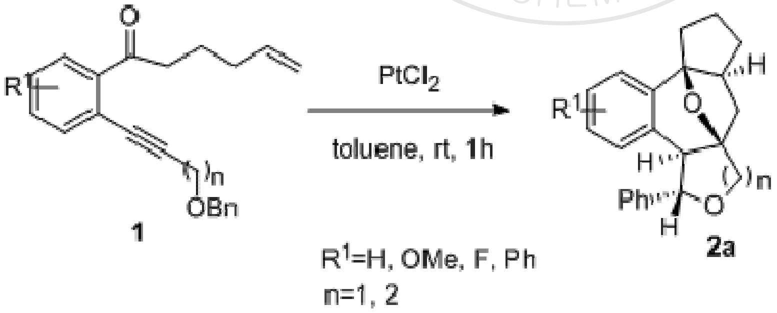
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Platinum-catalyzed Cyclization of Alkenyl Enynones and Subsequent Insertion into a Benzylic C-H

오창호* 김지희 유진 김소영 오부근

한양대학교 화학과

The discovery of new and efficient synthetic routes to polycycles containing a central seven-membered carbocycle is still an important challenge for organic and medicinal chemists, as numerous natural products, including taxol and its analogues, have a core skeleton of this type. We have developed novel platinum-catalyzed transformation of of 1-(2-(3-(benzyloxy)prop-1-ynyl)phenyl)hex-5-en-1-one (1) and its derivatives with a terminal alkene double bond in side chain underwent cyclization through a [3+2] cycloaddition in the presence of a platinum catalyst to give a tetracyclic compound 2a and its derivatives in good to excellent yields.



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발표코드: **MEDI.P-845**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and evaluation of 2-(2'-methoxy-4'-methylaminophenyl)benzoxazole

정순재 박정훈[1] 허민구[1] 양승대[1] 유국현[*]

동국대학교 화학과 [1]한국원자력연구원 방사선기기연구부

Amyloid plaques are one of the neuropathological hallmarks of Alzheimer’s disease (AD), and beta-amyloid (Aβ) is the main component of amyloid plaques. Thus, assessing the degree of Aβ deposition is an important tool for AD diagnosis. Herein, we report the synthesis of 2-(2'-methoxy-4'-methylaminophenyl)benzoxazole for the detection of amyloid plaques, and their biological properties as fluorescent probes *in vitro*. 2-(2'-methoxy-4'-methylaminophenyl)benzoxazole was tested using synthetic Aβ_{40} aggregates for their fluorescence response, which exhibited a strong fluorescence response ($F_{A\beta}/F_0$=36.1) and binding affinity (K_D=3.27±0.29 μM). We further tested the applicability to the fluorescence imaging of intracellular aggregated Aβ_{42} fibrils using SHSY5Y cells, and the results suggest that 2-(2'-methoxy-4'-methylaminophenyl)benzoxazole can be a useful marker of intercellular aggregated Aβ.

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발표분야: 의약화학

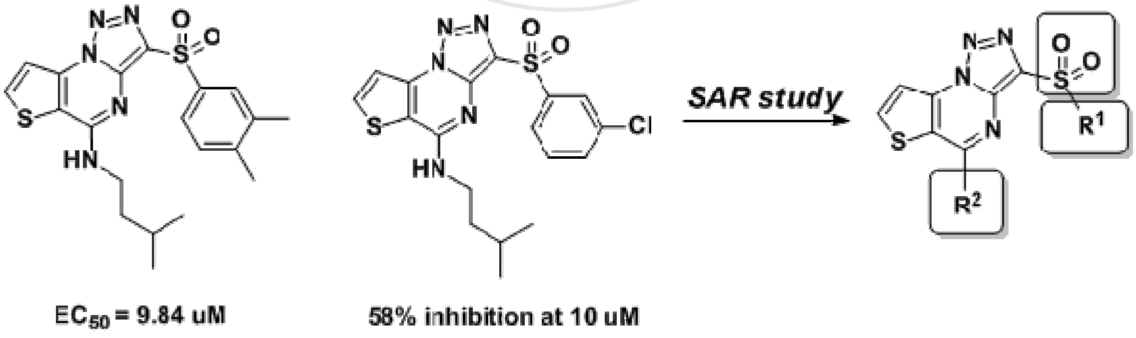
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of triazolothienopyrimidine derivatives as novel HIV-1 replication inhibitors

김준원 권정진[1] 조수연 박은정 박동식[1] 최지현[2] 황종연[2] 고윤애[3] 최인희[3] 이진화[4,*]

한국파스퇴르연구소 의약화학팀 [1]한국파스퇴르연구소 [2]한국파스퇴르연구소 의약화학 [3]한국파스퇴르연구소 의약화학그룹1 [4]한국파스퇴르연구소 late discovery program(LDP)

We identified a novel class of triazolothienopyrimidine (TTPM) compounds as potent HIV-1 replication inhibitors during a high-throughput screening campaign that evaluated more than 200,000 compounds using a cell-based full replication assay. Herein, we report the optimization of the antiviral activity in a cell-based assay system leading to the discovery of aryl-substituted TTPM derivatives (38, 44, and 45), which exhibited significant inhibition of HIV-1 replication with acceptable safety margins. These novel and potent TTPMs could serve as leads for further development.



EC$_{50}$ = 9.84 uM

58% inhibition at 10 uM

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of novel 7-aminopyrazolo[1,5-a]pyrimidine scaffold with inhibitory activity against hepatitis C virus

황종연 조수연[1] 박동식[1] 최지현 박은정[1] 권정진[2] 김준원[1] 이진화[3]

한국파스퇴르연구소 의약화학 [1]한국파스퇴르연구소 의약화학팀 [2]한국파스퇴르연구소 [3]한국파스퇴르연구소 late discovery program(LDP)

This pathogen is the major cause of acute hepatitis and chronic liver disease, including cirrhosis and liver cancer and thereby HCV is the leading indication for liver transplantation. Despite the recent approval of two direct acting antivirals (DAAs), telaprevir and boceprevir inhibiting the NS3/4A protease, standard of care for chronic hepatitis C is still a combination therapy of pegylated interferon-alpha (PEG-IFN-α) and ribavirin, which has limitations in HCV genotype 1 patients and causes severe side effects. Herein, we describe a novel 7-aminopyrazolo[1,5-a]pyrimidine (7-APP) derivative as a potent hepatitis C virus (HCV) inhibitor. A series of 7-APPs was synthesized and evaluated for inhibitory activity against HCV in different cell culture systems. The synthesis and preliminary structure-activity relationship study of 7-APP are reported.

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

Preparation of ^{68}Ga-labeled radiopharmaceuticals for tumor diagnosis

조보배 유국현

동국대학교 화학과

Recently, the design of surface-modified nanoparticles have been interested greatly in nanobiotechnology (NBT) due to the major applications, such as contrast media.Among the various nanoparticles, iron oxide was used to have applications in tagging for biosensing, probe of drug delivery and contrast media for magnetic resonance imaging (MRI).This research was focus on developing of nano-bio targeting composites using Fe_3O_4 nanoparticles and ^{68}Ga radioisotope, which could be useful for therapy in hyperthermia and diagnosis in the fields of PET and MRI applications. The surface of Fe_3O_4 nanoparticles that are used MRI imaging and hyperthermia can be reformed by citric acid to increase hydrophilic property. Nano-bio targeting composites can be obtained by combining Fe_3O_4 nanoparticles and NOTA as bifunctional chelating agent with ^{68}Ga radioisotope,This bi-functional imaging media will allow the earlier detection of tumor with a high degree of accuracy

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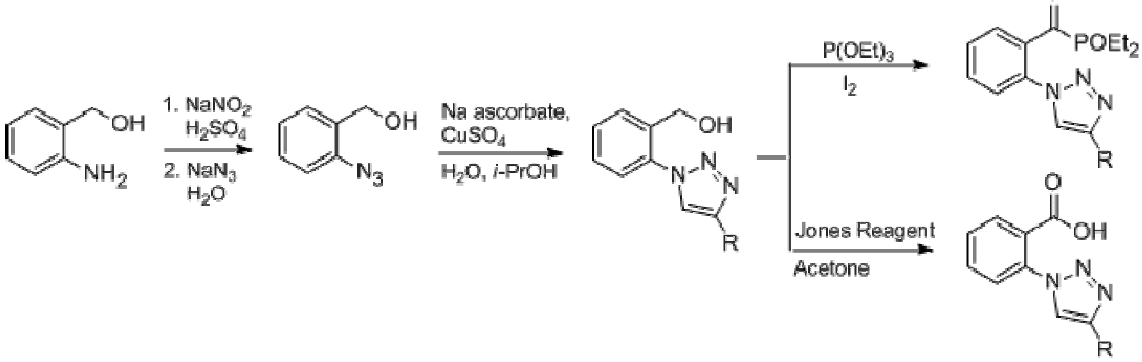
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Triazole Derivatives as an Anti-Inflammatory Drugs

김태우 Tasneem Islam[1] 정강연[2,*]

강릉원주대학교 환경응용화학공학과 [1]Department of Biological, Chemical and Physical Sciences, Roosevelt University, [2]강릉원주대학교 생명화학공학과

Efficient synthesis of a library of diclofenac analogs enabled cost effective biological testing of a range of novel NSAIDs with potential for improved drug efficacy and toxicity profiles. Utilizing click chemistry and Arbuzov reactions, a series of phosphonate and carboxylic acid derivatives of diclofenac were synthesized from 2-aminobenzyl alcohol. Anti-inflammatory properties of the products were tested with xylene induced ear edema in mice and compared to a diclofenac standard. Four of the synthesized compounds exhibited significantly better anti-inflammatory effects than diclofenac. Molecular modeling and in vitro COX-1 and COX-2 isozyme inhibition studies were also performed which support the in vivo studies.



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발표코드: **MEDI.P-850**
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Influence of ketamine induced slow oscillation by pretreatment ofT-type Ca2+ channel blocker

홍진리

과학기술연합대학원대학교(UST) 의약 및 약품화학

T-type calcium channels have been studied as therapeutic targets of neuropathic pain, hypertension and epilepsy pectoris. Many of potent T-type Ca2+ channel blockers have been synthesized and their inhibitory activity in vitro and in vivo was measured1). Inhibitory activity alone, however, seems not to be sufficient to explain their pain alleviation activity, because the feeling of pain alleviation is generally regarded as related simply to one's consciousness processing. Living animal lacks consciousness in deep-sleep stage and is unable to feel any pain, and it is uncertain that T-type Ca2+ channel blockers actually affect consciousness. To investigate the influence of T-type calcium channel blocking ability andconsciousness in deep-sleep state on neuropathic pain alleviation, an experiment on mouse's slow oscillation induced by anesthetic agent after oral administration of T-type Ca2+ channel blockers using EEG(Electroencephalogram) was performed. Here the experimental method and results obtained by using a T-type Ca2+ channel blocker KKJA1222s and an anesthesia inducing agent Ketamine/Xylazine(20:1) cocktail will be discussed.

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

Synthesis and Nrf2 activating ability of thiourea and vinyl sulfoxide derivatives

심영선

과학기술연합대학원대학교(UST) 생체분자과학

Parkinson’s disease (PD) is a progressive, degenerative condition of the central nervous system (CNS), caused by the degeneration of dopaminergic neurons in the substantia nigra of the midbrain. The hallmark physical symptoms of PD are tremor at rest, rigidity and hypokinesia (slowness of movement). Due to the therapy comprise mainly of improvement of the symptoms with L-Dopa or dopamine (DA) agonists, levodopa remains the mainstay of PD treatment. However, long-period L-DOPA therapy often causes many side reactions, including dyskinesia. To find compounds that can control PD, vinyl sulfoxide and thiourea derivatives were synthesized and evaluated for biological activity on a novel PD target, Nrf2 activator. Every compound exerted inconvenient activities on HO-1 induction compared with sulforaphane, well-known Nrf2 activator. The thiourea derivative with methoxy compound showed the best *in vitro* activity among the compounds synthesized in this study.

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Multifunctinal magnetic polyaniline nanocomposite for imaging-guided photothermal ablation of metastatic cancer cells

황승연 양재문[1,*] 허단[2]

연세대학교 나노메디컬 협동과정 [1]연세대학교 메디컬융합연구소/영상의학과 [2]연세대학교 의과대학

Theragnosis based on nanotechnology has been attracted as progressive strategy for effective cancer therapy. In particular, photothermal cancer therapy using nanoparticles absorbing near-infrared light has been spotlighted because target cancer cells can be killed by the generated extensive heats. Recently, our group reported that polyaniline could be used to the photothermal agent for cancer cells. To increase therapeutic efficacy for target cancer cells, here, imaging probe and biomarker-specific ligand were incorporated into polyaniline nanoparticles. We thus designed the well-tailored multifunctional nanocomplex, composing of polyaniline and magnetic nanoparticle, namely magnetic polyaniline nanocomposite (MPNC), for photothermal therapy and magnetic resonance (MR) imaging. In detail, MPNC was synthesized by thermal decomposition method in the presence of polyaniline as a ligand. The synthesized MPNC was stabilized in aqueous phase using functionalized polysorbate 80 molecules and metastatic cancer specific cancer-targetable ligands were immobilized on the surface of water-soluble MPNC. To characterize biomarker-specific MPNC, colloidal size, near-infrared absorbance, morphology, and magnetic property of were evaluated. In order to estimate targeted photothermal ablation and imaging potentials of the multifunctional nanocomplex, in addition, tumor bearing xenograft mouse model was established and biomarker-specific MPNC was intravenously injected. In conclusion, the prepared MPNC could bind to target metastatic cancer cells and effectively kill the target cells by irradiation of near infrared light. Furthermore, tumor site treated with biomarker-specific MPNC could be monitored by MR imaging.

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Synthesis and Biological Evaluation of Pyrrolidine Derivatives as Novel T-type Ca^{2+} Channel Blockers for Neuropathic Pain Therapy

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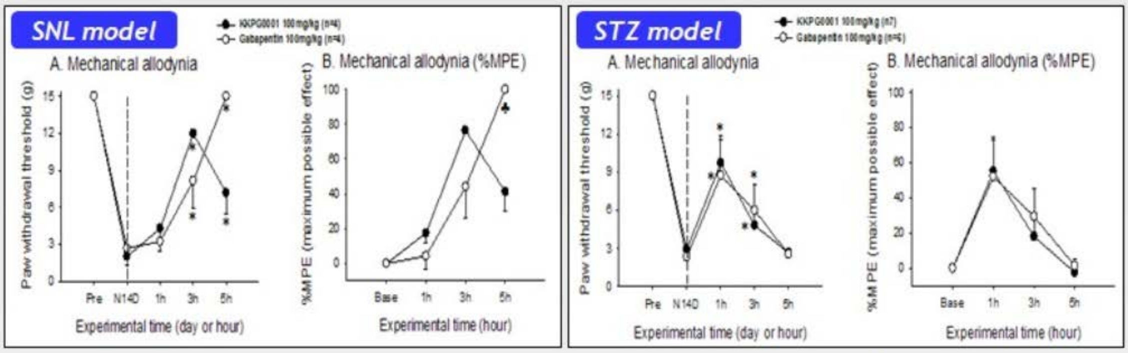
과학기술연합대학원대학교(UST) 의약 및 약품 화학 [1]한국과학기술연구원(KIST) 생체과학연구본부

Development of T-type Ca^{2+} channel blockers could lead to the treatment of hypertension, epilepsy, sleep disorders and neuropathic pain. T-type Ca^{2+} channels control muscle contraction, hormone release and cellular proliferation. $Ca_v3.2$ is the predominate T-type channel subtype in the dorsal root ganglion (DRG) with lower expression of both $Ca_v3.1$ and $Ca_v3.3$ detected. The major function of T-type Ca^{2+} channels in DRG sensory neurons is to support acute nociceptive signals. $Ca_v3.2$, therefore, is strongly implicated as contributing to the development of neuropathic pain. The goal of this study was to identify compounds that block the $Ca_v3.2$ channels and to evaluate their *in vitro* and *in vivo* efficacies. Several pyrrolidine derivatives were designed using a 3D ligand based pharmacophore model. The synthesized compounds were evaluated *in vitro* in HEK293 cells which stably express both $Ca_v3.1$ and $Ca_v3.2$ subunits using FDSS6000 assay and patch-clamp assay. Compound KKPG0001 was demonstrated to have good *in vivo* efficacy in mechanical and cold allodynia that was comparable to gabapentin through both the rat spinal nerve ligation model and STZ-induced diabetic neuropathy model.



After oral administration of gabapentin (○, 100 mg/kg, *n* = 4,6) and **KKPG0001** (●, 100 mg/kg, *n* = 4,7) to neuropathic pain-induced rats. *P<0.05 (gabapentin), $^{*}P$<0.05 (**KKPG0001**) vs pre-administration value (paired *t*-test), ♣P<0.05 gabapentin vs **KKPG0001** (unpaired *t*-test).

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In silico approaches for Identification of Histone H3 (K9) trimethyltransferase Inhibitors

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Histone lysine methyl transferase (HKMT) plays key roles in the post-transcriptional regulation of ERG-associated protein with SET domain (ESET) gene expression via trimethylation of lysine 9 on histone H3 of chromatin. Altered chromatin remodeling and transcription dysfunction are associated with abundant pathological states of neuronal disorders, such as Huntington's disease (HD). Discovery of small molecule HKMT inhibitors will suggest new methods for therapeutic development. We applied the combination of homology modeling and phamacophore-based virtual screening methods. Homology models of human ESET protein was generated based on the crystal structures of three human Suv39 families. Total 2.6 million compounds, which came from Chemdiv and Asinex database, were initially filtered by three different types of phamacophore. Then, 61,566 mapped compounds were performed to predict ADME and physicochemical properties, thereby analyzing its uses of drug. The 18,813 compounds in the obtained data were eventually determined for selective binding poses by using docking procedure in GOLD v5.0.1. Cluster process was based on chemical diversity and classified with fitvalue and docking scores for final selection of hits. These compounds may be promoted to a potential chemical probe against trimethyltransferase after passing *in vitro* and cellular activity evaluation.

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Transmembrane region prediction tools : Evaluation and analysis

최민학 허지영*

상명대학교 의생명공학과

생물체의 전체 genome sequence 의 ~25%는 integral membrane protein 에 해당된다고 알려져 있다. 이들 membrane protein 은 transport, signalling 등 생체 내 여러 가지 주요한 역할을 담당하고 있다. 하지만 RCSB PDB database 에서 살펴보듯이 3 차 구조가 밝혀진 membrane protein 의 수는 ~0.5%에 불과하다. 이러한 membrane protein structure 에서 membrane 을 관통하고 있는 Transmembrane (TM) 영역의 결정은 membrane protein 연구에서 중요한 역할을 담당하고 있다. 현재까지 membrane protein 의 TM 영역을 예측하는 다양한 tool 들이 개발되어있다. 우리는 대중적인 1 차 database 인 PDB, Uniprot 과, 3 차 구조가 알려진 TM protein 과 TM 영역만을 정리한 2 차 database 인 MPtopo, PDB_TM 을 평가 분석하였고, 결과적으로 PDB_TM 을 사용하여 TM 영역이 a-helix 로이루어진 protein 으로 구성된, 이를 TM helix 의 갯수로 구분한 true set 을 구성하였고, 그 결과 true set 은 총 749 protein, 861 chain 으로 구성되었다. 결정된 true set 을 통해서 TM prediction tool − DAS, HMMTOP, TopPred, TMHMM, SOSUI 를 포함한 총 26 개의 tool 들을 분석하였다. Tool 을 사용하여 얻은 예측 결과를 객관적이고 다양한 측면에서 평가 분석하기위해서 TM helix number, TM helix segment start-end 를 기준으로 Qp, Q3, Start-End Scoring measures, RMSD, correlation coefficient 등의 다양한 평가 방법을 결정하여 적용하였다. 우리는 membrane protein 의 3 차 구조에서 중요한 역할을 담당하는 TM 영역을 가장 정확하게 예측할 수 있는 tool 을 결정하기 위해서 extensive 한 true set 과 다양한 평가 방법을 사용하였고, 이러한 분석 결과를 통해서 현재까지 개발된 tool 들 중 더 정확한 tool 과 예측 방법을 알 수 있게 되었다. 본 연구 결과는 이후 정확한 tool 개발의 밑거름이 될 수 있는 유용한 정보를 제공한다고 볼 수 있다. 할 수 있을 것이다.

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Construction of a novel drug-like 2,5-piperazinedione derivatives using various amino acids via BAL resin on solid-phase.

이석형 김나연 안예희 공영대*

동국대학교 화학과

Solid-phase combinatorial chemistry has hold its place as an extremely powerful technique for the rapid generation of small, drug-like organic molecule libraries for the purpose of medicinal chemistry programs within the pharmaceutical industry. Heterocyclic skeletons serve as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. Compounds containing 2,5-piperazinedione have attracted significant interest in medicinal chemistry because 2,5-piperazinedione moiety, present in several natural and synthetic products, is biologically active on various pharmacological targets, displaying antihyperglycaemic, antiviral, antitumor, antifungal and antibacterial activities. Compounds containing amino acids are attractive class of scaffolds in drug research, due to its chiral nature, rigid structure. As a part of our ongoing drug discovery program, we has established the solid-phase parallel synthesis of 2,5-piperazinedione compound derivatives on the BAL linker as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Final compounds was obtained in good yields and high purities upon cleavage from resins.

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Solid-Phase Parallel Synthesis of some new a Novel Drug-like 2,4-Diaminosubstituted Thiazole Libraries Via Using BAL Resin

김용상 이지형 천수필 공영대*

동국대학교 화학과

Among organic small molecules, 5-memberd heterocyclic compounds have received particular attention in combinatorial chemistry, since they are important structural components of bioactive molecules. In this regard, owing to the fact that thiazole derivatives exhibit a wide range of important biological activities, and was reported in many potent biologically active molecules. For example, thiazoles exhibits the activities against cyclin-dependent kinase (CDK) and glycogen synthase kinase-3 (GSK-3). Thus as a part of an ongoing drug discovery process, we have been studying the potential of resin-bound 2,4,5-thiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. And as a result, the thiazole of heterocyclic components, being evaluated the core structure of the bioactive molecules, and they serve as attractive targets for combinatorial library construction via solid-phase parallel synthesis. We had previously report a useful method for the solid-phase synthesis of 2,4-diaminosubstituted thiazole derivatives using a sulfone traceless linker. Herein we would like to present a novel solid-phase synthetic better than existing methods optimized method for combinatorial generation of 2,4,-diaminosubstituted thiazole derivatives through resin-bound BAL resin. Also we are studying cleavage condition on solid-support under TFA. Therefore, we expect our efficient approach will be obtained many compound in good yields and high purity upon cleavage from the BAL resin.

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Solid-phase synthesis of a novel drug-like 2-thiohydantoin derivatives via BAL resin.

이재민 양정원 임성현 공영대*

동국대학교 화학과

The solid phase synthesis of heterocyclic combinatorial libraries is a powerful strategy to have drug discovery process. And solid-phase synthesis of heterocyclic core skeleton serves as the core components of a large number of substances that process very efficient for the construction of drug-like library. As a part of our ongoing drug discovery program, we have been exploring a potential of resin-bound 2-thiohydantoin derivatives since they are easily obtained from various natural amino acids. In this present, we would like to show several results of combinatorial generation of 2-thiohydantoin derivatives from solid-phase synthesis. Through making the various isothiocyanate substituted amino acids building blocks, we could obtain linear compounds in solid-phase synthesis.

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Synthesis of 2-Amido/amine substituted benzo[d]oxazine Derivatives via Thiourea Linker on BAL Resin.

<u>김은미</u> 정세린 JUVEKARVINAYAK 공영대*

동국대학교 화학과

Synthesis has become an extremely powerful technique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. Therefore, we have been exploring the potential of resin-bound 2-amido/amine substituted benzo[d]oxazine derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Especially, we were interested in construction the variously substituted 2-amido/amine substituted benzo[d]oxazine library because of their broad biological activities. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of 2-amido/amine substituted benzo[d]oxazine library through resin-bound benzo[d]oxazine via thiourea linker on BAL resin.

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Synthesis of 5,6-Disubstituted-2-Aminothiazolo[4,5-*b*]pyrazine Derivatives as Wnt2/β-catenin Pathway Inhibitors

이지형 곽세훈 김하영 공영대*

동국대학교 화학과

The Wnt signaling is one of the key signaling pathways that regulate cell proliferation, differentiation, and morphogenesis. Wnt proteins constitute a family of highly conserved secreted glycoproteins that play multiple roles in the development and progression of diseases. Small-molecule inhibitors of this pathway are desired because it is believed their clinical use would suppress cancer cell growth. As a result, there has been an interest in identifying small molecule inhibitors of Wnt signaling as tool compounds for research or as precursors to new generations of anticancer drugs. Several potent small-molecule inhibitors have been reported; however, the development of therapies to specifically target the Wnt pathway in cancer cells is still in its infancy. An earlier search, employing high throughput screening, has demonstrated that 2,3,6-trisubstituted quinoxaline derivatives were highly potent anti-cancer biological activities toward Wnt2/β-catenin pathway. However, in our previous paper we could not find out good druggable lead compound. Thus, based on our previous results, we have tested whether development of a new core skeleton based on the bioisostere concept compared with that of quinoxaline may improve the physicochemical properties as well as the cell proliferation of A549/Wnt2 cells. To identify small molecule inhibitors of Wnt/β-catenin pathway, we synthesized 5,6-disubstituted-2-aminothiazolo[4,5-*b*]pyrazines derivatives via tandem reactions of various pyrazines and isothiocyanates has been developed.

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Parallel Synthesis of Novel Drug-like 2-Quinolinyl Piperazine Derivatives as Antitumor Agents

곽현정 이은실[1] 김나연 공영대*

동국대학교 화학과 [1]동국대학교 의약화학연구실

The importance of G2/M-specific cell cycle inhibitor in the mediation of normal and pathological processes has motivated considerable efforts to identify cell proliferation. Recently we reported the anticancer activities of 5 or 6- substituted quinoxaline compounds containing piperazine groups. Especially, 1-(3,5-dimethoxyphenyl)-4-[(6-fluoro-2-methoxyquinoxalin-3-yl)aminocarbonyl]piperazine, induced G2/M arrest in cell cycle and an apoptosis in cancer cells. This hit compound has also significantly inhibited growth of drug resistant cancer cells, and has shown potential use in combination therapy with known anticancer drugs such as palcitaxel, doxorubicin, gemcitabine, 5-FU and cisplatin. However, most of the first quinoxaline hit compounds showed several hundred nM activity toward cancer cell lines as well as there were showed low water solubility. Therefore, we needed much stronger active hit compound with good physicochemical properties for the final lead compound selection process. So, we focused on the development of a quinolone core skeleton to improve more active quinoline derivatives containing piperazine then quinoxaline derivatives containing piperazine of previous studies. In connection with a project for exploring the novel potent G2/M-specific cell cycle inhibitors, we have designed some target compounds for quinolinyl-piperazine-based library for optimization of the structural features of the primary screening results through high throughput screening efforts.

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A Construction of 1,3,4-Oxadiazole and 1,3,4-Thiadiazole Libraryvia Solution-Phase Organic Synthesis.

양승주 최지혜 공영대*

동국대학교 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In this family, 1,3,4-oxadiazoles and 1,3,4-thiadiazoles have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as antiimflammatory, antimicrobial, anticonvulsant, and antihypertensive. In addition, these heterocycles serve as intermediates in the preparation of various biologically important compounds. In this reason, we developed a regioselective, reagent-based method for the cyclization reaction of 2-amino-1,3,4-oxadiazole and 2-amino-1,3,4-thiadiazole core skeletons. The thiosemicarbazide intermediate were reacted with EDC.HCl in DMSO or p-TsCl, TEA in NMP to give the corresponding 2-amino-1,3,4-oxadiazoles and 2-amino-1,3,4-thiadiazoles through regioselcective cyclization processes. The regioselectivity was affected by substituent in p-TsCl mediated cyclization. It is shown in select set of thiosemicarbazide. 2-Amino-1,3,4-oxadiazole was also shown in the reaction of p-TsCl mediated cyclization. The resulting 2-amino-1,3,4-oxadiazole and 2-amino-1,3,4-thiadiazole core skeleton are functionalized with various electrophiles such as alkyl halide, acid halides, and sulfornyl chloride in high yields.

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Synthesis of N-[2-(diethylamino)-ethyl]-4-18F-fluorobenzamide (18F-FBZA) using microfluidics.

홍유진 유국현

동국대학교 화학과

Malignant melanoma is one of the most critical cancers because of its high metastatic potential. Therefore, the early diagnosis and accurate staging of the disease is an important method to increasing survival. N-[2-(diethylamino)-ethyl]-4-18F-fluorobenzamide (18F-FBZA) formally proved that it has an affinity for melanoma model, suggesting that labeling of such benzamide with 18F could potentially produce melanin-targeted PET probes. We study the convenient several steps using micro-fluidics. Especially, the amidation is a key step of synthesizing the benzamide derivatives which is pose high sensitivity for melanin lesions with high tumor uptake. In our research, we improve the process of synthesis of 18F-FBZA through the micro-fluidic technology that have advantages such as the accuracy temperature control, continuous process and easy to scale up.

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Gold Nanoparticles Conjugates of Various Ionic Liquid Type Photosensitizers for Photodynamic Therapy

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인제대학교 PDT 연구소 [1]인제대학교 나노공학부

Water soluble ionic liquid type photosensitizers were synthesized and used for making gold nanoparticles conjugates which were characterized by IR, UV-vis, and NMR spectroscopic and Mass spectrometric analyses, and transition electron microscopy. And photodynamic effect of those gold nanoparticles conjugates has been evaluated by in vitro study using MTT assay.

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Synthesis of Gold Nanoparticles Conjugate of Ionic Liquid Type Purpurin-18-N-butylimide and In Vitro Study

윤일[*] 심영기[1] 장민아[1] 이태헌[1]

인제대학교 PDT 연구소 [1]인제대학교 나노공학부

Ionic liquid type purpurin-18-N-butylimide (P18NB) was synthesized with N-methyl-D-glucamine (NMGA). Gold nanoparticles conjugate of P18NB-NMGA was prapared and was characterized by IR, UV-vis, and NMR spectroscopic and Mass spectrometric analyses, and transition electron microscopy. In vitro study was carried out for photodynamic activity of the gold nanoparticles conjugate.

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Synthetic studies and their biological activities of regioselective aryl 1,2,3-triazole derivatives for dopamine receptors.

곽주명 고훈영

인하대학교 화학과

Functionalized five-membered heterocyclic with two or three heteroatoms, such as imidazoles, thiazoles, triazoles and others, are key structural units in many pharmaceutical preparations. Among them, 1,2,3-triazole derivatives are useful molecules which exhibit a wide range of biological activities and appear as key structural units in many important pharmaceuticals. 1,2,3-triazole structure is one of key scaffolds and building blocks in the construction of complicated organic compounds. Though our previous studies on the discovery of potent and selective ligands against dopamine receptor, 1,2,3-triazole library having mixed two regio isomers is designed and synthesized by click chemistry. These constructed libraries have potent binding affinities mixed two regio isomers. In this study, the synthetic pathway for regioselective isomers by using of metal catalyzed click chemistry has been studied, and also, it will be discussed their binding affinities.

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

Identification of Novel Chemotypes for TREK-1 Antagonists using Combined Structure-based and Ligand-based Approach

AMBILY NATH 배애님[1,*]

과학기술연합대학원대학교(UST) 의약및 약품화학 [1]한국과학기술연구원(KIST) 생체과학연구본부

Gene knockout experiments in mouse models have disclosed TREK-1, the prototypical K2P channel, as a potential target for antidepressants, anesthetics and anti-ischemic drugs. The present investigation has employed a combined structure-based and ligand-based approach to explore novel chemotypes for TREK-1 antagonists. A 3D model of TREK-1 was built using the X-ray crystal structure of TRAAK K2P channel as template. The verified model was docked with quaternary ammonium (QA) ions using eight scoring functions of four commercial docking protocols (CDOCKER, SURFLEX, GLIDE and GOLD) and GoldScore (GScore) was chosen over others because it had the best correlation with experimental data. Twenty six known antagonists that showed good inhibitory profile for TREK-1 constituted the dataset to characterize binding interactions by docking with protein model. A common feature pharmacophore (Hypo1) was generated from six highly active compounds (0.1 ?M ≤ IC50 ≤1 ?M) from the dataset and the remaining served as test set. Two types of virtual screening (VS) have been carried out against Asinex, ChemDiv and Ionchannel libraries in search of novel compounds. The validated Hypo1 was applied to pharmacophore-based VS whereas the most potent compound (IC50= 0.06 ?M) among the inhibitors was subjected to 2D similarity-based VS. The retrieved hits ranked by FitValue, Lipinski’s rule of five and ADME properties were docked with TREK-1 model. Finally, 54 lead compounds selected based on high dock score, key interactions, molecular weight and scaffold diversity are currently under in vitro screening. The present in silico study is expected to identify TREK-1 specific inhibitor scaffolds.

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

Synthesis and SAR of novel urotensin-II receptor (UT) antagonists

임채조* <u>최준영</u>[1] 이규양

한국화학연구원 대사증후군치료제연구센터 [1]과학기술연합대학원대학교(UST) 의약 및 약품화학

The urotensin-II (U-II) is a cysteine-linked cyclic peptide and their cell-surface receptor (UT) which is a G-protein-coupled receptor that was originally identified as orphan receptor (GPR14) and is expressed in many tissues, including blood vessels, heart, liver kidney, skeletal muscle, and lung. Interaction of U-II ligand with UT is also intimately involved in cardiorenal diseases including hypertension, heart failure and chronic renal failure. In continuing our efforts to discover novel UT antagonists, we recently have identified biphenyl derivatives and systematically examined the effects of various heterocycles linked to biaryl group to UT binding activity. Furthermore, we also investigated some 5-membered heteroaryl group on biphenyl moiety. The details of synthesis and SAR results will be presented.

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

Synthesis and optimization of novel urotensin-II receptor (UT) antagonists

임채조* 이혜인[1] 이규양

한국화학연구원 대사증후군치료제연구센터 [1]과학기술연합대학원대학교(UST) 의약 및 약품화학

The urotensin-Ⅱ (U-Ⅱ), a cystein-linked cyclic undecapeptide, is known as the one of the most potent vasoconstrictor. U-II ligand binds to an urotensin-II receptor (UT) as specific G-protein coupled receptor, which plays an important role in the regulation of cardiorenal function. UT is widely expressed through cardiovascular, central nervous and renal system. Furthermore, UT has received a great deal of attention as potent target for cardiovascular treatment. As part of our drug discovery program in the development of potent UT antagonists, we have identified a series of biaryl derivatives and extensively investigated the effects of various heteroaryl group of biphenyl to UT binding activity. The details of synthesis and structure-activity relationships (SAR) results will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

mGluR1 Antagonists for Treatment of Neuropathic Pain

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Neuropathic pain is a complex, chronic pain state with numerous causal factors. In many cases neuropathic pain is initiated by damage to nerves, but other origins of neuropathic pain include compression of nerve fibers by tumors, scar tissue, and inflamed tissue. Glutamate is a predominant excitatory neurotransmitter of central and peripheral nervous systems. Glutamatergic activity is mediated via ligand gated ionotropic glutamate (iGlu) receptor and G-protein coupled metabotropic glutamate (mGlu) receptors. Currently eight mGluR subtypes have been cloned and are classified into three groups on the basis of their sequence homology, pharmacology, and signal transduction mechanisms. Group I mGluRs (mGluR1 and mGluR5) are post synaptic receptors. It has been reported that the Group I mGluRs play key roles in the central sensitization of pain and other neurologic disorders. In this study, novel compounds with a bicyclic core structure were designed and synthesized on the basis of the reference compound with an IC$_{50}$ value of 6 nM.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of tetrahydrothieno[2,3-c]pyridine derivatives as mGluR5 negative allosteric modulators

남민아

상명대학교 자연과학대 화학과

Glutamate is major excitatory neurotransmitter of mammalian in central nervous system and peripheral nervous system. Glutamate receptors are related to mediate glutamate for post-synaptic excitation in neural cell, involved in pathologies of many brain diseases.Metabotropic glutamate receptors belong to the type of C class of GPCR(G protein coupled receptors) and they are divided into three groups with eight subtypes on the basis of their sequence homology, pharmacology, and signal transduction mechanism. Group 1 consists of the mGluR1 and mGluR5, which are predominantly identified in post-synapses in the brain region, including the hippocampus, cerebellum, thalamic nuclei, and spinal cord. Recently studies show that selective mGluR5 antagonists may play a role in the treatment of neuropathic pain and other brain diseases. In this study, we report the synthesis and biological evaluation of novel tetrahydrothieno[2,3-c]pyridine derivatives as selective mGluR5 antagonists for treatment of neuropathic pain.

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

Novel 5-HT$_7$ Receptor Antagonists for Treatment of Depression

염미영 김영재[1] 문봉진 추현아[2,*]

서강대학교 화학과 [1]과학기술연합대학원대학교(UST) 의약및약품화학 [2]한국과학기술연구원 (KIST) 생명보건본부

5-HT$_7$ Receptor is the most recently described member of 5-HT receptor family. The 5-HT$_7$ receptor has been detected both in periphery and central nervous systems. Although biological functions of the 5-HT$_7$ receptor are poorly understood, preliminary evidence suggests that it may be involved in depression control of circadian rhythms and relaxation of vascular smooth muscle. Knockout animal studies have provided demonstrative proofs that 5-HT$_7$ receptor is engaged in the pathomechanism of depression. Thus, 5-HT$_7$ receptor is potentially a good target for treatment of depression. Based on the known 5-HT$_7$ receptor ligands, compounds with a novel scaffold were designed, synthesized and biologically evaluated against the 5-HT$_7$ receptor. The synthesis and biological activities will be discussed in detail.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold nanorod-Photosensitizer Complex for Photodynamic / Photothermal Dual Therapy

김승범 이우경[1,*]

인제대학교 나노시스템 [1]인제대학교 나노공학부

In this study, photosensitizers(PS) were complexed with gold nanorod(GNR) to enhance the effect of anticancer therapy by introducing the additional PTT effect of GNR to the PDT effect of PS. PS with (-) charge were prepared and incorporated into GNR multilayer complex by the layer-by-layer preparation method using poly(allylamine hydrochloride)(PAH) as positive polymer layer and PS as negative layer. Each coating step was characterized with UV?vis spectroscopy and Zeta potential measurements. Photodynamic / photothermal effects of GNR-PS complexs were evaluated by in vitro MTT assay. The complexs showed rod morphology and higher drug contents with increasing polyelectrolyte layers. NIR irradiation increased the temperature of buffer including GNR. Dual therapy of GNR-PS complexs was expected to show more anticancer effect than photodynamic therapy alone.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Radiolabeling of benzamide derivatives via Al^{18}F chelation for tumor PET imaging

김희정 김동연[1] 박정훈[2] 양승대[2] 허민구[2] 유국현

동국대학교 화학과 [1]화순전남대학교 병원 [2]한국원자력연구원 방사선기기연구부

^{18}F is the most widely used PET radioisotope because of excellent imaging properties, and thus, the development of ^{18}F-labeled bioactive molecules has become an important area. Recently, ^{18}F-labeling method using Al?F complex in aqueous solution was developed that offered a simple ^{18}F-labeling procedure without drying steps. We designed and synthesized novel Al^{18}F-labeled benzamide derivatives as a potential PET agent for malignant melanoma. The novel radiotracers were synthesized at good radiochemical yields (~50% decay corrected yield) and high specific radioactivity (5~7 GBq/μmol), respectively.

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Synthesis of $B_{12}H_{11}SH$ substituted cholesterols for efficient boron delivery in neutron capture therapy

박상하 이종대*

조선대학교 화학과

Cholesterols with $B_{12}H_{11}SH$ known as BSH were synthesized for liposomal boron delivery systems in neutron capture therapy. The current synthesis is based on the *S*-alkylated BSH with alkyl halides. The BSH substituted cholesterol liposome, which was prepared from dimyristoylphosphatidylcholine (DMPC), cholesterol, BSH substituted cholesterol, and polyethyleneglycol-conjugated distearoylphosphatidylethanolamine (PEG-DSPE) (1:0.5:0.5:0.1), exhibited higher cytotoxicity than BSH at the same boron concentration and IC_{50} values of the BSH substituted cholesterol-liposome and BSH toward colon 26 cells were estimated as 25 and 78 ppm of boron concentration, respectively.

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

Transferrin-Loaded *nido*-Carborane Liposomes: Tumor-Targeting Boron Delivery System for Neutron Capture Therapy

김소연 이종대*

조선대학교 화학과

The *nido*-carborane lipid as a double-tailed boron lipid was synthesized from heptadecanol in five steps. The boron lipid formed stable liposomes at 25% molar ratio toward DSPC with cholesterol. Transferrin was able to be introduced on the surface of boron liposomes (Tf(+)-PEG-CL liposomes) by the coupling of transferrin to the PEG-CO2H moieties of Tf(-)-PEG-CL liposomes. A boron concentration of 22 ppm in tumor tissues was achieved by the injection of Tf(+)-PEG-CL liposomes at 7.2 mg/kg body weight boron in tumor-bearing mice. After neutron irradiation, the average survival rate of mice not treated with Tf(+)-PEG-CL liposomes was 21 days, whereas that of the treated mice was 31 days.

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발표코드: **MEDI.P-877**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Liposome Formation of B-10 Enriched $B_{12}H_{11}S$-Substituted Lipids for Boron Delivery System on BNCT

황조현 이종대*

조선대학교 화학과

We succeeded in the synthesis of the double-tailed boron cluster lipids 4a-c and 5a-c, which have a $B_{12}H_{11}S$ moiety as a hydrophilic function, by *S*-alkylation of $B_{12}H_{11}SH$ (BSH) with bromoacetyl and chloroacetocarbamate derivatives of diacylglycerols for a liposomal boron delivery system on neutron capture therapy. Calcein encapsulation experiments revealed that the liposomes, prepared from the boron cluster lipid 4b, DMPC, PEG-DSPE, and cholesterol, are stable at 37 °C in FBS solution for 24 h.

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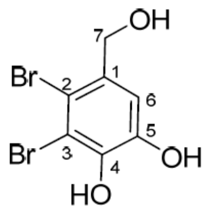
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-Human Rhinoviral Activity of Bromocatechols Isolated from the Korea Red algae, Neorhodomela aculeata

최필주 김희진[1] 이명재 이석준[2] 함정엽[1,*]

강릉원주대학교 화학신소재학과 [1]한국과학기술연구원(KIST) 천연의약센터 [2]관동대학교 의과대학 기초과학교실

The oceans are home to 90% of the world’s living biomass, which makes up about half of the total global biodiversity. Thus, the marine environment is an extraordinary reservoir of bioactive natural products, many of which exhibit chemical and structural features not found in terrestrial natural products .The oceans are a rich source of bioactive compounds, which only started to attract interest from pharmaceutical companies and research institutions approximately 50 years ago. Since then, more than 14,000 different natural products from marine organisms have been described, and hundreds of patents describing new bioactive marine natural products have been filed. More than 500 species of marine algae are distributed along the coast of Korea. Some of these algae are sources of food and traditional medicines, while others may serve as important resources for bioactive natural products. The Rhodomelaceae family are rich sources of several monoaryl, diaryl, and triaryl bromocatechol structural types with various biological activities, including anticancer, antioxidative, antimicrobial, and anti-thrombotic effects.The aim of the present study was the extraction of the red alga, Neorhodomela aculeata, which showed antiviral activity against human rhinovirus toward HeLa cells.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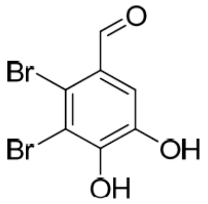
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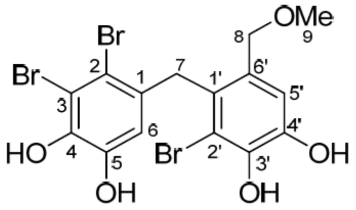
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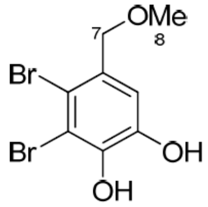
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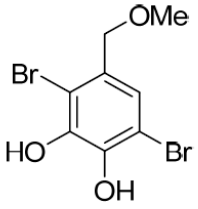
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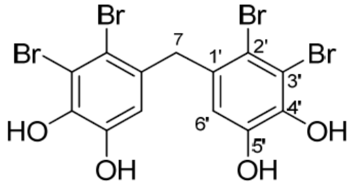
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일시: 2013년 4월 17~19일(수~금) 3일간
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발표코드: **MEDI.P-879**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification of mGluR5 negative allosteric modulators for treatment of neuropathic pain.

김지영 배애님[1] 이재균[2] 최기항 조용서[1] 민선준[3]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 생체과학연구본부 [2]한국과학기술연구원(KIST) 케모인포매틱스연구단 [3]한국과학기술연구원(KIST) 뇌의약연구단

Glutamate is the major excitatory neurotransmitter of mammalian in central nervous system and peripheral nervous system. Glutamate receptors are related to mediate glutamate for post-synaptic excitation in neural cell, involved in pathologies of many brain diseases. They are classified into two types of receptors depending on the mechanism of activation; ionotropic glutamate receptors (iGluRs) and metabotropic glutamate receptors (mGluRs). Metabotropic glutamate receptors belong to the type C class of GPCR (G protein coupled receptors) and they are divided into three groups with eight subtypes on the basis of their sequence hormonology, pharmacology, and signal transduction mechanism. Group I consists of the mGluR1 and mGluR5, which are predominantly identified in post-synapses in the brain region, including the hippocampus, cerebellum, thalamic nuclei, and spinal cord. Recently studies showed that selective mGluR5 antagonists may play a role in the treatment of neuropathic pain and other brain diseases. Accordingly, we have synthesized a series of quinoline derivatives and tested their inhibitory activities against mGluR5 receptors. Indeed, we identified one compound showing good potency under IC50 value of 1 μM. In addition, it was found that it has excellent stability profile. At last, in vivo study revealed that this compound exhibited favorable analgesic effects in spinal nerve ligation model of neuropathic pain, which is comparable to gabapentin.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] 연회비 환불 및 발표 취소

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발 표 취 소

본 논문은 발표취소된 논문입니다.

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A Highly Stable α-Helix constrained by a Hexenyl Propionate Cross-link

유지연 김영우*

동국대학교 약학대학

The α-helix is the most common secondary structure of proteins and plays a critical role in mediating many important protein-macromolecule interactions. Based on the notion that short helical peptides may be useful for modulating such interactions, a library consisting of unbiased α-helical peptides would be a powerful tool to efficiently identify new, biologically active molecules. Although various chemical strategies have been developed to stabilize α-helical conformation of a short stretch of peptides using a covalent crosslink, they are not appropriate for building such libraries, especially because deconvolution of active peptides is difficult using typical peptide sequencing methods due to the stable covalent cross-links. Here we present a new helix-stabilizing strategy by utilizing a hexenyl propionate tether. A peptide constrained by this ester-containing linkage showed a notably enhanced helicity, indeed compatible to that induced by the most widely employed "all-hydrocarbon stapling" system. In addition, the hexenyl propionate moiety is considerably stable at a physiological pH. Furthermore, the hexenyl propionate linkage can readily be cleaved in the presence of a palladium catalyst to yield a linear peptide that can be analyzed by typical peptide sequencing methods. These results strongly support the valuable potential of this new cross-linking system for the practical application to the α-helix library approach.

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Synthesis and Biological Evaluation of the Mitochondrial Permeability Transition Pore (mPTP) Inhibitors for the Treatment of Alzheimer's Disease

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The role of mitochondrial β-Amyloid peptide(Aβ) has been highlighted in Alzheimer's disease(AD) pathogenesis. Aβ is produced from transmembrane amyloid precursor protein(APP) by sequential actions of β- and γ-secretase. Aβ is implicated in the pathogenesis of Alzheimer's disease by interaction of Aβ with cyclophilin D(CypD). CypD, adenin nucleotide translocator(ANT), voltage-dependent anion channel(VDAC), and benzodiazepine receptor(PBR) compose the mitochondrial permeability transition pore(mPTP). The interaction of Aβ with CypD enhances the translocation of CypD to the mPTP and results in mPTP opening. After the mPTP opening, cytosolic solutes influx into the mitochondrial matrix, and then mitochondrial swelling causes cell death. Therefore, blockage of CypD or PBR can be an effective therapeutic strategy in Alzheimer's disease. Based on the pharmacophore-based virtual screening, we identified novel scaffolds KKPN0001 and KKPN0002, and the synthesis and biological evaluations of those compounds were performed. The 80 newly synthesized KKPT compounds were biologically evaluated in vitro and in vivo. And their biological data showed the improvement in symptoms of AD. Now the optimization of novel mPTP inhibitors is in progress.

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Naturomimetic Approach을 이용한 생리활성 천연물의 전합성 및 유도체화 연구

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최근 자연계에서 발견된 천연물이 인간에게 유용한 생리학적 활성을 나타내어 신약 또는 그의 선도물질로 이어지는 경우를 흔히 볼 수 있다. 그 예로 Tamiflu, Taxol, Vincristine, Morphine, Codeine 과 같은 천연물 및 그 유도체는 시중에서 항암제, 진통제등으로 널리 이용되고 있다. 특히, 이러한 천연물은 유기합성을 통한 화합물에 비해 개발기간이 단축되고 임상 실험 등 환자 투여 시 부작용문제가 적다는 장점이 있어 신약개발 분야에서 크게 주목 받고 있으며 국내뿐만 아니라 전 세계적으로 천연물을 이용한 신약개발의 비중은 크게 증가하는 추세이다. 이에 본 연구팀은 자연에서 발견된 인간에게 유용한 생리활성을 가지는 천연물의 전합성과 이를 기반으로, 천연물 유도체화 연구를 통한 천연물 신약개발에 주력하고 있다. 또한, 보다 효과적인 유도체화 연구를 위해 본 연구진이 고안한 Naturomimetic Approach 개념을 도입하여 천연물의 모체를 제조한 후, C-C, C-N 등의 결합반응을 통한 천연물 유도체 합성 및 생리활성 탐색연구를 수행 중에 있다. 본 포스터 발표에서는 Naturomimetic Approach 의 개념과 함께 최근에 진행된 Amorphastilbol, Arylnaphthalene Lignan 류 생리활성 천연물의 전합성 및 유도체화 연구에 대해 보고하고자 한다.

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Galactosylated Magnetic Nanocomplexs for ASGPr-specific siRNA delivery and MR imaging

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Hypercholesterolemia, is associated with low-density lipoprotein (LDL)-cholesterol levels in the blood, can lead to premature cardiovascular diseases. In recent, one method for treatment of hypercholesterolemia has reported that the regulation of PCSK9 can increase LDL receptors to reduce LDL concentration in the blood. In particular, siPCSK9 can explore to inhibit the production of target PCSK9 proteins in cytosol as a means of post-transcriptional regulator of LDL receptor expression. However, the delivery of siRNA molecules to the target cells is a challenge because of non-specific off-targeting effect, immune stimulation problem, and absence of optimal delivery vehicles. To leap these obstacles, developing biomarker-specific nanovector is important for siRNA-based therapy. In this study, we thus fabricated glycosyl magnetic nanovector (gMNV) that are capable of targeting asialoglycoprotein receptor (ASGPr), a biomarker expressed on hepatocyte membrane, for siPCSK9 delivery and the simultaneous monitoring of targeting by MR imaging in particular. The physicochemical properties and cytotoxicity of gMNVs were reported using a variety of analytic techniques. In addition, the targeting efficiency of siPCSK9-loaded gMNVs and MR imaging potential were confirmed. As a result, our studies demonstrated that gMNVs enabled the targeted delivery of siRNA to ASGPr-expressing hepatocytes for regulation of PCSK9 level. In conclusion, the well-defined nanocomplex will be helpful to study of RNAi and biomarker-specific molecular imaging.

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Synthesis and Biological evaluation of the 3,5-disubstituted Indol as PIM Kinase Inhibitors.

MORE KUNAL 이진호*

계명대학교 화학과

Pim kinases are the small family of serine-theronine kinases which play role in survival, apoptosis, differentiaon and proliferation of both normal and cancerous hematopoietic cells. Pim kinases regulated through activation of cytokine receptor recruiting JAKS for induction of STAT-dependant transcription of Pim gene. Overexpression of these Pim genes has been reported to cause some solid tumors and many hematologic cancers such as chronic lymphocytic leukemia. Discovery of Pim-1 inhibitors has intensively pursued attention as potential and selective anti-cancer agents in recent years. Indole scaffold is continuously drawing interest for development of newer drug moiety due to its wide range of activities like anticancer, antibacterial, antifungal, anti-malarial, anticonvulsant and anti-inflammatory. Novel series of 3,5-disubstituted indole were synthesized and screened against Pim kinases. Synthesized compounds showed potent inhibitory activity against Pim kinases.

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Synthesis and antioxidative activity of Polyphenolic acid derivatives

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계명대학교 화학과

Oxidative stress resulted from excessive reactive oxygen species (ROS) is highly related to the occurrence of diseases such as cancer, diabetes, inflammation, neurological disorders and cardiovascular disease. The biomolecular damage caused by the attack of ROS to living organisms can be effectively quenched by antioxidants. Phenolic acids have shown the potential protective role against oxidative damage related diseases. In the present study, antioxidative activities (DPPH, ABTS, FTC, TBA) of gallate and 3,4,5-trihydroxyphenylacetate derivatives were compared. It was found that antioxidant activity of two phenolic acids showed different patterns of dependency on the structure of substituent.

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The studies on 1-substituted indole derivatives as GPR109A agonists

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Indole-2-, 3- or carboxylic acids were synthesized and biologically evaluated as the agonists on GPR109A. The 1-position of indole was diversified with a variety of groups including variously substituted nicotinoly, 3-(thiazol-5-yl)propanoyl, 3-(1,2,3-triazol-4-yl)propanoyl, 3-(1,2,4-oxadiazol-5-yl) propanoyl, pyrazin-2-carbonyl, and piperazin-1-carbonyl moieties to elucidate the structure-activity relationships. The activation activity of synthesized compounds on GPR109A was evaluated using the GPR109A overexpressed cell lines. In addition the selectivity on G-protein signaling over β-arrestin signaling was determined.

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The Role of Korea Chemical Bank in "Hit to Lead" process ofDrug Discovery

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한국화합물은행은 산?학?연 등에서 기탁한 25 만여 종의 다양성이 확보된 화합물을 관리하고 있으며 현재까지 490 여개 작용점에 대한 고효율약효시험(HTS)에 활용되어 Hit 를 대상으로 한 선도물질화 연구를 지원하고 있다. 한국화합물은행에서는 HTS 후 도출된 Hit 평가 과정에서 Hit 화합물의 순도 및 물리화학적 물성평가, pharmacophore 검색을 통한 SAR 자료, 작용점에 대한 최근 연구개발 동향 및 Hit 골격과의 연관성, Pre-ADME 검색을 통한 선도물질성, 3D-QSAR 결과 등을 관련기관에 제공하고 있다. 아울러 Hit 발생 빈도가 높은 화합물 골격에 대한 조사를 통하여 false positive 에 대한 일반적 정보를 제공하여 선도물질개발을 위한 Hit 평가를 좀 더 효율적으로 진행할 수 있도록 하고 있다. 그 결과 독창적인 골격을 지닌 Hit 가 다량 도출되고 있으며, 그 중 항암제, 당뇨병 및 난치성 질환과 관련된 Hit 화합물로 후속연구가 진행 중에 있으며 이러한 “Hit to Lead"의 몇 가지 사례 및 이 과정에서 화합물은행의 역할에 대하여 발표하고자 한다.

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Anticholinesterase Activities of Organic Extracts of Chinese Propolis

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In our continuing search for anti-cholinesterase compounds, chinese Propolis was examined and here we report the isolation and structure determination of the purified anti-cholinesterase compounds.From the 100% methanol extract of Chinese Propolis, solvent partition fractions were prepared by using n-hexane, chloroform, butanol and water, and among them chloroform fraction showed strong anti-BuChE and anti-oxidative activities.Using various chromatographic methods and by the bioassay-guided fractionation, three BuChE inhibitory compounds, C-1b-1, C-1b-2 and C-1b-3, were purified. Also, they structure of three compounds, were elucidated by GC-MS and NMR experiments.These three compounds (C-1b-1, C-1b-2, C-1b-3) showed strong BuChE activity as 74.01, 84.75, 81.38% at 100μg/mL. While they showed relatively low AChE inhibitory activity as 6.11, 21.76, 7.06% at 100μg/mL, they showed much stronger BuChE inhibitory activity.From these results, we concluded that the three isolated compounds from chinese Propolis, C-1b-1, C-1b-2 and C-1b-3, are BuChE selective inhibitors and antioxidative. Thus, these could be the candidates for functional foods, cometical resources and AD therapeutics. * BuChE : butyrylcholinesterase * AChE : acetylcholinesterase

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PharosDre@ms 3.0: IT-based Drug Discovery Solution

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Structure-based drug design methods have had a significant impact on the creation of high-value compounds entering the market as drugs, or at least entering clinical trials. The core technology of structure-based drug design, virtual screening can find lead compounds more faster and less expensive than experimental HTS, it provides the key to reduce the number of compounds to be evaluated by experimental assays. We present a new structure-based drug discovery solution, PharosDre@ms 3.0, for accurately docking ligands into protein binding sites. This solution identifies potential binding sites of the protein by cavity detection algorithm. A Monte Carlo conformational search for generating ligand poses in the binding site is used. Ligands are minimized in the environment of the binding site using MMFF94 force field for evaluating protein-ligand interaction energies. Thus, it changes high cost and low efficieny to cost-effective alternatives. Using high-performance computing power, preclinical and clinical phase can be done at reduced time and cost. Drug discovery using PharosDre@ms 3.0 helps bio-venture companies that focus on the research find leads with row cost and fast time.

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Preparation of CD44 targeted gold liposomes

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Most primary human tumors, as well as tumor vascular endothelial cells, express the CD44 family of cell surface proteoglycans, the natural ligand for which is hyaluronic acid (HA). Additionally, we also prepared gold coated liposomes (GCL) for tumor diagnosis (re). So, we prepared HA labeled GCL (HA-GCL) to target CD44 positive tumor cells to enhance diagnostic effect. To conjugate HA on the surface of GCLs, we synthesized thiol group labeled HA. The particles size and zeta potential were measured by particle size analyzer. HA labeling on GCL's surface was confirmed by UV spectrometry. While particles size of GCL were around 153 ± 8 nm, HA-GCLs were slightly increased to 203±21nm because of HA labeling. In addition, HA labeling efficiency is up to 90% on GCLs. In this study, we developed HA-GCL, which should be useful for diagnosis of CD44 expressed tumors.

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Preparation of linalool encapsulated nanoparticles for cancer therapy

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A lot of cancer patients have been suffered from serious side effect of chemo drugs. So, we sought advanced anti-tumor drug to reduce side effect. Linalool is a natural product, which has potential for cancer therapy without side effect. Therefore, we focused on development of linalool-nanoparticles (LNPs) to deliver linalool at tumor site. LNPs was prepared using linalool and 1, 2-distearoyl-sn-glycerol-3-phosphoethanolamine-N- [amino(polyethylene glycol)-2000] (DSPE-PEG-2000) which was generated in 8 % (v/v) Tween20 by voltexing. Size and zeta potential were measured by electrophoretic light scattering (ELS). Morphology was confirmed by scanning electron microscope (SEM). The size of LNP is around 60 nm and loading efficiency is up to 90%. In this study, we successfully prepared linalool encapsulated nanoparticles, which should be useful for cancer therapeutic study.

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Synthesis of Novel ^{64}Cu-Labeled RGD Conjugates for Improved PET Imaging

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목적: 신생 혈관 내피세포와 종양으로 인한 신생 혈관 생성시 발현되는 αvβ3-Integrin 의 표지를 위해 개발하고 있는 dimer cyclic RGD 는 monomer cyclic RGD 에 비해 αvβ3-Integrin 에 대한 uptake 가 높고, 체내 간 섭취 감소 및 blood clearance 를 증진시키고자 glucosamino 를 붙이고, tracer 의 lipophilicity 를 제거하였다. 따라서 NODAGA, DOTA, NOTA 의 각 chelator 에 dimer cyclic RGD 와 glucose 를 붙여 ^{64}Cu 로 표지된 새로운 혈관신생 자극인자 방사성의약품을 개발하고자 하였다.방법: 각 chelator 의 한쪽에는 glucosamino 를 붙이고, 다른쪽에는 cyclic RGDfK 를 각각 2 개씩 붙여 glyco imer cyclic RGDfK 를 합성하였다. 우선 체내 혈청에서의 안정성 평가를 위해 serum stability test 를 30 m, 60 m, 120 m, 24 h 동안 실시하였다. 다음으로 U87MG glioma cancer cell 이 형성된 누드마우스에 64Cu 가 표지된 3 종의 dimer cyclic RGDfK 230 μCi(8.5 MBq)/22 g/0.1 mL 씩을 꼬리 정맥에 주사한 후, 일정 시간별 영상을 획득하여 tumor 에 미치는 영향을 비교 평가하였다. 또한 각 장기에 대한 64Cu 표지된 3 종의 Glyco dimer cyclic RGDfK 의 장기섭취율을 비교하기 위해 각각 10 μCi(370 KBq)씩 꼬리 정맥으로 주사하고, 동물들을 희생시켜 장기와 종양조직내의 dimer cyclic RGD 의 섭취 정도를 감마계수기로 측정하고 장기섭취율로 계산하여 비교하였다.결과: serum stability test 에서는 3 종의 dimer cyclic RGDfK 모두 평균 화학적 순도가 95 % 이상으로 20 h 이상 안정하다는 것을 ITLC 결과로 확인하였다. 다음으로 tumor uptake 영상에서는 3 종의 glyco dimer cyclic RGDfK 모두 16 h 이상 tumor uptake 가 지속되는 것을 확인 할 수 있었다.결론: ^{64}Cu 가 붙은 3 종의 glyco dimer cyclic RGDfK 모두 혈청에서의 안정성을 확인할 수 있었고, tumor uptake 는 monomer cyclic RGDfK 에 비해 더 오래 지속되어 PET/CT 에서의 tumor 진단시 더욱 유리 할 수 있다는 가능성을 확인하였다.

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연구성과물(화합물) 기탁제

__황순희__ 김선우 이현규

한국화학연구원 한국화합물은행

국가는 연구성과의 활용성 증대를 위해 연구 주체들의 자발적인 협력을 유도하고 원활한 커뮤니케이션 창구를 구축하기 위해 8 대 연구성과물 전담기관을 지정하여 운영하고 있다. 한국화합물은행은 2004 년 7 월 과학기술부 ‘특정연구개발사업’ 연구성과물 기탁 및 등록제 화합물분야 중심기관으로 선정, 2012 년 5 월 '국가연구개발사업'으로 도출된 화합물을 기탁관리하는 연구성과물(화합물) 전담기관으로 지정되어 운영되고 있다.연구성과물(화합물)로 얻어진 저분자 라이브러리, 천연물 라이브러리, 조합화학 라이브러리 등 다양한 골격의 화합물이 산.학.연을 통해 한국화합물은행으로 기탁되고 있다. 한국화합물은행(www.chembank.org)은 기탁된 화합물에 대해 기탁필증을 발급하고 있으며, 기탁된 화합물 현황은 매년 각 기관에 전달되고 있다.한국화합물은행에서는 연구성과물(화합물)로 얻어진 다양한 화합물을 모아 체계적으로 관리하며 스크리닝용 플레이트를 생성하고 고효율약효시험(HTS)에 화합물을 제공하여 연 평균 40 여건의 다양한 질병 타겟에 약효시험을 수행하고 있으며, 각 단계별 관리정보는 화합물의 구조정보 및 약효검색 결과 DB 와 연동시켜 종합적으로 운영하고 있다.한국화합물은행은 화합물 및 정보를 매개체로 신약연구와 관련된 합성 및 고효율약효시험 기관간을 연결시켜 잠재적 가치를 갖는 산재된 화합물의 무한가치 창출에 기여하고자 한다.

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Formation of amorphous form of Clopidogrel Hydrogen Sulfate

윤선경

한밭대학교 화학공학과

In this study, the preparation of amorphous form of Clopidogrel hydrogen sulfate (CHS) from its polymorphic forms was carried out. Based on the solubility data, the amorphous form and form I was found to be monotropically related, whilst form I and form II are enantiotropically related. Furthermore, the supersaturation generated serves as a window for preparing the various solid forms of active pharmaceutical ingredients. The solid forms obtained from the crystallization process were characterized by Powder X-ray diffraction (PXRD), Scanning electron microscopy (SEM) and Optical microscopy (OM). The results indicated that the amorphous form can only be prepared at high supersaturations. In the order of supersaturation; amorphous > form I > form II crystallization. These results contribute to a better understanding of the polymorphic nature and crystallization mechanism of API's in terms of the preparation, solid-state characterization and solvent-mediated transformations of amorphous, form I and form II of Clopidogrel hydrogen sulfate.

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Sugar coating on pharmaceutical ingredient using solution crystallization

이경실

한밭대학교 화학공학과

Processing of crystalline solid with a particular field of application in mind and shows crystallization can be used as tool to generate materials with particular properties and how to tailor these properties by crystallization. The fact that crystallization is a tool for product design will be proved a coating solid drug forms, such as pills, granules and tablet. On the other hand, the problem of conventional coating process is cracking and splitting on the coating's surface, fast dissolution rate and non-uniformities in the coating's thickness, because the final coating is formed as an amorphous coating. A new coating process by crystallization was developed using solution method. In this study, evaluated coater performance based on three criteria: Product quality, product yield and product time. Quality can be characterized as a function of two factors, coating mass uniformity and coating morphology. Crystallization process is applied to obtain a uniform and crystalline coating. From this point of view, the ultimate objective of this study is to examine how a crystalline coating can be formed by crystallization and how operating conditions affect the surface morphology and the crystal growth rate of the solid drug coating. Crystal form can be determined by solubility as a thermodynamic feature and various parameters as a kinetic feature. Product parameters of interest are specific size or size distributions, certain purities and morphology (crystal shape), modification of polymorphs or solvates, long shelf life, a certain color, porosity, bioavailability or filterability.

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Development of Potential Anticancer Agents: Pyridone-based Histone Deacetylase Inhibitors for Metabolic Stability

조미선 이철호 한균희*

연세대학교 생명공학과

Histone deacetylases (HDACs) play a key role in epigenetic regulation and they are therapeutic targets for cancer. Abnormal expression of HDACs is presented in various cancer cells and most zinc-dependent HDACs induce proliferation, dedifferentiation, and anti-apoptotic effects in cancer cells. We designed and synthesized a new series of pyridone-based HDAC inhibitors that have a pyridone ring in the core structure and a conjugated system with an olefin connecting the hydroxamic acid moiety. Consequently, most of the selected pyridone-based HDAC inhibitors showed similar or higher inhibition profiles in addition to remarkable metabolic stability against hydrolysis relative to the corresponding lactam-based HDAC inhibitors. Furthermore, the selectivity of the novel pyridine-based compounds was evaluated across all of the HDAC isoforms. One of these compounds, (E)-N-hydroxy-3-{1-[3-(naphthalen-2-yl)propyl]-2-oxo-1,2-dihydropyridin-3-yl}acrylamide, exhibited the highest level of HDAC inhibition (IC_{50}= 0.07 ?M), highly selective inhibition of class I HDAC1 and class II HDAC6 enzymes, metabolic stability in mouse liver microsomal studies, and effective growth inhibition of various cancer cell lines. Docking studies indicated that a long alkyl linker and bulky hydrophobic cap groups affect *in vitro* activities. Overall, the findings reported herein regarding pyridone-based HDAC inhibitors can be used to guide future research efforts to develop new and effective anticancer therapeutics.

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Smart Protein Design System: Watson

김한조 정우성 서영주 장병하 윤정혁[1]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

Protein drugs have several superior characteristics like higher specificity and less adverse effects especially for rare diseases, while they are easily degraded in human body by a lot of different proteases, which causes low bioavailability and short life time. Different kinds of technologies including PEGylation, glycosylation, and protein fusion, are being actively developed not only to deal with this problem, but also to enhance protein's overall characteristics. Here we present a novel statistical model which can predict the probability of proteolytic event for a protein 3D structure. To achieve this goal, we carefully designed peptide sequence fingerprint (PSFP) and construct a probability calculation model. Statistical characteristics of this fingerprint are analyzed. As different kinds of fingerprint are actively used in small molecule area, we assume that protein-based fingerprint will have different strengths according to their algorithms. Compared to other rule-based systems already published, this fingerprint-based system is less biased and simpler to update. As a part of our Smart Protein Design System, Watson is used for our BioBetter development.

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Molecular modeling studies on structural requirement and underlying mechanism of pyrimidoazepine analogs for 5-HT2C receptor activation

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5-HT2C receptors, one of the members of aminergic G-protein coupled receptor families, are potential target for anti-obesity agents. Our pyrimidoazepine analogues that we designed and synthesized for targeting this receptor displayed agonistic or antagonistic functional activities on varying the substituents, which in turn will cause different therapeutic effects. Computational approaches, such as classification using Bayesian algorithm and recursive partitioning, a molecular docking to the homology model, and molecular dynamics simulations were adopted to reveal structural basis of these moieties to different functional activities, and underlying mechanism of how the receptor changes their conformations upon structural changes of bound ligands. The classification models revealed that aniline moiety of analogues was the determinant for functional activity of 5-HT2C receptor. The docking studies of these compounds using homology model of 5-HT2C receptor demonstrated that agonistic or antagonistic activities of ligands were attributable to the loss of broad van der Waals interactions between hydrophobic features of ligands and hydrophobic residues in TM3 and TM5, which confirmed our results of classification models. Further molecular dynamics simulation of 5-HT2C receptor homology model bound to agonists and antagonists clearly showed different conformational changes, which were measured by “ionic lock” stability at the bottom of TM3 and TM6. Our molecular modeling study identified the molecular features that were associated with different functional activities of 5-HT2C receptor, and substantiated that they actually changed the receptor conformation, which has taken a closer look at the underlying mechanism of 5-HT2C receptor activation.

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Structure-Activity Relationship and Mechanism of Action of Bicyclic Furanones as Anti-Influenza Agents

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As our ongoing search for new anti-influenza agents, we have performed a series of high-throughput screenings (HTS) with more than ten thousand compounds from the Korea Chemical Bank in KRICT to discover hit molecules active against both Type A (H1N1 and H3N2) and Type B influenza viruses. Several hit compounds were identified based on the evaluation of activities. Considering cytotoxicity profiles and the synthetic practicability of the hit compounds, a bicyclic furanone was selected to further optimize the activities. The structure-activity relationships of the bicyclic compounds will be presented. In addition, we will discuss the preliminary results about the mechanism of action of the compounds optimized.

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Synthesis and biological evaluation of heteroarylphenylcyclohexyl acetic acid derivatives as diacylglycerol acyltransferase-1 inhibitors

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Triacylglycerols (triglycerides, TG), a major type of neutral lipid, are a heterogeneous group of molecules with a glycerol backbone and three fatty acids (FAs) attached by ester bonds. Excess accumulation of triglycerides can participate in the pathogenesis of several metabolic disorders such as obesity, insulin resistance and type II diabetes and cardiovascular disease. Dietary TG is cleaved to monoacylglycerol and free fatty acids (FFA) by lipases in the gut lumen, which is moved to the enterocytes and reorganized by diverse enzymes. DGAT (Acyl-CoA: diacylglycerol acyltransferase), which has two isoforms (DGAT-1 and DGAT-2), is a transmembrane enzyme that functions in the final step of TG biosynthesis. DGAT-1 inhibition is expected to impair the TG and chylomicrons formation in the enterocytes to reduce postprandial TG levels in the blood. We will present the synthesis of heteroarylphenylcyclohexyl acetic acid derivatives and their biological evaluation as DGAT-1 inhibitors.

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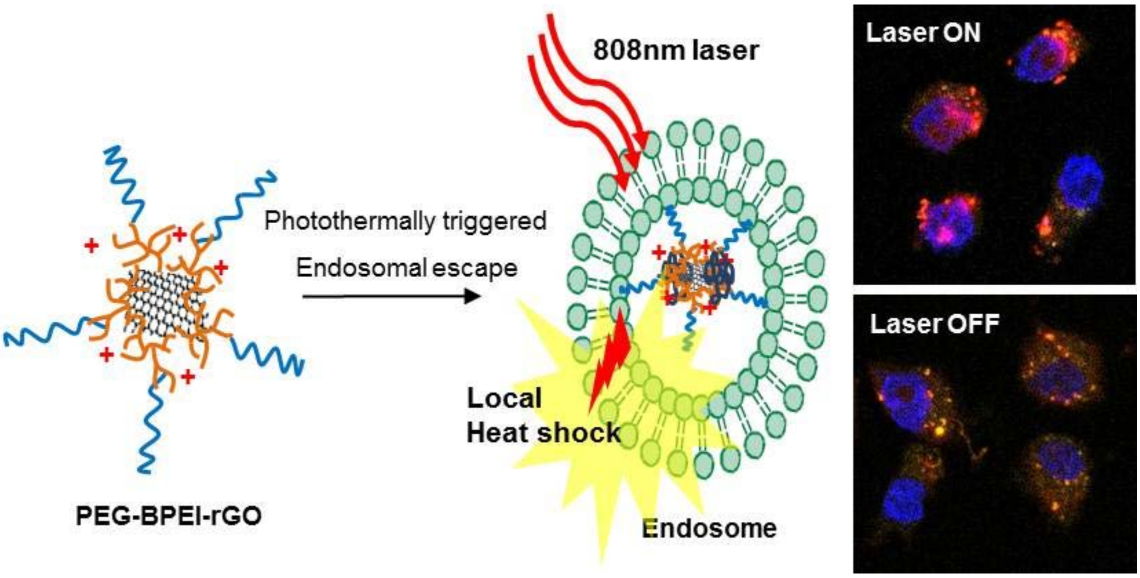
Near infrared light stimuli triggered gene delivery using a funtionalized reduced graphene oxide

김현우 김원종*

포항공과대학교 화학과

Recently, External stimuli responsive spatially and temporally controlled gene delivery vectors have received a huge attention, because it could allow highly advantageous in medicine for minimizing adverse effects. Among various external stimuli, light is provides a safe and convenient opportunity to release a gene at a want of time and in a target area, which is considered to enhancing gene delivery efficiency. Photothermal effect also can be used one of transfection strategy using by light, which is called as 'photothermal transfection (PTT)'. Meanwhile, Graphene Oxide (GO) has attracted increasing interest for its potential of applications in biomedical fields such as biological imaging, drug/gene delivery and cancer therapy. GO has unique features such as facile synthesis, high water dispersibility, capability of easy surface functionalization, and good biocompatibility which are suitable for biomedical applications. Moreover, owing to GO's high optical absorption in the NIR region, a new arrow for GO is in the biomedical field using photothermal effect of GO. However, to be an efficient gene delivery vector GO should be modified with cationic polymer such as polyethylenimine (PEI). And thus, in this study, we developed nanosized, reduced graphene oxide sheets with covalently conjugation of branched polyethyleneimine and PEGylation (PEG-BPEI-rGO). And confirmed the potential of locally and remotely activated photothermal transfection in cells using PEG-BPEI-rGO with NIR irradiation.


808nm laser
Laser ON
Photothermally triggered
Endosomal escape
Local
Heat shock
PEG-BPEI-rGO
Endosome
Laser OFF

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Ultrahigh Stabilization of Gold Nanorods using Chemical Reagents for the DNA-Conjugation

주장호 이재승*

고려대학교 신소재공학부

Gold nanorods (AuNRs) have been hardly used for applications because of their low stabilities. To solve this problem, we have first synthesized AuNRs using cetyltrimethylammonium bromide (CTAB), and have chemically improved their mechanical and chemical stabilities by a library approach. We hypothesize that certain negatively charged chemical agents would permeate the interlocked layers of CTAB on the surface of the AuNRs, and would gather more extra CTAB. Therefore, we have carefully chosen 11 chemical agents, and screened them spectroscopically for our purpose by measuring the shift of the λmax, and extinction at λmax. Based on the enhancement of stabilities, we develop a novel, reproducible, and facile method to synthesize polyvalent DNA-AuNR conjugates, and investigate how to control their melting properties. Zeta potential is used to reveal the fundamental mechanism of the ligand exchange, and reinforcement of the AuNRs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Controlling Nanoparticle Seed Structures Using a Polymer Library

김병호 이재승*

고려대학교 신소재공학부

To date, the precise control of the structures of tiny silver nanoparticles, or silver seeds, has been hardly achieved owing to the difficulties lying in the analysis of how these structures affect the grown products. To solve these problems, we investigate twenty-four polymers with respect to their molecular weights, functionalities,and charges, each of which turns out to playsignificant roles in theformation of the seed structures and their growth into larger nanostructures.Interestingly, the grown products exhibitvarious optical properties observed by UV-vis spectroscopy, depending on which polymer is used to control the seed structure.A mechanism depicting the seedstructures ‘stitched by polymer threads’ is proposed, which clearly explains the experimental observations.

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A comparative kinetic-study of CO oxidation catalyzed by Fe_2O_3 submicron clusters and Fe_2O_3 powder

유승균 이성한[1]

연세대학교 화학과 [1]연세대학교 화학 및 의화학과

Fe_2O_3 clusters with spherical shape were prepared by using a solvothermal method and Fe_2O_3 powder with the particle size of 20-50 μm was prepared by decomposition of iron nitrate. The XRD results showed the samples to be monophase Fe_2O_3 having rhombohedral structure. FE-SEM and HR-TEM results indicated that the Fe_2O_3 clusters are porous spheres with the size of ~490 nm in diameter. The samples were examined as catalysts for the CO oxidation to compare their catalytic properties. The catalytic reaction was carried out in a flow of $CO/O_2/He$ mixture at atmospheric pressure in the temperature range of 100-500℃. The reaction was found to be catalytic below 300℃. Rates of CO_2 formation were measured in a flow of $CO/O_2/He$ (10/5/15 cm^3/min) mixture in the temperature range of 100-300℃. Apparent activation energies obtained from the Arrhenius plots were 15.0 kcal/mol for the Fe_2O_3 powder catalyst and 15.1 kcal/mol for the Fe_2O_3 cluster catalyst. The p_{O2} and p_{CO} dependencies of reaction rate were measured at a various partial pressures of CO and O_2 at 275℃ for the CO oxidation. Both the catalysts showed zero'th order with respect to p_{O2}. The p_{CO} dependence was found to be 1.0-order for the Fe_2O_3 pwder catalyst and 0.7-order for the Fe_2O_3 cluster catalyst. Reaction mechanism for the CO oxidation over Fe_2O_3 catalyst was suggested from the kinetic data and rate law was derived from the reaction mechanism.

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High efficiency white organic light-emitting diodes fabricated using a broad-bandwidth red phosphorescent emitter for lighting application

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부산대학교 화학과

High color rendering white organic light-emitting devices (WOLEDs) were developed using a broad-bandwidth red phosphorescent iridium complex, bis[2-(1-naphthyl)benzothiazolato-N,C2′]iridium(III) acetylacetonate [Ir(absn)2(acac)]. The red phosphorescent emitter Ir(absn)2(acac) was used to fabricate blue-red and blue-green-red WOLEDs by combining blue-emitting bis[2-(4,6-difluorophenyl)pyridinato-N,C2′]iridium(III) picolinate (FIrpic) and green-emitting tris-fac-(2-cyclohexenylpyridine) [Ir(chpy)3] in multiple-emissive layers. Mixed host emissive layers were employed using host TCTA and DCzPPy for efficient charge carrier injection. The effects of the emissive layer thickness and the doping ratios of different color dopants on WOLED performances were investigated. The WOLED based on ITO/TAPC/TCTA:FIrpic (10%):Ir(absn)2(acac) (4%)/TCTA:Ir(chpy)3 (9%, 6 nm)/DCzPPy:FIrpic (13%):Ir(absn)2(acac) (4%)/BmPyPB/LiF/Al exhibited an external quantum efficiency of 10.7%, a power efficiency of 23.0 lm/W, a very high color rendering index (CRI) of 88.1, and a correlated color temperature (CCT) of 2629 K at 1,000 cd/m2.

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Atomic Layer Deposition of Tin Monosulfide using Bis[bis(trimethylsilyl)amino]tin(II) and Hydrogen Sulfide

한규석 성명모*

한양대학교 화학과

Thin films of tin monosulfide (SnS) have been deposited by the atomic layer deposition (ALD) using bis[bis(trimethylsilyl)amino]tin(II) and hydrogen sulfide (H_2S) as precursors. The film growth rate was 0.41?/cycle at deposition temperature of 120~200°C. A linear growth rate characteristic of ALD was observed, with no chemical contamination. Film properties are studied using XPS, XRD, Raman and Hall measurements. SEM images show that the films are polycrystalline with grain size increasing with film thickness. Using UV-VIS spectroscopy study, the fabricated SnS films have low optical band gap around 1.45eV and strong absorption coefficient in visible range, which mean that the fabricated SnS films can be a promising photovoltaic material.

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Solution processed AgNWs-reduced graphene oxide (rGO) transparent electrode for organic photovoltaic devices

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Transparent electrodes have been known and well-studied as an essential element of optoelectronic devices. Indium tin oxide (ITO) has been widely used in a variety of optoelectronic devices because of low sheet resistance and high optical transmittance. However, it has several drawbacks such as color, brittleness, high indium cost, and high processing temperature used in its production. Therefore, flexible and solution-processable transparent electrodes have been required for flexible solar cells and display applications. Recently, solution-processable transparent electrode based on a silver nanowire (AgNW) ink is attracting interest as a promising candidate because it shows high optical transmittance, low sheet resistance, and flexibility. However, they still have a long-term stability issue, which makes them difficult for practical use. When AgNW films are exposed to air and water, AgNW can be easily oxidized, leading to sharp increase of sheet resistance and hazeness of the AgNW films. Therefore, it is necessary to suppress the oxidation of AgNWs for enhancement of the long-term stability of the AgNW films. Here, we demonstrate reduced graphene oxide (rGO)-coated AgNW films which exhibit excellent thermal oxidation and chemical stabilities. The reduced graphene oxide (rGO)-coated AgNW films exhibited high optical transmittance and low sheet resistance, which is comparable to ITO transparent electrode. In addition, it was found that AgNW-rGO films exhibited highly enhanced long-term stability due to excellent gas-barrier property of rGO passivation layer onto AgNW film. Furthermore, the organic solar cells with AgNW-rGO hybrid transparent electrode showed good photovoltaic behavior as much as solar cells with AgNW transparent electrode.

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One-Step Encapsulation of Individual Yeast Cell with Rationally Designed Catalytic Peptide

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한국과학기술원(KAIST) 화학과 [1]*한국폴리텍대학 바이오캠퍼스 바이오나노소재과*

Biomineralization, the evolved process of mineral formation in nature, has been utilized in versatile applications involving both academic interests and industrial interests: drug delivery, surface functionalization, carbon dioxide capturing, and water purification. In particular, cell encapsulation is the emerging field of interdisciplinary study (i. e. nanobiotechnology) inspired by biomineralization, such as silica, titania, iron oxide. Although some groups reported a few strategies of cell encapsulation, it generally adopted layer-by-layer technique (LbL technique) using positively/negatively charged and cytocompatible polymers. However, LbL technique is time-consuming and causes loss of products in multiple steps. In this context, we designed catalytic peptide inspired by silicatein-a, the silica-forming enzyme in glass sponge, and carried out peptide-induced encapsulation of individual yeast cell using tetraethyl orthosilicate (TEOS) without any further steps. The resulting yeast@silica showed high viability and efficiency of encapsulation. In addition, time delay of division process of yeast@silica and lyticase tolerance were studied. Considering the simplicity of process, the peptide-induced cell encapsulation could be utilized in other cells and fields.

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Synthesis of diketopyrrolopyrrole (DPP)-based small molecule donors containing thiophene or furan for photovoltaic applications

김유정 임은희*

경기대학교 화학과

Two π-conjugated small molecules based on diketopyrrolopyrrole (DPP) were synthesized using the Suzuki coupling reaction to determine the effects of furan and thiophene on the OPV performance. Two small molecules contain furan and thiophene, respectively, next to a DPP core. Organic photovoltaic cells (OPVs) were fabricated using two DPP-based oligothiophenes as donors. The improved photovoltaic properties of DPP4T will be explained by the optical properties and the film morphology.

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Synthesis and Photovoltaic Properties of oligothiophenes containing diketopyrrolopyrrole (DPP)

조아라 임은희*

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In this study, a series of solution-processable π-conjugated small molecules based on thiophene and DPP have been synthesized using the palladium-catalyzed Suzuki coupling reaction. The oligomers were designed to have solubilizing alkyl groups to facilitate solution-processing. Two oligomers have the same conjugated backbone of five thiophene rings and differ only in the direction of hexyl side chains (α- and β- position). The relationship between the different direction of side chains and photovoltaic properties were investigated in terms of band gap and film morphology. The optical and physical properties of these materials were characterized by UV-visible, photoluminescence (PL), cyclic voltammetry (CV), TGA and DSC measurements. Finally, the organic photovoltaic cells were fabricated using new materials as the active layer.

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Synthesis and luminescence spectra of $Eu^{2+/3+}$-doped $LaAlO_3$ phosphors

이민호 정우식*

영남대학교 화학공학부

Europium(III)-doped lanthanum aluminate ($LaAlO_3$) powder was prepared by calcining a mixture of alumina and Eu(III)-doped lanthanum carbonate hydroxide ($LaCO_3OH$) powder that had been obtained from boiling an aqueous solution containing La(III) salt, urea and EuF_3. The $LaAlO_3$ powder was characterized by X-ray diffraction, ^{27}Al MAS NMR spectroscopy, and scanning electron microscopy. The blue emission lines in luminescence spectra of Eu(III)-doped $LaAlO_3$ powder became more intense with increasing calcination temperatures.

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Proton beam-induced morphology change of Au nanorods

이윤지 송재희*

순천대학교 화학과

Chemically synthesized gold nanorods were irradiated with proton beam, and the morphology change of as-made Au nanorods was monitored by UV-Vis absorption measurements and TEM analysis. Proton beam current and irradiation time were adjusted systematically and the effects of the two factors were investigated. Average aspect ratio of as-made gold nanorods was in the range of 4.5. As the beam irradiation time was increased, the aspect ratio was observed to be gradually decreased.

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Size-controlled synthesis of Pd nanocrystals through proton beam irradiation

송재희

순천대학교 화학과

We present a facile one-pot synthetic route for the production of palladium nanoparticles via a simple proton beam irradiation process at room temperature. The synthesis of size-controlled palladium nanostructures was realized just by changing the mean current of the proton beam and by controlling the molar concentration ratios of surfactants to Pd precursors in an aqueous phase-based solution without the addition of any harsh reductants. As the beam current was increased under the same Pd ion concentration conditions, the average diameter of the prepared Pd nanoparticles tended to be decreased. We also found that the size of the synthesized Pd nanocrystals was decreased as the molar ratio of surfactants to palladium ion was increased.

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Facile one-pot synthesis of Ag NPs and CNT-Ag NPs composites through proton beam irradiation

이윤지 송재희*

순천대학교 화학과

A facile one-pot synthetic route is presented for the preparation of silver nanocrystals via a simple proton beam irradiation process at room temperature. Size and shape of the prepared silver nanostructures were controlled just by changing the stabilizing reagents and by controlling the molar ratios of stabilizer to silver ions. The size of the resulting Ag nanocrystals was observed to be easily varied by changing the stabilizer from hexadecyltrimethylammonium bromide to sodium dodecyl sulfate. The size of the prepared silver nanocrystals was also found to be decreased as the molar ratio of hexadecyltrimethylammonium bromide to silver ion was increased. Composites of carbon nanotubes with metal nanoparticles are particularly useful for use in catalysis, energy storage, and nanotechnology. Among them, CNT-Ag nanocomposites drew significant attention due to their potential applications as catalyst, and advanced materials. In this study, a new synthetic route to decorate carbon nanotube (MWCNT) with silver nanoparticles (Ag-NPs) is presented via a simple proton beam irradiation process at room temperature. The characterization of the MWCNT/Ag composites has been done by using FE-TEM and EDS analysis.

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Low-Temperature Growth of Carbon Nanotubes from Organocobalt Precursor and Benzene

JIN ZHENYU LIYINSHI 임지나 박인혜 민요셉*

건국대학교 화학공학과

We report low temperature growth of carbon nanotubes on SiO_2/Si substrates in vacuum reactor by alternately supplying Co precursor (dicobalt hexacarbonyl tert-butylacetylene, DCHCBA) and benzene. Our growth sequence consists of DCHCBA pulse-purge-benzene-pulse, which is akin to that for atomic layer deposition. The sequence was repeated to control the growth behavior of CNTs. The DCHCBA precursor and benzene play roles of catalyst and carbon source, respectively. Carbon nanotubes, which show clear G-bands and radial breathing mode in Raman spectra, are grown even at 400 ℃. D- to G-band ratio, which is a measure of crystalinity in CNTs, is ~ 0.5 for the CNTs grown at 400 ℃. However the ratio is improved at higher growth temepratures and/or by repeating the growth sequance.

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Optical Capacitance-Voltage Characteristics of Organic-Inorganic Alloy Film Grown by Molecular Layer Deposition

LIYINSHI 박인혜 임지나 **JIN ZHENYU** 민요셉*

건국대학교 화학공학과

Organic-inorganic alloy films were deposited onto p-type silicon substrates by molecular layer deposition (MLD) using trimethylaluminum, *p*-phenylenediamine and water. The electrical properties of the alloy films were investigated on Au/alloy/p-Si capacitors by capacitance-voltage (CV) and current-voltage (IV) measurements. Interestingly when the CV was measured with a frequency of 1 MHz under a white light, CV curve shows a dramatic increase in the capacitance in a range of positive bias. Furthermore the degree of the increase in the capacitance is strongly influenced by a power of the light. Here we discuss the origin of this phenomenon by comparing with an optical CV curve of Au/Al_2O_3/p-Si capacitor.

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Photoresponsive Azobenzene-Functionalized Monolayers

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Although azobenzene molecules in organic solutions undergo reversible trans/cis photoisomerization, it has been reported that closely packed azobenzene self-assembled monolayers (SAMs) are photochemically unreactive on flat surfaces. Efforts to afford free volume required for the conformational change between the trans and cis forms have been made by fabricating (i) unsymmetrical azobenzene disulfide SAMs and (ii) mixed azobenzenethiol and alkanethiol SAMs. However, instability problem accompanied by cleavage of the S-S disulfide and phase separation occurs in these SAMs consisting of two components on a gold surface. We have designed azobenzenethiols (ortho-Az) substituted with alkyl groups at the ortho positions and investigated their photoisomerization characteristics in solution as well as in SAMs on a flat gold surface. Photoswitching between the trans and cis states was confirmed by UV-vis absorption spectroscopy and contact angle measurements. Reversible variations in the surface morphology between the worm-like structure and the smoother structure were successfully manipulated by continuous alternating irradiation with UV and visible light (Figure 1). The collective molecular photoswitches (light-sensitive molecular reeds) are successfully visualized in phase-separated nanodomains by atomic force microscopy (AFM).References[1] Han, M.; Ishikawa, D.; Honda, T.; Ito, E.; Hara, M. Chem. Commun. 2010, 46, 3598.[2] Han, M.; Ishikawa, D.; Honda, T. Soft Matter. 2011, 7, 10594.

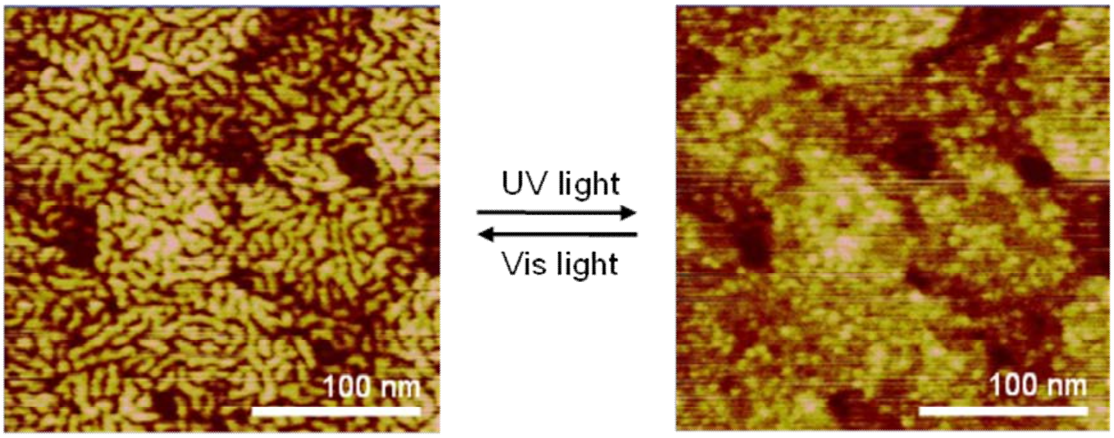

Figure 1. AFM images of ortho-Az SAMs on Au(111).

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Mussel-Inspired Green Synthesis of Silver Nanoparticles on Graphene Oxide Nanosheets for Enhanced Catalytic Applications

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울산과학기술대학교(UNIST) 친환경에너지공학부

We report a novel green approach for the synthesis of silver nanoparticles on the surface of graphene oxide (GO) nanosheets and demonstrate its utility for active catalyst for reduction of nitroarenes. By introducing the mussel-inspired motif of dopamine (Dopa) on the surface of graphene oxide, silver nanoparticles were easily synthesized by the simple mixing without additional reductant or stabilizer at room temperature. This hybrid Ag/GO-Dopa composite is characterized with various techniques including FT-IR, UV/vis, AFM, TEM, XRD, and ICP/MS. Also, the catalytic activity of the hybrid Ag/GO-Dopa is monitored with UV/vis spectroscopy. We observed that Ag nanoparticles are well decorated on the GO-Dopa sheets with a good dispersity and stability in aqueous solution and Ag/GO-Dopa has a superior catalytic activity for the reduction of nitroarens due to the high surface area of graphene nanosheets and the catalytic activity of Ag nanoparticles.

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Preparation of Highly Uniform and Well Dispersed Hollow Carbon Nanocapsules by using Protective Silica Shells

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A novel process for the preparation of highly uniform and well dispersed hollow carbon nanocapsules with mesoporous shell was developed. Highly monodisperse silica nanoparticles were coated with octadecyltrimethoxysilane to produce core/shell nanostructures. The core/shell nanostructures were further coated with outer silica shells to create core/inner-shell/outer-shell nanostructures. The organic moieties in the nanostructures were polymerized by using concentrated sulfuric acid and carbonized at 600 ^{o}C under an inert atmosphere. This outer silica shell prevented the aggregation of carbon during the high temperature treatment. Finally, the nanocomposites were dispersed in sodium hydroxide solution at 90 ^{o}C for 20 h with vigorous stirring to remove the core, inner shell and outer shell of the silica. The carbon nanocapsules were collected by centrifugation and washed with deionized water and ethanol. The core size and shell thickness of the carbon nanocapsules could be easily controlled by varying the reaction parameters. Subsequent PEGylation of the surface of the carbon nanocapsules facilitated their stable dispersion in aqueous solution. The drug-loading and drug-release properties of the PEGylated carbon nanocapsules were also studied.

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Applications of metal-organic frameworks (MOFs) in adsorptive removal of bisphenol-A from water

박은영 정성화*

경북대학교 화학과

Recently, metal-organic frameworks (MOFs) attract much attention due to huge porosity, and easy tunability of their pore size/shape and many potential applications. Bisphenol-A (BPA) has been adsorbed over a MOF, Cr-benzenedicarboxylate (MIL-53) to understand the applicability of MOFs for the adsorptive removal of hazardous endocrine disturbing chemicals from water. MIL-53 shows very fast adsorption in an hour and the maximum adsorption capacity of MIL-53 is higher than that of commercial activated carbon adsorbent. Moreover, unlike the carbon adsorbents, MIL-53 showed very high efficiency over the adsorption especially at very low concentrations of BPA. Therefore, porous MOFs such as MIL-53 can be one the potential class of adsorbents for efficient decontamination of water.

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Effect of acidity and basicity of metal-organic frameworks (MOFs) on adsorption of naproxen and clofibric acid

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Liquid-phase adsorption of PPCPs (pharmaceuticals and personal care products) such as naproxen and clofibric acid was investigated with the virgin and modified MIL-101s (Cr-benzenedicarboxylate) [1] The modification was done by grafting aminomethanesulfonic acid (AMSA) and ethylenediamine (ED) on coordinatively unsaturated sites (CUSs) of the MOF which generates acidic (-SO3H) and basic (-NH2) groups, respectively. Both for the adsorption rate and adsorption capacity, ED-MIL-101 showed the highest removal efficiency. On the contrary, the performance of the acidic AMSA-MIL-101 was very poor. Therefore, the adsorption mechanism may be explained with an acid-base interaction between the PPCPs and the adsorbents. Moreover, the adsorption of naproxen over ED-MIL-101 was shown to be less favorable at both low (6), which may be due to protonation and deprotonation of the adsorbents and adsorbates, respectively. The base-functionalized MOF (ED-MIL-101) can be reused several times by simply washing the spent MOF with ethanol. As a result, commercial implementation of ED-MIL-101 for the removal of PPCPs may be viable because of its high adsorption capacity, facile regeneration and rapid uptake of PPCPs References[1] Z. Hasan, E.-J. Choi, S. H. Jhung, Chem. Eng. J., 2013, http://dx.doi.org/10.1016/j.cej.2013.01.002.

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Preparation and optical properties of three-dimensional macroporous silver inverse photonic crystals

이명진 강태연 채원식*

한국기초과학지원연구원 강릉센터

콜로이드 입자로 제조되는 광결정(photonic crystal) 물질은 구성하는 콜로이드 입자의 크기에 따라서 광밴드갭이 자외선에서 적외선까지 조절되는 특이성을 갖고 있으며, 이러한 광결정 물질들의 빛과의 상호작용은 최근 광기술 분야에서 주목 받고 있다. 본 연구에서는 나노 및 마이크로 크기의 폴리스티렌(polystyrene) 콜로이드 입자를 이용하여, 제어된 환경하에서 용매 증발을 통한 자기조립 (self-assembly) 공정으로 광결정 물질을 제조하였다. 광결정체의 입자간 공극(interstitial pore) 내에 전기화학적으로 은(Ag)을 증착한 후 주형으로 사용된 폴리스티렌 입자를 선택적으로 제거함으로서 거대기공성(macroporous) 플로즈몬 금속 광결정 물질을 얻을 수 있었다. 전기화학적 방법을 통해 제조된 구경이 제어되는 은 역광결정체(inverse photonic crystal)의 광밴드갭은 퓨리에변환 적외선(FT-IR) 분광 현미경을 사용하여 측정하였다. 표면 플라즈몬 공명 주파수는 은 나노구조체의 크기나 형태 등에 의해 달라지는데, 광여기시 은 나노구조체 주변의 전자기장을 증폭하는 표면 플라즈몬 효과에 의한 분자의 형광 증강현상을 시분해 형광 공초점 현미경(time-resolved fluorescence confocal microscope)으로 확인하였다. 이와 같은 연구결과는 광결정체의 광밴드와 플라즈몬 금속의 고유한 공명 주파수를 표면적이 큰 기공성 물질로 제어함으로서 다양한 분야에서 활용할 수 있는 첨단 소재기술을 제공할 것으로 기대된다.

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150 ℃ 저온 용액 공정의 ZnO 산화물 반도체 소자의 전기적 성질 및 안정성에 관한 연구

황재은 김홍두[1]

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ZnO TFTs 는 낮은 온도에서 성막 하여도 좋은 전기적 성질을 나타내고, 공기 중에서도 높은 안정성을 나타내는 장점 때문에 최근 박막 트랜지스터로의 응용에 큰 관심을 끌고 있다. 기존의 ZnO 박막 성장에는 sputtering, MOCVD, PLD 등 진공증착법이 사용되었지만, 최근 낮은 생산 비용과 대량 생산의 장점을 갖고 있는 용액공정을 이용한 연구가 활발히 진행되고 있다. 본 연구에서는 전구체를 이용한 합성을 통해 얻은 물질로 용액공정을 통해 ZnO TFTs 소자를 구성하여 전기적 성질과 안정성을 연구하였다. 150℃ 열처리 공정을 통해서 SiO2 절연체를 이용한 bottom gate 소자인 경우 0.6cm2/Vs, SOG 를 이용한 top gate 소자인 경우 ~3cm2/Vs 의 이동도를 얻었다. 또한, 100℃ 열처리 공정을 통해서도 반도체 특성을 나타내고, 시간에 따른 높은 안정성을 확인 할 수 있었다.

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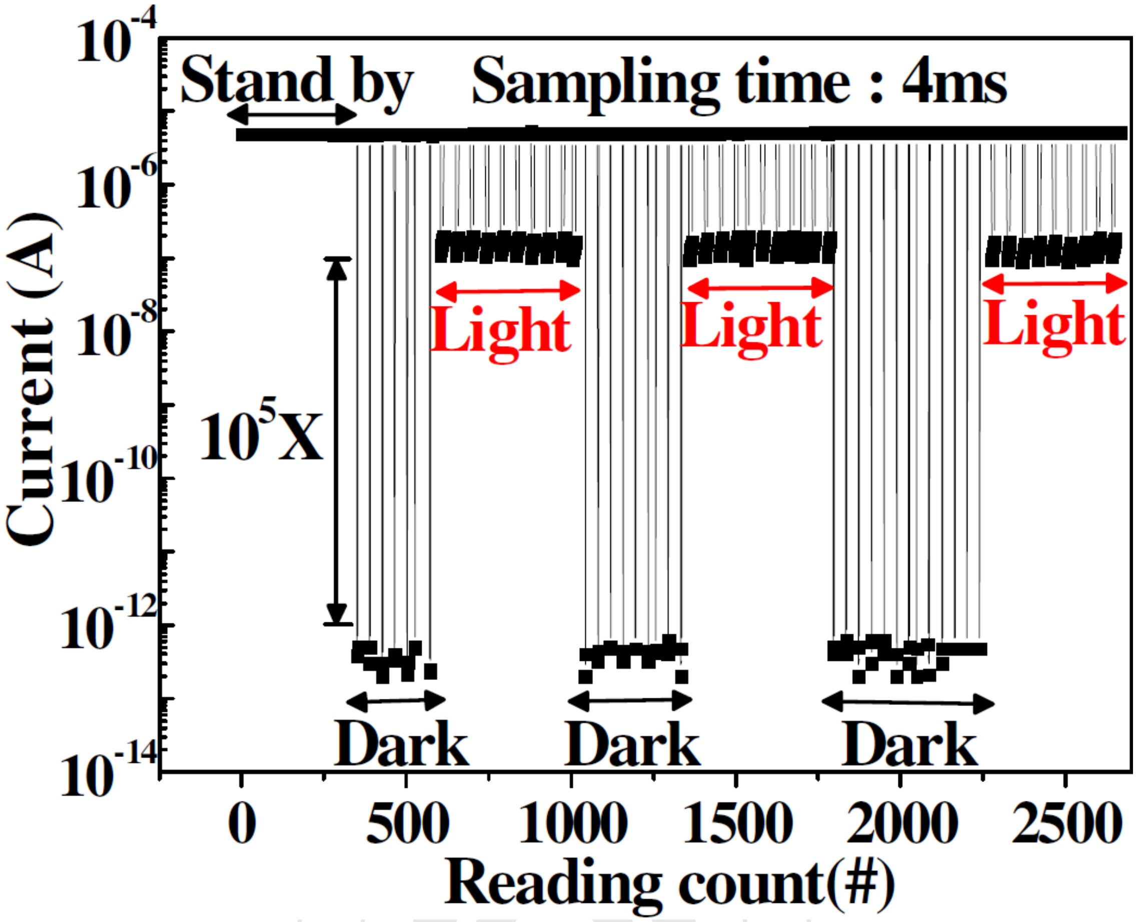
High Performance Transparent Photosensor Array Utilizing Triple Oxide Semiconductor

박서경 박성호* 채원석 한만소

대진대학교 화학과

We proposed a novel photo sensor architecture utilizing transparent amorphous oxide TFT as both switching and sensor elements. The optimized triple layered TFT reveals negligible Vth, and photo current distributions with various device dimensions and aging time, which provides the solution to a workable transparent oxide sensor in terms of manufacturability and scalability. In addition, the operation principle of an oxide sensor TFT proposed in this poster allows for us to realize high performance (>150Hz) sensor array.


Stand by
Sampling time : 4ms
Light
Light
Light
10^5X
Dark
Dark
Dark
Current (A)
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
0
500
1000
1500
2000
2500
Reading count(#)

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A Role of Graphene as an Agent for Directing and Stabilizing Layered Structure in Nanohybrids of Graphene and Layered Titanate

김인영 박수혜[1] 황성주*

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학나노과학과

Novel layer-by-layer ordered nanohybrids of layered titanate-reduced graphene oxide (RGO) are synthesized in the form of powdery composite and freestanding film. The powdery nanocomposite of layered titanate-RGO is synthesized via a reassembling between TiO_2 nanoparticles and RGO nanosheets, which is followed by a phase transformation of anatase TiO_2 to lepidocrocite-structured layered titanate. The hybridization between layered titanate nanosheets and RGO is effective not only in promoting the phase transition of anatase TiO_2, but also in improving the thermal stability of the layered titanate, indicating the role of RGO nanosheets as an agent for directing and stabilizing layered structure. The nanocomposite of layered titanate-RGO does not show any reflectance edge in diffuse reflectance UV-vis spectra, strongly suggesting a modification of electronic structure of titanate component upon hybridization with RGO. The strong electronic coupling between two components is evidenced by the visible-light-induced generation of photocurrents after the hybridization with RGO. Another form of layered titanate-RGO freestanding film is fabricated by a vacuum-assisted filtration of the mixed colloidal suspension of layered titanate and RGO nanosheets. The maintenance of layered crystal structure of the freestanding film is interpreted as a result of the stabilization of layered titanate component with RGO under the heat treatment. The incorporation of RGO nanosheets into the layered titanate freestanding film gives rise not only to the enhancement of surface roughness but also to the increase of hydrophilicity. The present finding clearly demonstrates the merits of hybridization with RGO to tailor unusual physicochemical properties of layered metal oxide.

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Development of Acid-Base Detection Sensors using Inkjet-Printed Crystal Violets

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한양대학교 화학공학과 [1]한양대학교 응용화공생명공학부

Crystal violet 은 triphenylmethane dye 의 일종으로 보라색을 띠며 산과 염기에 반응하는 성질을 가지고 있다. 산과 반응하여 기존의 보라색이 청색을 거쳐서 노란색으로 색 변화가 일어나며, 염기와 반응하여 색이 흐려지는 블리칭현상이 일어난다. 이러한 특성을 이용하여 crystal violet 용액을 종이 위에 잉크젯 프린트함으로써 산-염기 증기에 반응하는 센서를 개발하였다. 산의 종류와 농도를 조절함으로써 증기에 노출되어 노란색으로 변하는 반응과 증기가 증발하면서 보라색으로 되돌아가는 역반응의 색 변화 및 반응시간을 각각 실험하였고, 산과 염기에 반복적으로 노출시킴으로써 약 7 회까지 뚜렷한 색 변화와 가역성을 보이는 것을 확인 하였다. 센서 이미지의 CMYK 값과 Uv-vis 스펙트럼 분석을 통하여 색 변화에 대한 수치적 결과를 얻었다. 개발된 센서는 종이를 기질로 사용하고 특별한 장비의 개조가 필요하지 않아 생활 속에서 매우 편리하게 센서와 패턴을 제작할 수 있다는 장점을 가진다.

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Fabrication of Metal-Metal Oxide Composite via Electrostatic Interaction between Layered Metal Oxide Nanosheets and Noble Metal Ions

박수혜 황성주*

이화여자대학교 화학·나노과학과

As precursors, titanoniobate (Ti_5NbO_{14}) nanosheets are prepared by soft-chemical exfoliation process of the pristine potassium titanoniobate. Titanoniobate has a low photocatalytic activity due to the slow electron-hole transport rate. To overcome this limitation, titanoniobate nanosheets are composed with noble metal ions such as Ag^+ by electrostatic interaction. The successful hybridization of Ag^+ ion and titanoniobate nanosheets is identified by powder X-ray diffraction (XRD). Also, field emission-scanning electron microscopy (FE-SEM) image shows porous house-of-card morphology of the hybrid. Elemental mapping analysis (EDS) confirms homogeneous distribution of the composite between Ag^+ ions and titanoniobate nanosheets. The diffuse reflectance spectra (DRS) demonstrate that Ag-Ti_5NbO_{14} can absorb visible light ($\lambda > 420$ nm). The Ag-loaded titanoniobate nanosheets show higher organic pollutants decomposition rate than the unloaded sample. Also, we expect oxygen production reaction from water using Ag-Ti_5NbO_{14}.

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A Novel Biomolecule-assisted Method for the Preparation of Coaxial MoS2/Carbon Nanotube Composites with High Performance for Lithium Ion Batteries

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서울대학교 융합과학기술대학원 나노융합학과 [1]서울대학교 화학부

We developed a novel process to synthesize coaxial MoS2/carbon nanotubes by a biomolecule-assisted hydrothermal route, in which L-cysteine, an ordinary amino acid, plays an important role in controlling the morphology of the composites and serves as the binder to help the nucleation and growth of MoS2 on the surface of the carbon nanotubes. Through TGA data, it is found that the polypeptide formed by L-cysteine can be transformed into amorphous carbon through high temperature heat treatment. Furthermore, L-cysteine can make unique structured nanocomposites owing to its multifunctional groups. The composites exhibit high capacity and stable cycling performance when used as an anode material for lithium ion batteries. The specific capacity of a composite with 1:4 molar ratio of MoS2 to carbon nanotubes is almost 830 mAh g?1 after 30 cycles at a current density of 100 mA g?1. Even at a very high current density of 1600 mA g?1, the composites show a stable capacity of almost 530 mAh g?1 after 30 cycles. The improvement in the electrochemical performance of the composite can be attributed to their coaxial structure and the synergistic effects of carbon and MoS2.

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구리-아민 착화합물의 MOF구조를 통한 인쇄전자용 구리전극 패턴화 연구

<u>황재은</u> 김신희 김홍두[1]

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공기 중에서 안정하며 낮은 온도에서 구리로 변환되는 구리-아민 착화합물은 환원시 구리염에 비해 낮은 온도인 150 ℃에서 구리로 분해되며, 14.4 wt% 정도의 구리함량을 갖는다. 이 착화합물은 구리고체의 비저항값(1.68 μΩ·cm)에 가까운 1.84 μΩ·cm 을 나타내지만 열처리 시, 온도 상승으로 인해 점도가 급격히 떨어져 패턴 고정이 곤란하며, 접착성이 떨어지는 단점이 있다. 이를 개선하기 위한 방법으로 첨가제를 사용한 연구와 MOF 구조를 이용해 점도를 높이기 위한 연구를 하였다. 개선된 착화합물의 구리 잉크는 27.4 ~ 18.5 μΩ·cm 정도의 비저항값을 나타나며, 패턴 고정과 접착성이 향상되었으므로 인쇄전자용 전극으로 사용 될 가능성을 보여주었다

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Facile One-pot Synthesis of Mesoporous Carbon Nanospheres from Glucose and its Application for Electrochemical Capacitor

JINXING 김지만[1,*]

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Porous carbon materials have attracted considerable attention in recent years due to their applications in many areas, such as gas separation, adsorption of small gas molecules, catalysis, energy storage and capacitors, because of high specific surface areas, large pore volume, low density, thermal conductivity, good chemical, mechanical stability and satisfied conductivity caused by the nanostructure. Porous carbons with various shapes such as plates , rods , spheres, rattle-type tube, hollow mesoporous spheres and flower-like sphere, have been synthesized. Among them, submicrometer-size carbon spheres with satisfactorily narrow size distributions have the potential to be used as building blocks to fabricate photonic band gap crystals or other nanodevices. As a continuation of our previous studies, here, we have synthesized Mesoporous carbon naospheres (MCNS) using readily available low cost sources and water as solvent. The reaction ration of each component was optimized and the MCNS were characterized by TEM, SEM, XRD, Microtrac-Nanotrac and N_2 sorption isothermal etc. And the sample test of electrocatalytic performance.

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Layered yttrium hydroxynitrate as an adsorbent of tungstate ion

이기룡 변송호*

경희대학교 화학과

Water pollution due to heavy metals is caused by several sources such as metal plating, mining, and painting, and also by agricultural sources such as fertilizers and fungicidal sprays. The toxic heavy metals, when present in the water more than the permitted limit, become injurious to the health. With regard to heavy metal pollution, there have been growing interests in the development of new materials to remove toxic metal ions even in low concentration from the contaminated water. The layered yttrium hydroxide matrix containing Tb^{3+} was applied to detect (trace) amount of tungstate ions in the present work. Rare earth complexes present sharp and intense emission lines upon ultraviolet light irradiation due to the rare earth-centered luminescence generated from the effective intramolecular energy transfer, so called ‘antenna effect’, from the coordinated ligands to the central rare earth ion. Small amount of tungstate ions adsorbed on the layered yttrium hydroxide induced a strong green luminescence by harvesting and transferring the energy to the layered yttrium hydroxide layer. The efficient energy transfer from the oxygen-to-tungsten charge transfer band to Tb^{3+} would provide an effective way to detect and remove (trace) amount of tungstate ions from water.

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Metavanadate-induced photoluminescence of layered gadolinium hydroxide

박이슬 정희진 변송호*

경희대학교 화학과

Stable luminescent colloidal solutions were prepared by simply mixing Eu^{3+}-doped layered gadolinium hydroxychloride (LGdH:Eu) and its oleate exchanged form (LGdH:Eu-Ole) with meta-vanadate (VO_3^-) ions in water and chloroform, respectively. In water, the reaction between LGdH:Eu and VO_3^- led to rapid formation of $GdVO_4$:Eu with spindle-like morphology. Interestingly, approximately 100 nm sized $GdVO_4$:Eu particles were well dispersed to form a stable translucent colloidal solution without any stabilizing agent, probably due to remnant hydroxyl groups on the surface of nanoparticles that facilitate the hydrogen bonding with water molecules. The LGdH:Eu-Ole was readily exfoliated in chloroform to form a transparent colloidal solution. When we added aqueous $NaVO_3$- solution to the colloidal solution, small amount of VO_3^- ions were adsorbed on the surface of exfoliated LGdH:Eu-Ole nanosheets. Both colloidal solutions exhibited efficient energy transfer from the ligand-to-metal charge transfer (LMCT) band of meta-vanadate to Eu^{3+} ions as well as highly enhanced f ? f transitions, resulting in the bright red emission under the commercial 254 nm UV irradiation. These luminescent colloids of $GdVO_4$:Eu and metavanadate-adsorbed LGdH:Eu-Ole showed potential utility as a new class of multimodal probe for biomedical applications.

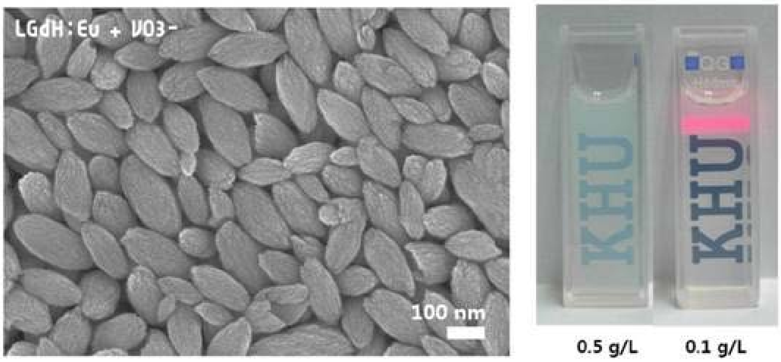

Figure 1. FE-SEM image and photograph of aqueous colloidal solution of $GdVO_4$:Eu.

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Synthesis and structural property of layered gadolinium hydroxide

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Layered gadolinium hydroxide (LGdH-OH), which is polymorph of hexagonal gadolinium hydroxide (h-Gd(OH)$_3$), was synthesized by exchanging Cl^- anions with OH^- anions in the gallery of layered gadolinium hydroxychloride (LGdH-Cl) precursor at room temperature. While LGdH-OH and h-Gd(OH)$_3$ have the same chemical formula expressed as $Gd(OH)_3$ except H_2O content, the structure of LGdH-OH composed of positively charged layers and charge-compensating interlayer anions is quite different from that of h-Gd(OH)$_3$ but similar to the LGdH-Cl host. The structural difference between the layered and the hexagonal polymorphs was compared through X-ray diffraction (XRD), selected area electron diffraction (SAED), infrared (IR) spectroscopy, and thermogravimetric analysis (TGA). The structure of LGdH-OH began to collapse by liberation at 100°C and totally transformed to h-Gd(OH)$_3$ over 300°C. The slurry of LGdH-OH is readily dispersed in water, and the colloidal suspension is stable for one month at ambient condition. Stable aqueous colloidal solutions containing LGdH-OH nanosheets can be easily synthesized in reproducible large-scale at room temperature.

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A New Electron Transporting Material for Effective Hole- Blocking and Improved Charge Balance in Highly Efficient Phosphorescent Organic Light Emitting Diodes

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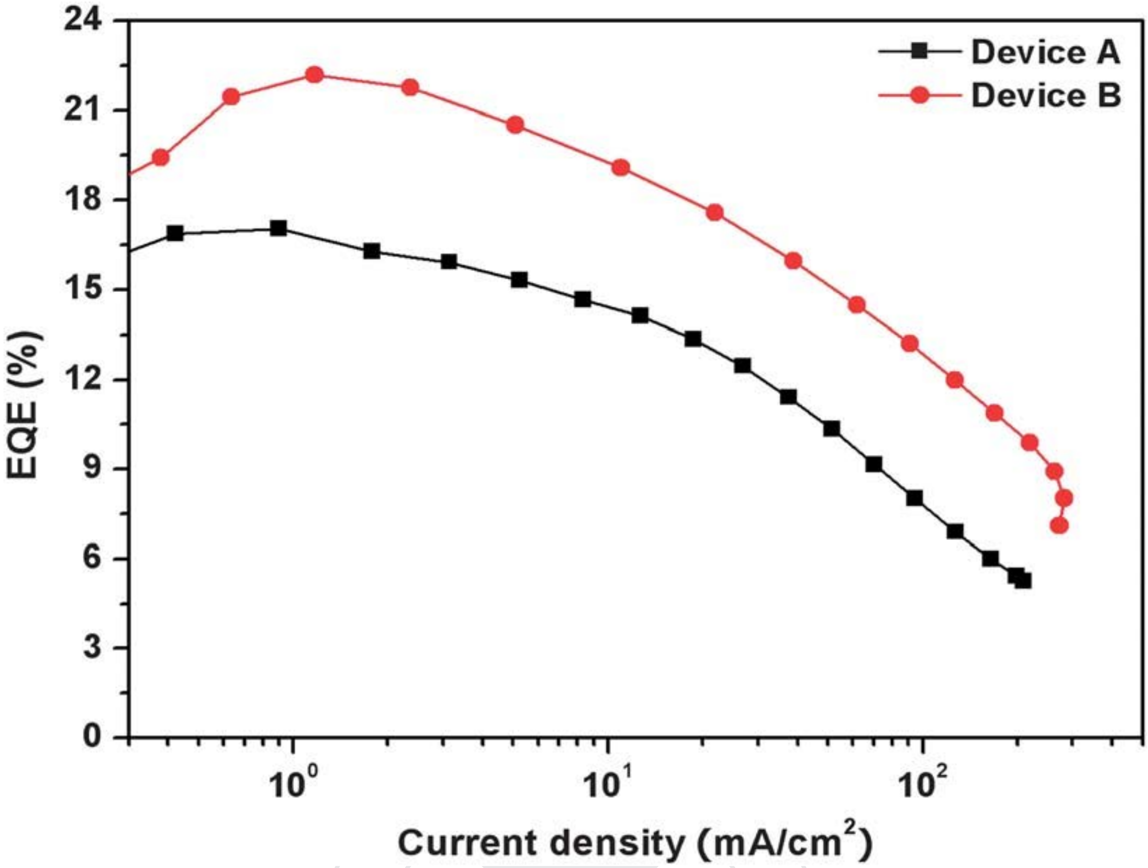
A highly efficient new benzoimidazole phosphine oxide based electron transporting material, bis(1-phenyl-1H-benzo[d]imidazole)phenylphosphine oxide (BIPO), was designed, synthesized by condensation,nucleophilic substitution and oxidation reactions, and confirmed using various spectroscopic studies. It shows a thermal stability (5% weight loss) of 451 ℃ with a glass transition temperature of 129 ℃ from the thermogravimetric analysis and differential scanning calorimetry studies. BIPO used as an efficient electron transport layer (ETL) in a green emitting phosphorescent organic light emitting diode, ITO/4,4'- bis[N-(1-naphthyl)-N-phenyl-amino]biphenyl (30 nm)/4,4',4"-tris(carbazole-9-yl triphenylamine 10 nm)/(4,4'-N,N'-dicarbazole)biphenyl (CBP) host doped with $Ir(ppy)_3$ dopant (5%) (30 nm)/ETL (40 nm)/LiF(1 nm)/Al (100 nm), serves as an effective hole-blocking material and improves the charge balance in the device, resulting in higher device efficiencies of 22.19%, 68.3 cd/A and 24.4 lm/W with a maximum luminance of 72 080 cd/m^2 compared to those (17.03%, 52.0 cd/A and 20.9 lm/W with a maximum luminance of 33 490 cd/m^2) of a device using a widely used ETL,1,3,5-tris(m-pyrid-3-ylphenyl)benzene. These results show that the new BIPO ETL could be very useful in efficient organic light emitting diodes.


24
21
18
15
12
9
6
3
0
EQE (%)
10^0
10^1
10^2
Current density (mA/cm^2)
Device A
Device B

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New n-channel Conjugated Polymer for Organic Thin Film Transistors

김란 황재영[1] 권순기[2] 김윤희*

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Organic thin film transistors have currently been the subject of intensive research activity due to their promising attributes for the manufacturing of low-cost, large-area and flexible electronic devices. In particular, acenes and heteroacenes are efficient hole-transporting (p-type) semiconductors, whereas rylene diimides, especially perylene and naphthalene derivatives, are so far the most successful air-stable electron-transporting (n-type) materials. In this study, we have synthesized new polymer for organic thin film transistors(OTFTs). The ability to extend the π system of polymers not only leads to broadened light absorption spectrum but also increases the electron affinities to facilitate electron injection and transport. After annealing, polymer films exhibit excellent OTFT characteristics under ambient stability.

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Metal oxide structures for high performance lithium ion battery electrode materials

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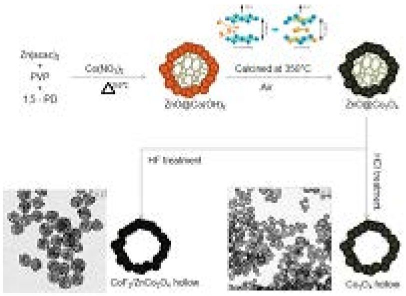
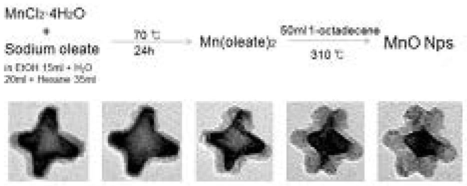
한국과학기술원(KAIST) 화학과

Researchers have studied about various lithium ion battery anode materials such as carbon, metal oxides, alloys, metal sulfides to improve their recyclability and charge density. It is well known that especially metal oxides nanostructures which have many active sites commonly used as a lithium ion battery anode material. For example, cobalt oxides have maximum charge density about 900 mA/g theoretically because eight Lithium ions can be substituted one cobalt atom. Maximum charge density of commercial carbon anode material is only 372 mA/g. Therefore the cobalt oxides can replace carbon as lithium ion battery anode material on a long time basis. In this study, we synthesized various types of cobalt oxides, manganese oxides, and iron oxides nanostructures for lithium ion battery electrode material. Their recyclability and charge density were measured through half-cell tests. In addition to this, the metal oxide nanostructures were coated with carbon to enhance their physical and chemical stability and electrical conductivity.



<Cobalt oxides synthetic scheme>



<Manganese oxides synthetic scheme>

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2D-to-3D conversion of layered perovskite $Sr_2Ta_2O_7$ into Li-intercalated defect perovskites

김정미 김영일*

영남대학교 화학과

Ammonolytic reaction between layered perovskite $Sr_2Ta_2O_7$ and Li_2CO_3, where [Li]:[Sr] = 0~0.67, resulted in the perovskites with substantial amounts of vacancy defects both on the cation and anion sites. Above process can be described as Li+ insertion into the layered lattice of $Sr_2Ta_2O_7$ with an aid of charge-balancing O^{2-}/N^{3-} exchange. A control experiment conducted in air, using $Sr_2Ta_2O_7 + 0.25Li_2CO_3$, lead to only a partial decomposition of $Sr_2Ta_2O_7$. Inductively coupled plasma spectroscopy and combustion analysis indicated that the Li evaporation was minimal during the ammonolytic heating, and that the anion vacancy increased by raising the mixing ratio of Li_2CO_3 to $Sr_2Ta_2O_7$. Investigations by X-ray powder diffraction and solid state Li-7 nuclear magnetic resonance spectroscopy show that Li populated the octahedral site without any Li/Ta ordering.

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Microenvironments and different nanoparticle dynamics in living cells revealed by a standard nanoparticle

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(주)바이테리얼즈 부설연구소 [1]RIKEN, ASI Japan

For quantitative analysis of nanoparticle diffusions and submicro-environments in living cells, use of newlysynthesized silica-based fluorescent nanoparticle (Si-FNP) as a standard nanoprobe is successfullydemonstrated. The appropriate characteristics of a standard probe were fully analyzed in vitro by singlemolecule detection, transmission electron microscopy, and dynamic light scattering. Using fluorescencecorrelation analysis in single living cells, we quantitatively compared the diffusional properties of thestandard Si-FNP with a diameter of 50 nm, peptide coated Si-FNP, streptavidin coated Qdot, and GFPmolecule which have different sizes and surface properties. The result demonstrates that the standard Si-FNPwithout coat is minimally trapped in the vesicles in the process of cellular endocytosis. Interestingly, a largeproportion of Si-FNP introduced into the cells by electroporation diffuses freely in the cells during a cell cyclesuggesting free diffusing NPs are hardly trapped in the vesicles. The simple but highly sensitive method willprovide insight into strategies to understanding the hydrodynamic process of nanoparticle delivery intoliving cells as well as the cellular microenvironment in the view of submicro-size.

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Cytotoxicity and gene expression of sarcoma 180 cells in response to the surface morphology of Fe3O4@Au nanoparticles

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The biological interaction of nanomaterials to tumor cells is of fundamental importance to develop new strategies for the design of efficient nanoscale therapeutic complexes on cancer therapy. Among nanomaterials, non-spherical core-shell nanoparticle (NP) becomes attractive research theme due to its unique shape ? dependent physical properties and fascinating multi-functionality. In this paper, two different shaped Au-coated iron oxide core-shell NPs (spherical and spiky Fe3O4@Au NPs) were designed. Then it was investigated the shape effects of these particles on cytotoxicity and global gene expression in sarcoma 180 cells. The investigated cells after treatment for 7 days showed > 90% viability at the spiky NP of concentrations up to 50 µg/mL, indicating that the spiky NPs were not toxic. Meanwhile, the cells exposed to spherical NP showed 50% decrease in their relative cell viabilities. To understand the cytotoxicity differences, total 33,315 genes expressions were monitored in the NP-treated cell by microarray analysis where 171 genes were up-regulated and 181 genes were down-regulated in the spiky NP-treated cell, based on the arbitrary difference of gene expression in the 2-fold change. The major genes in the up- and down-regulated categories included Il1b, Spp1, Il18, Rbp4, and Il11ra1 that are mainly related with cell proliferation, differentiation, and apoptosis. Therefore, these results suggested that an alteration on NP shape could induce the different regulation of cytotoxicity and gene expression in tumor cells.

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Controlled Synthesis of Mesoporous Calcium Silicates with Ultrahigh Drug/Protein Loading Capacity and Their pH-Triggered Release Behaviors

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한국기초과학지원연구원 전주센터 [1]한밭대학교 응용화학과

We have developed a facile method for the synthesis of mesoporous calcium silicates (CS) using a poly (allylamine hydrochloride; PAH), assisted CS-PAH with a large specific surface area (SBET = 348.4 m2g-1) and pore volume (Vp=1.42 cm-3g-1). TEOS was employed as silicon source, which rapidly hydrolyzes and reacts with amine groups of PAH and Ca2+ to form nanosheets as building blocks in basic media. The excess of Ca2+ enriches the surfaces and results in well-defined 3D network structures of CS-PAH. Ibuprofen (IBU) and FITC labeled bovine serum albumin (FITC-BSA) were chosen as a model drug and protein respectively for testing loading and delivery proficiency of CS-PAH. Ultrahigh DLC (drug loading capacity) and the linear relationship between cumulative amounts of their released have been found under controlled pH conditions. Excitingly, the highest DLC reported so far (3.1 mg IBU is loaded in per mg carrier) has been achieved in this work. Furthermore, CS-PAH can entirely transform to hydroxyapatite after the drug release in simulated body fluid (SBF), implying the good bioactivity and biodegradability of CS-PAH. Thus, the CS-PAH drug-delivery system combines the advantages of large specific surface area, large pore volume, extremely high DLC, adjustable drug-release rate, and good bioactivity. Therefore, is promising for reducing systemic side effects.

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Highly Dispersed Water Adsorbents, $CaCl_2$, in Porous Silica Materials for Adsorption Cooling System

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한국생산기술연구원 [1]연세대학교 화공생명공학과

A water adsorbent, $CaCl_2$ was highly dispersed in porous silica materials by freeze drying to apply for adsorption cooling system. Silica gels (SS-SIL 52 and SS-SIL 230), a precipitated silica (Zeosil-142) and a fumed silica (Aerosil 200) were used as porous supports. The composites “salt in porous materials” (CSPM) exhibit higher dispersion of the salt in the silica media when these were freeze-dried (-40 °C) than dried at relatively high temperature (60 °C). Moreover, the size of the salt in the freeze-dried CSPM is smaller than that of the CSPM dired at high temperature. The small size and the high dispersion of the salt particles make the CSPM to improve the water sorption properties (sorption capacity and stability).

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For conductivity enhancement of Poly(3,4-Ethylene dioxyThiophene):Poly(StyreneSulfonate) (PEDOT:PSS) with organic solvent treatment

황기환 서현진 부진효*

성균관대학교 화학과

The poor conductivity of poly(3,4-ethylene dioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) film hinders to use for a flexible electrode in solar cells. In this report we demonstrate that the conductivity of PEDOT:PSS film can be enhanced by modifying structures in a mixture of PEDOT:PSS aqueous solution and various organic solvents such as polar protic (2-propanol, methanol, ethanol, formic acid) and aprotic solvents (acetone and acetonitrile). To comparatively study the structural effects on the resulted electrical properties, the films are spin-coated on glasses and ITO. At the same time, a contact angle goniometer is used for clarifying a mechanism of wettability of PEDOT (hydrophobic) and PSS (hydrophilic) on the observed conductivity. The structures and electrical properties are investigated by FE-SEM (Field Emission Scanning Electron Microscopy), AFM (Atomic Force Microscopy), and 4-point probe, respectively.

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Low Temperature Sol-gel synthesis and Structural Characterisationof P_2O_5-CaO-Na_2O glasses

이인호 Jonathan C. Knowles[1,*] 공명선[*]

단국대학교 나노바이오의과학과 [1]Division of Biomaterials and Tissue Engineering, Eastman Dental Institute, University College London

Ternary phosphate-based glasses in the system P_2O_5-CaO-Na_2O have been successfully synthesized using a new low-temperature sol-gel method. The glasses have a fixed P_2O_5 content of 45 or 50 mol% and the CaO:Na_2O ratio was varied. The synthesized systems which remained fully amorphous have been characterized using X-ray diffraction (XRD) and their thermal properties have been examined by differential thermal analysis (DTA). The structure of the phosphate network has been studied as a function of composition using Fourier transform infrared (FTIR) spectroscopy and ^{31}P nuclear magnetic resonance (NMR). The XRD results reveal that none of the glasses contain any crystalline phases, while the DTA results reveal increases in the glass transition, crystallization and melting temperatures with a decrease in the Na_2O content. The FTIR and ^{31}P NMR results show that dried gel has a structure dominated by Q^0, Q^1 and relatively small amounts of Q^2 groups, whereas that of the stabilized sol-gel derived glass is composed of mainly $Q^1$and Q^2 species. These results provide several interesting insights into phosphate sol-gel chemistry and indicate their suitability for further study with a view to developing biomedical applications of these glasses in the future.

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Porously Stacked Nanocomposites of Ruthenium-Substituted Manganese Oxide Nanosheets Applicable for Supercapacitor Electrode

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

The exfoliated 2D nanosheets of Ru-substituted manganese oxides and their lithiated nanocomposites are synthesized by the soft-chemical exfoliation reaction of Ru-substituted Manganese dioxide ($K_{0.45}Mn_{1-x}Ru_xO_2$) material and the following flocculation with Li^+ cations for restacking of these nanosheets, respectively. Powder X-ray diffraction analysis clearly demonstrates the successful substitution of Ru ions for the layered structure of $K_{0.45}MnO_2$ and the intercalation of Li^+ ions into layered $Mn_{1-x}Ru_xO_2$ by self-assembly process. According to X-ray absorption spectroscopic analysis, tetravalent Ru^{4+} ions are stabilized in the octahedral sites of layered $Mn_{1-x}Ru_xO_2$ structure. According to electron microscopic analysis, the lithiated $Li\text{-}Mn_{1-x}Ru_xO_2$ nanocomposites are composed of the porous assembly of layered $Mn_{1-x}Ru_xO_2$ nanosheets with Li^+ cations. The lithiated $Li\text{-}Mn_{1-x}Ru_xO_2$ nanocomposites show mesoporous structure with remarkably expanded surface area. The promising capacitance performance is obtained for the $Li\text{-}Mn_{1-x}Ru_xO_2$ nanocomposites with large specific capacitance and excellent cyclability, which are much superior to those of unsubstituted $Li\text{-}MnO_2$ nanocomposite. The present finding provides strong evidence for the usefulness of Ru substitution and exfoliation-self-assembly in enhancing the electrode performance of layered MnO_2 material.

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Application of core-shell $ZnFe_2O_4$ particles as magnetically recyclable catalysts

강경태 정진승

강릉원주대학교 화학과

Photofunctional magnetic $ZnFe_2O_4$, $ZnFe_2O_4@SiO_2@TiO_2$, $ZnFe_2O_4@mTiO_2$ particles were successfully fabricated via a simple surface modification process.The phase structures, morphologies, particle sizes, and chemical compositions of these particles have been characterized by field emission scanning electron microscope (FESEM), transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDX). Photocatalytic experiment of the $ZnFe_2O_4$, $ZnFe_2O_4@SiO_2@TiO_2$, $ZnFe_2O_4@mTiO_2$ particles was carried out in 2,4,6-TCP solutions illuminated under Xe light in a photochemical reactor.

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A Facile Fabrication of Biocompatible $CoFe_2O_4$Particles

강경태 이명진[1] 정진승

강릉원주대학교 화학과 [1]한국기초과학지원연구원 강릉센터

During the past few decades, spinel ferrite materials have been widely investigated for their excellent magnetic and electrical properties as well as for their numerous applications in different technological fields and in biomedicine.Among the various spinel ferrite materials, $CoFe_2O_4$ has attracted remarkable research interest because of its excellent chemical stability, good mechanical hardness, high coercivity, moderate saturation magnetization, a positive anisotropy, constant, large magneto-strictive coefficient, wear resistance, and electrical insulation. The magnetic properties of $CoFe_2O_4$ particles have been adjusted finely by controlling the size of the primary $CoFe_2O_4$ nanograins and the secondary superstructed composited particles formed by an aggregation of the nanograins.Microstructure and physical properties of the $CoFe_2O_4$ particles are investigated by field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), superconducting quantum interference device (SQUID), X-ray diffraction (XRD).

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Direct Formation of Graphene Nanomesh on Au Nano-Network as a Metal Catalyst

정인섭 조상현 김수진[1] 문정혁[1] 박성호[1,*]

성균관대학교 에너지과학과 [1]성균관대학교 화학과

Graphene, an atomically thin carbon layer that has 2-D hexagonal lattice, is one of promising candidates for electronic devices due to its unique electrical, mechanical, and optical properties. However, it still requires more improvements in terms of on-off ratio and band gap to be used for field-effect transistor (FET). For that reason, graphene nanomesh (GNM) is one form of graphene showing semiconducting behavior due to quantum confinement effect unlike semi-metal like graphene. Here, we present direct formation of graphene nanomesh on insulating substrates (SiO2) by chemical vapor deposition (CVD) technique with the assistance of Au nano-network as metal catalyst. We confirmed that few layers of graphene formed between the substrate and metal, which can be explained by carbon diffusion mechanism recently reported. We investigated the properties of graphene with a variety of characterization tools such as SEM, HR-TEM and Raman, etc and the edge effects by comparing with as-prepared graphene from Au film. Finally, we fabricated simple GNM-based FET devices in order to see the charge transfer characteristics such as on-off current ratio, bandgap and mobility, etc. Further, we confirmed the change of electronic properties depending on pore sizes of GNM which strongly relies upon the pore size of Au nano-network.

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Comparison of Electrocatalytic Activity of Pt Nanoparticle and Graphene Hybrid Composite and Analogous CNT Composite

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성균관대학교 화학과 [1]성균관대학교 에너지과학과

We synthesized Pt nanoparticles (NPs) and graphene hybrid materials using facile method. 30 nm Pt NP solution and graphene solution were prepared by wet-chemical synthesis and reducing agent system respectively. Pt NP solution and graphene solution were mixed, and anodic aluminum oxide (AAO) was used as template to deposit the Pt NPs and graphene (Pt/G) mixed films. This facile synthesis has considerable advantages. Pt/G films can be fabricated with various sizes, morphologies of Pt NP and different ratios of Pt/G. In this experiments, Pt/G films show higher hydrogen desorption area and better durability than pure Pt films. We furthermore synthesized Pt NP and carbon nanotube (Pt/CNT) composites with analogous method. Electrochemical properties and activities of Pt/G and Pt/CNT films were compared by cyclic voltammogram, carbon monoxide oxidation and methanol oxidation. In this experiment, Pt/G films have higher electrochemical activities than Pt/CNT films.

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Melting Infiltration Assisted Synthesis of Ordered Mesoporous Molybdenum Disulfide (MoS_2)

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The layered nanomaterials including transition metal dichalcogenides (TMDs) are expected to have great potential in nano-electronics, sensing and energy harvesting. As the layered TMDs can be made into porous structure with structural flexibility, energy devices such as photovoltaics, and capacitors can be envisaged. Furthermore, the layered structures allow ionic or molecular intercalation, suggesting possible applications in lithium ion batteries (LIBs), hydrogen storage, catalysis and electrochemical double layer capacitors.MoS_2 is a widely used compound with many applications in catalysis and as solid lubricants, mainly due to the weak interlayer interaction of the material. MoS_2 is a TMD with properties that make it a material with promising applications such as solid state LIB cathode, industrial catalysts for hydrodesulfurization of crude oil.Herein, highly ordered mesoporous MoS_2 materials successfully obtained *via* simple melting infiltration assisted impregnation of precursors and heat treatment under H_2 atmosphere by using ordered mesoporous silica materials as hard templates. Synthesized meso-MoS_2 exhibit ordered meso-structures, high specific BET surface area, and well-developed crystalline framework.

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Facile preparation of lotus-root shaped mesoporous TiO_2 materials and their DSSC performances

홍진연 배상은 허성*

한국외국어대학교 화학과

TiO_2 is adopted for a promising candidate of photovoltaics, photocatalysis, hydrogen storage, and other useful photon-related applications. Various synthetic methods for shaped TiO_2 are being investigated to improve its properties and develop new potential applications. In this presentation, lotus-root shaped mesoporous TiO_2 was facilely prepared by using cetyltrimethylammonium hydroxide (CTAOH) template. The thermal treatment of amorphous as-prepared lotus-root shaped TiO_2 was performed at 500 °C and 700 °C. Pure anatase TiO_2 phase was obtained at 500 °C and it has high BET surface area of 93.2 m^2 g^{-1}. At 700 °C, a portion of rutile phase was generated but the surface area decreased to 30.0 m^2 g^{-1}. These crystalline lotus-root shaped mesoporous TiO_2 materials have well-developed bimodal porosity with pore dimensions of 10.6 nm and 28.0 nm, respectively. Photon-to-current conversion efficiencies of lotus-root shaped mesoporous TiO_2 were examined by Gratzel type dye-sensitized solar cells (DSSCs). Efficiency of both DSSCs prepared by mixing Degussa P25 and mesoporous TiO_2 increased about 10% compared with standard electrode using only P25. Incident photon to current efficiencies (IPCE) of the all DSSCs were quite similar each other but impedance analysis indicated that mesoporous TiO_2 mixed cell has lower resistance than P25 cell. Thus, photovoltaic efficiency could be improved due to the decrease of resistance by using lotus-root shaped mesoporous TiO_2 with nanocrystalline P25.

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Preparation and Characterizations of Bimodal Mesoporous Silicas

배상은 허성*

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In order to prepare bimodal mesoporous silicas (BMSs), cetyltrimethylammonium hydroxide (CTAOH) was used instead of rather conventional cetyltrimethylammonium bromide (CTAB) template. Extra base catalysts were not required during the preparation of BMS materials. In addition, varying amounts of nonionic auxiliary templates such as Brij-76, Brij-72, Brij-52, and Brij-30 were added into the reaction mixture. All these mixed template syntheses led to BMS materials with two different length scales of mesopores. The small pore was generated by CTAOH template while large pore was produced by auxiliary template. The bimodal porosity is therefore systematically controlled by changing the chemical structure of auxiliary template. Powder X-ray diffraction (PXRD), transmission electron microscopy (TEM), and N_2 adsorption/desorption analysis were used to investigate the BMS materials. The detailed pore structures were revealed from the Brunauer-Emmett-Teller (BET) isotherms and Barrett-Joyner-Hallenda (BJH) pore size distribution curves. Depending on the type of auxiliary template, BMS materials exhibited very distinct nanostructures.

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Sonochemical synthesis of $CuGaS_2$ nanoparticles in ethylene glycol with amines

박승욱 차준호[1] 차지현* 정덕영*

성균관대학교 화학과 [1]성균관대학교 화학

I-III-VI_2 ternary chalcopyrite semiconductors are materials having potential applications for electro-optical devices and infrared-radiation generation and detection. In particular, $CuGaS_2$ have a large direct energy band gap of 2.46eV. We synthesized $CuGaS_2$ nanoparticles by employing sonochemical process under ambient conditions. We used ethylene glycol, hydrazine, alkyl amines as the solvents. We prepared three types of hexagonal, wurtzite and chalcopyrite $CuGaS_2$ as amine reagents. The $CuGaS_2$ nanoparticles with a chalcopyrite structure were annealed in air to burn out the remaining organic materials which improved crystallinity. The morphologies, compositions of $CuGaS_2$ nanoparticles were investigated by X-ray diffraction, Raman spectroscopy, scanning electron microscopy, X-ray fluorescence spectroscopy, Inductively coupled plasma.

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Copper-Tin-Zinc Metallic precursors by Borohydride Reduction for Cu_2ZnSnS_4

이한경 정덕영

성균관대학교 화학과

Cu_2ZnSnS_4(CZTS) thin films are one of the most viable materials for low-cost, thin film solar cells. In order to reduce the cost of producing CZTS thin films, it is necessary to use a non-vacuum process. We synthesized copper-tin alloy metal precursor by chemical reduction. Copper-tin alloy was synthesized by reduction method using $NaBH_4$ as a reducing agent in glycol at room temperature. Copper-tin-zinc precursors were also fabricated from CZTS nanoparticles which synthesized by sonochemical method. Using zinc metal precursor with solvent, CZTS nanoparticles were obtained. The characteristics of copper-tin-zinc nanoparticles were analyzed with powder X-ray diffraction, scanning electron microscopy, inductively coupled plasma atomic emission spectroscopy.

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Characterization and Synthesis of Cobalt Hydroxide Film by Ammonia Gas Transfer

김보미 정덕영

성균관대학교 화학과

Nanostructured cobalt hydroxide films were prepared using "Ammonia Gas Transfer Method". Petri dishes containing an aqueous solution of 0.1M $CoCl_2$ and one containing a dilute solution of NH_4OH were placed in the same enclosed container. Substrates were fixed to touch with surface of precursor solution. Reactions were carried out under ambient condition and mild stirring. After 18h, cobalt hydroxide films were grown perpendicular to the substrate with thickness of 6μm. As-prepared films were densified by pressing and finally thickness of films were about 1.4μm. The films were characterized using X-ray powder diffraction, scanning electron microscopy, UV-Vis spectroscopy, FT-IR, ICP-AES. Hall measurement showed that this material is a p-type semiconductor. This cobalt hydroxide films can be applied to the solar cells or thin film transistors(TFT).

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Preparation of Cu_2ZnSnS_4 Thin Films by Solution Deposition

차준호 정덕영[1]

성균관대학교 화학 [1]성균관대학교 화학과

The Cu_2ZnSnS_4 (CZTS) thin films were prepared by solution deposition on molybdenum coated soda-lime glass substrate for solar cell devices. The Cu-Zn-Sn alloy was electrochemically co-deposited in ternary metal salt solution, tartaric acid, and tri-sodium citrate at room temperature. Subsequently, a methanolic solution of (Zn-Sn)-thiourea complex was casted by spin coating on electrodeposited uniform thin films which were slightly Zn-poor and Sn-poor compared with the stoichiometric composition. The CZTS thin films were prepared by annealing Cu-Zn-Sn alloy thin films in Ar + H_2S (2%) gas atmosphere at 500℃ for 1h. The structural, morphological, and compositional properties of CZTS thin films has been investigated by using scanning electron microscopy (SEM), X-ray diffraction (XRD), and electron probe micro-analyzer (EPMA) respectively. These properties were discussed in relation to their potential for photovoltaic application.

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Molecular aggregationeperformance relationship in the design of novelcyclohexylethynyl end-capped quaterthiophenes for solution-processed organictransistors

한승훈 권순기[1,*] 김윤희[*]

경상대학교 화학과 [1]경상대학교 나노신소재공학부

The synthesis and characterization of cyclohexylethenyl end-capped quaterthiophenes is reported.Additionally, an investigation of the performance of organic field-effect transistors based on thesequaterthiophenes in view of the relationship between the solid-state (or aggregate) order andthe electronic performance is described. UVevis absorption measurements revealed that the quaterthiophenewith an asymmetrically substituted cyclohexylethynyl end-group induced the formation ofH-type aggregates, whereas the quaterthiophene with a symmetrically substituted cyclohexylethynylend-groups favored the formation of J-type aggregates. Two-dimensional grazing-incidence wide-angleX-ray scattering studies were performed to support the molecular structure-dependent packing offilms of the new quaterthiophenes. Solution-processed quaterthiophenes were tested as the activelayers of p-type organic field-effect transistors with a bottom gate/top contact geometry. The field-effectmobility of devices that incorporated asymmetric quaterthiophene molecules was quite high, exceeding0.02 cm2/V s, due to H-aggregation and good in-plane ordering. In contrast, the field-effect mobility ofdevices that incorporated symmetrical quaterthiophenes, was low, above 5 10 4 cm2/(V s), due to theformation of J-aggregates and poor in-plane ordering. A comparison of the symmetrical and asymmetricalquaterthiophene derivatives revealed that the molecular aggregation-dependent packing,determined by the cyclohexylethynyl end groups, was responsible for influencing the organic field-effecttransistor performance.

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Germanium-Silicon and Germanium-Tin Alloy Nanocrystals for High-Performance Lithium Ion Batteries

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Composition-tuned germanium-silicon ($Ge_{1-x}Si_x$) and germanium-tin ($Ge_{1-x}Sn_x$) alloy nanocrystals were synthesized using a gas-phase laser photolysis of tetramethyl germanium, tetramethyl silicon, and tetramethyl tin. A complete composition tuning of cubic phase $Ge_{1-x}Si_x$ alloy nanocrystals was achieved using the partial pressure of precursors in a closed reactor. Ge and Sn precursors produced cubic phase $Ge_{1-x}Sn_x$ ($x_{1-x}Sn_x$-Sn (x=0.1~0.4) hetero-junction nanocrystals due to their limited miscibility. We investigated the composition-dependent electrochemical properties of these nanocrystals as anode materials of lithium ion battery. $Ge_{1-x}Si_x$ nanocrystals (at x=0~0.3) exhibited excellent cycling performance with capacity as high as 1100 mAh/g (with 10 wt % reduced graphene oxide) at a charge/discharge rate of 160 mA/g (after 50 cycles). Incorporation of Sn (x = 0.05; $Ge_{0.95}Sn_{0.05}$) significantly increased the capacities (1010 mAh/g) and rate capabilities (650 mAh/g at a rate of 8A/g), which promises outstanding electrode materials for the development of high-performance lithium ion batteries.

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Hydrogen and Carbon Monoxide Generation from Laser-Induced Reaction of Nanodiamonds in Water

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Nanodiamonds (ND) were found to generate hydrogen (H2) and carbon monoxide (CO) from water at a remarkable rate under pulsed laser (532 nm) irradiation. The transformation of diamond structure into graphitic layers takes place to form an onion-like carbon structure. The CO generation suggests the oxidation reaction of C layers, $C+H_2O\rightarrow CO+2H^++2e^-$, which produced unique laser-induced reaction; $C+H_2O\rightarrow CO+H_2$. We suggest that the gas generation reaction proceeds with the graphitization. Au, Pt, Pd, Ag, and Cu nanoparticles on the ND enhance both gas evolution rates (~2 times for Au) and graphitization and specifically, Au was found to be most efficient amongst other nanoparticles. The enhancement effect was ascribed to effective charge separation between the metal nanoparticle and ND. The Au-ND hybrid on the reduced graphene oxide produced consistently a greater photocurrent than the ND upon visible light irradiation.

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Synthesis of high yield Silver Nanowires and Their Application

임영록 조용재 명윤 백승혁 박정희*

고려대학교 소재화학과

Silver nanoparticles and nanowires High-yeild size controlled were synthesized by solvothermal method. The diameter of the silver nanoparticles is controlled in the range 50 ~ 100nm and the length of silver nanowires is controlled in the range 1~40μm. The morphology and structure of the products were analyzed by scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HRTEM), and UV-vis Absortion Spectra.

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Controllable Synthesis of One- and Two-Dimensional GaS and GaSe Nanomaterials

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Layer-structured semiconductor materials such as group Ⅲ monochalcogenides have highly anisotropic electrical, optical, and mechanical properties, which result from the strong intralayer covalent bonding and the weak interlayer van der Waals interaction.Hexagonal GaS and GaSe crystallizes in layered structure with double layer of nonmetal atoms, consisting of S(Se)-Ga-Ga-S(Se) sheets, stacking along c axis, is structurally similar to graphite. We controlled synthesis and characterization of layer-structured GaS and GaSe nanosheets via a catalyst-assisted vapor-liquid-solid (VLS) growth mechanism during Gasub>2Ssub>3 or Gasub>2Sesub>3 powder evaporation. And their Cu doping was achieved by solution-phase cation exchange reaction.The morphology, chemical composition, and crystal structure of the as-synthesized GaS and GaSe nanomaterials were investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy (HR-TEM), and X-ray diffraction pattern.

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Phase and Composition Tuned Tin Chalcogenide Nanocrystals Using Laser Photolysis.

임형순 명윤[1] 조용재[1] 김창현[1] 김한성[1] 백승혁[1] 정찬수[1] 박정희[1]

고려대학교 미세소자공학협동/마이크로소자공학 [1]고려대학교 소재화학과

We synthesized polytypic tin sulfide nanocrystals, SnS, Sn2S3, and SnS2, by means of novel gas-phase laser photolysis of tetramethyl tin and hydrogen sulfide. A facile composition tuning through the pressure of gas (addition of dimethyl selenium) yields a series of orthorhombic phase SnX and hexagonal phase SnX2, where X = SxSe1-x. Various polytypic hybrids such as SnS-Sn2S3-SnS2, SnS-SnS2, Sn2S3-SnS2, and SnSe-SnSe2 were synthesized. This resulted in the ability to tune the band gap over a wide range (1.0~2.3 eV). Their photon energy conversion properties were investigated by fabricating photodetector devices using the nanocrystal-reduced graphene oxide nanocomposites. The enhanced photoconversion efficiency was observed from the polytypic hybrid nanostructures. This original synthesis method for tin chalcogenide nanocrystals is expected to help expand applications in high-performance energy conversion systems.

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Development of eco-friendly plasma electrolytic oxidation process for highly functional metals

김성철

(주)아스플로 기술연구소

Plasma electrolytic oxidation (PEO) is a novel technique to fabricate thick and hard ceramic coatings on metals such as Al, Mg, Ti, and their alloys. Since PEO is primarily a oxidation of the substrate, the interfacial adhesion tends to be superior to that of most deposited coatings that involve mechanical interlocking at the coating to substrate interface. The crystalline phases in the PEO coating confer higher hardness than the amorphous oxides grown during conventional anodizing.Composite ceramic coatings were formed on aluminium by plasma electrolyte oxidation (PEO) using aqueous alkaline electrolytes. The effect of the electrolyte contents on the growth mechanism, element distribution and properties of oxide layers were studied. The composition, microstructure and element distribution analyses of the PEO treated layers were carried out by XRD and SEM & EDX. Electrical insulation property was measured by breakdown voltage with AC withstanding voltage tester. The coated samples obtained display uniform light-gray color. Smooth surfaces with relatively low roughness and strong adhesion with the substrates could be achieved through carefully control of the growth factors.

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Thermal properties of Erythritol with carbon materials as graphene

전권영 인영용* 홍다은

(주)그랜드텍 전자재료사업부 재료팀

Thermal properties of heat transportation system (HTS) depend on thermal conductivity of phase change material (PCM), temperature of heat transfer oil, and heat transfer method as direct or indirect. Among those properties, thermal conductivity is most important for increasing speed of heat charging/discharge. In this study, erythritol as a PCM was mixed with carbon materials as graphene to increase thermal conductivity. The results provide useful information for development of heat storage system.

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Oligo-Thiophene Modified Ag NP/Silica Core/Shell Nanoparticles for Efficient Bulk Heterojunction Solar Cells

이우철 임주현 이진규* 홍종인*

서울대학교 화학부

In this poster, silver nanoparticles (NPs) were introduced into the active layer to utilize localized surface plasmon (LSP) and light scattering to realize high-performance OPVs. Herein we present a systematic exploration of the characteristics of photovoltaic devices incorporating a blend of poly(3-hexylthiophene) (P3HT), PCBM, and surface-modified silver/silica core/shell NPs in the active layer. Ag NPs were coated with silica to prevent direct contact between the surface of the Ag NPs and other molecules in the active layer, which would inhibit electron quenching and exciton recombination. Oligothiophenes (OTs) were attached to the hydrophilic surface of Ag NPs coated with silica (Ag@Si), thereby enabling dispersion of the OT/silica-coated Ag NPs (Ag@Si@OT) in organic solvents as well as the inhibition of aggregation of the NPs in the film. Bulk-heterojunction devices having 1 wt% Ag@Si@OT relative to P3HT exhibited an improvement in the PCE value from 2.71% to 3.04%. Even with 50 wt% Ag@Si@OT relative to P3HT, the open-circuit voltage was sustained. This result demonstrated that the oligothiophene surface modified silica shells efficiently inhibit charge trapping by the silver NP core.

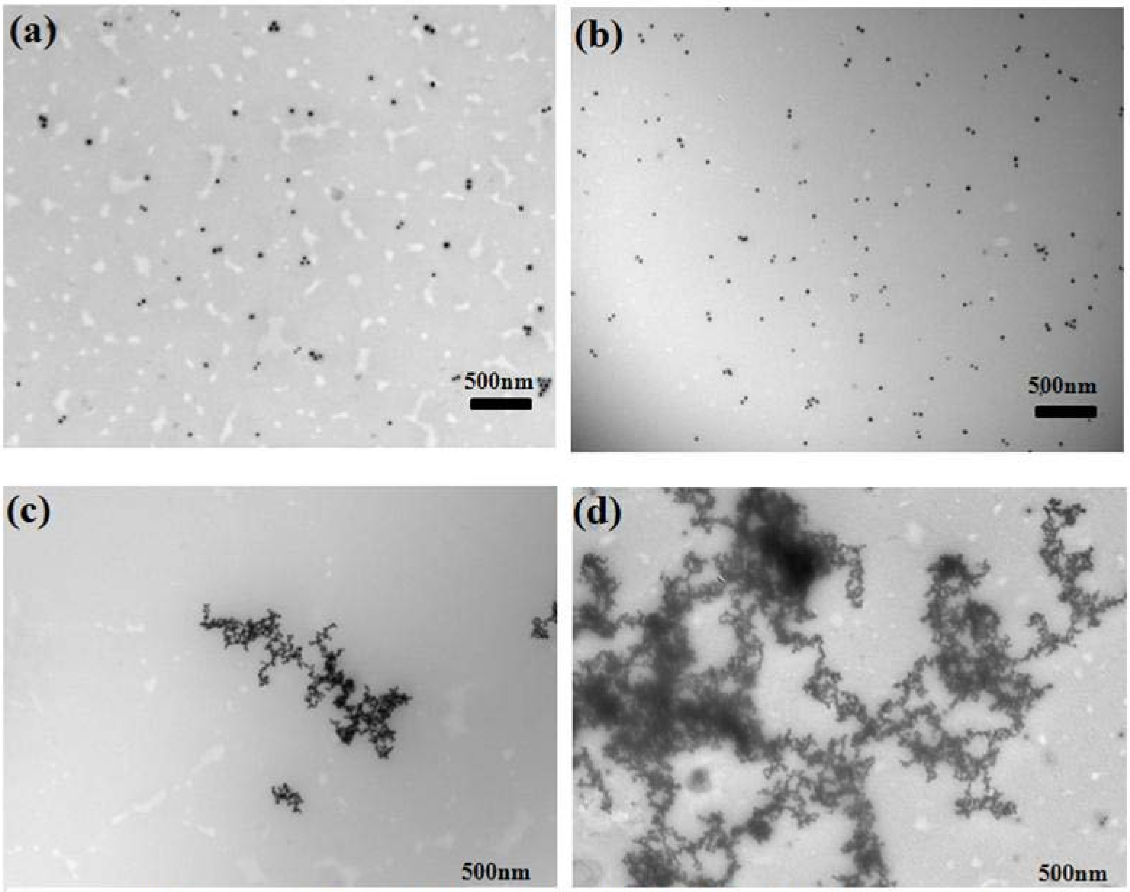

Figure 1. TEM images of blended film with the P3HT:PCBM (1:1) and nanoparticle components (a) 1 wt%, (b) 3wt % Ag@Si@OT NPs and (c) 1wt%, (d) 3wt% Ag NPs (scale bar = 500 nm)

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Producing carbon material by pyrolysis of methane

인영용* 홍다은 전권영

(주)그랜드텍 전자재료사업부 재료팀

Natural gas is a naturally occurring hydrocarbon gas mixture consisting primarily of methane, with other hydrocarbons, carbon dioxide, nitrogen and hydrogen sulfide. That is also important source of industrial producing of carbon and hydrogen. There are many studies about producing carbon from natural gas. Pyrolysis without catalyst is simplest method among them and doesn’t produce CO_2 as a byproduct during process. In this study, characteristics of produced carbon were investigated according to reaction temperature, flow rate of the methane gas, etc.

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Preparation and Characterization of Graphene by Chemical Exfoliation

홍다은 인영용* 전권영

(주)그랜드텍 전자재료사업부 재료팀

그래핀은 sp^2 탄소원자들이 벌집격자를 이룬 형태의 2 차원 나노시트 단일층으로서 뛰어난 전기적, 기계적, 열적 특성으로 인해 획기적인 신소재로 각광받고 있다. 본 연구에서는 그래핀의 대량생산에 가장 적합한 화학적 박리법 중에서 가장 널리 사용되고 있는 hummers method 를 응용하여 그래핀을 제조하여 X-ray diffraction, Scanning electron microscopy, transmission electron microscopy, thermogravimetric analysis, X-ray photoelectron microscopy 등을 통해 그래핀의 특성 및 성질을 확인하였다. 진행된 연구의 결과는 metal oxide/carbon, conductive polymer/carbon 등과 같이 탄소복합소재를 이용한 전극 제조 연구에 유용한 정보를 제공할 것이다.

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Synthesis of Zn_2GeO_4 Nanowires and their characterization

백승혁* 김한성 장동명 정찬수 박정희* 안재평[1]

고려대학교 소재화학과 [1]한국과학기술연구원(KIST) 산업화지원센터

Zn_2GeO_4 nanowires has been achieved by a thermal evaporation of a Ge and Zn mixture. X-ray diffraction (XRD) analysis indicates the product is Zn_2GeO_4 Rhombohedral structure (JCPDS card 80-0580). Scanning electron microscopy (SEM) characterizations show that the structures consist of straight form and zigzag form. We can control both straight and zigzag form. Though Transmission electron microscopy (TEM) analysis, we informed this product arrangement and crystal lattice.

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Thermo-induced Plasmonic Coupling in Gold/Poly(N-isopropylacrylamide) Hybrid Plasmonic Nanostructures for Surface-Enhanced Raman Scattering

이지은 김동하*

이화여자대학교 화학나노과학과

Surface Plasmon resonance (SPR) is an enhanced electromagnetic field induced by the interaction between the light and the surface plasmon in noble metal. The assembly of plasmonic nanostructures can induce near field coupling of surface plasmons between adjacent particles, leading to the generation of hot spots that are useful for enhancing Raman scattering. Noble nanostructures associated with responsive polymeric materials can be exploited to probe dynamic SP coupling behavior induced by swelling-shrinking transitions in polymer chains triggered by a specific environmental stimulus. The volume phase transition in the polymer layer causes changes in the refractive index in the vicinity of the surfaces and induces changes in the characteristic inter particle distance. Here, we designed a unique plasmonic-coupling-based sensing device composed of Au nanoparticles (AuNPs) separated from a Au film through a thermo-responsive polymer layer. Concretely, AuNPs having stimuli-responsive polymer chains tethered to the Au surface were first fabricated through surface initiated atom transfer radical polymerization. By this way, a modulated interaction between the AuNPs and the underlying Au film could be established. The optical and sensory properties of the stimuli-responsive SPR sensing devices were investigated by both in-situ and scan-mode SPR analysis.

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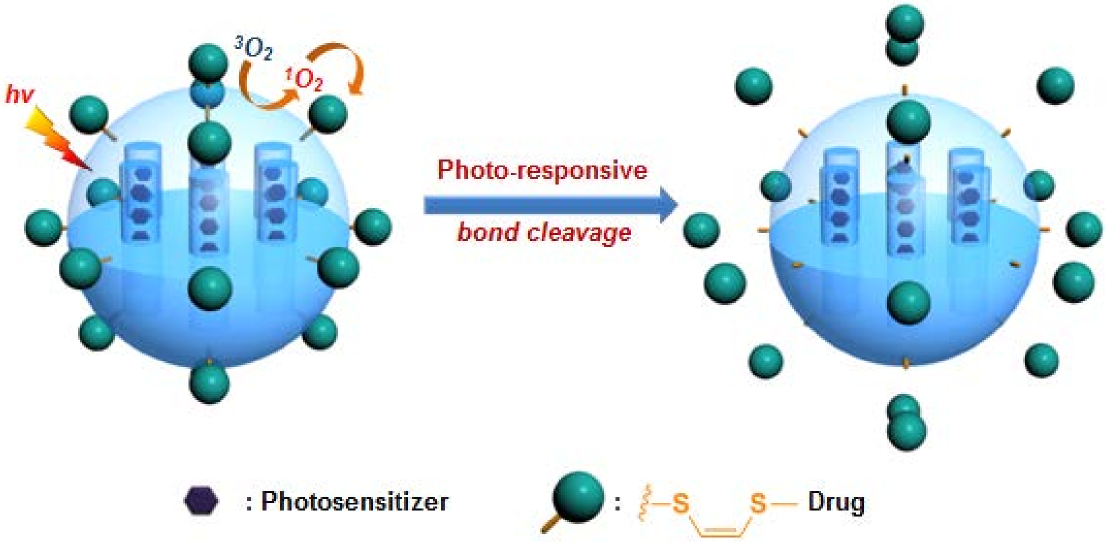
Stimuli-responsive drug releasing mesoporous silica sensitive to long-wavelength light driven by photosensitizer

이준석 김원종*

포항공과대학교 화학과

A mesoporous silica nanoparticle (MSN) based stimuli-responsive drug releasing system was prepared. The system was highly sensitive to long-wavelength light by the cascade reaction driven from photo-activated photosensitizer. The model drug was decorated on the surface of MSN via singlet oxygen sensitive linker (Linker-COOH) where the long-wavelength light sensitive photosensitizer (PS) was loaded in the mesopore structure by utilizing surface-pore biphasic structure of MSN. Singlet oxygen actively generated through the photo-activation of PS by the irradiation of long-wavelength light readily broke the linker to release model drug on the surface. An improved drug releasing profile triggered by the irradiation of long-wavelength light was observed under high responsiveness to light. It can be concluded from result that our novel system has the high potential for further application on biomedical field as a spatially and temporally controlled drug releasing system.


hν
$^3O_2$
$^1O_2$
Photo-responsive
bond cleavage
: Photosensitizer
: S S — Drug

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Temperature and electric-field dependent structure of poly(vinylidene fluoride) (PVDF) from molecular dynamic simulation

김영준 유택희[1]

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

Poly(vinylidene fluoride), PVDF, is known to exhibit good piezoelectric properties. PVDF forms many crystal phases. At room temperature and pressure, α-PVDF is thermodynamically stable and β-PVDF is kinetically stable. Although β-PVDF exhibits good piezoelectric pyroelectric properties, α-PVDF does not. To understand each phase, chain motions and structure change in crystalline and amorphous of PVDF has been studied by using molecular dynamic simulations. The force field parameters used in this simulation were determined in previous work of Karasawa and Goddard 1 which is validated by comparing our quantum mechanical calculation. PVDF polymer of each phase is simulated over a wide range of temperatures, pressures and electric-field. We study relation between rotation degree of molecular chain motions and electric character of PVDF polymer, between electric-field and changing structure of PVDF. This result is useful for understanding electric character of PVDF polymer.Reference:[1] N. Karasawa and W.Goddard, Macromolecules 25, 7268 (1992)

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DNA-templated silver nanoclusters: a sensitive and selective fluorescence probe for potassium ion sensing

이지현 김원종*

포항공과대학교 화학과

Noble metal nanoclusters, a few metal atoms aggregates, have emerged as promising substitutes for quantum dots and organic dyes. Among these metal nanoclusters, Ag nanoclusters (AgNCs) having typical size below 1 nm has been emerged as excellent fluorescence probe for biological/chemical sensing and biolabeling/imaging. Outstanding features of DNA-templated Ag nanoclusters (DNA-AgNCs) as facile synthesis, water soluble, remarkable quantum yield, excellent photostability, high biocompatibility and small size compared to other fluorophores as quantum dot or organic dye, are utilized as optical fluorescence probe for biological/chemical sensor, biolabeling and cell imaging. Also, potassium ion plays an important role in biological systems as maintaining of extracellular osmolarity, regulating concentration of other ions and balancing the pH in living cells. Herein, taking advantages of the high aqueous-solubility and sequence specific spectroscopic feature of DNA-AgNCs, we developed a novel strategy for detecting potassium ion using DNA-AgNCs as fluorescent probes. By modulating intrinsic fluorescence of DNA-AgNCs in response to potassium ion is achieved less than 1 minute.

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컬러기반 전기영동 디스플레이 구동을 위한 유기 칼라 입자의 표면 개질

김주연 서경수[1,*]

ETRI 반사형표시소자연구실 [1]한국전자통신연구원 전자종이연구팀

본 연구에서는, 전기영동 이미지 필름 제작을 위하여, 화이트 입자 기반 칼라 구동을 위한, 칼라 유기 입자의 표면 개질하고자 한다. 표면 개질은 stober 방식을 통하여 실리카로 코팅을하고, sperical 하면서도 균일한 크기를 가지는 입자를 제조하고자 하였다. 이렇게 표면 개질된 칼라 유기 입자의 오일상에서의 분산 안정성을 높이기 위하여 분산 안정제를 첨가하였으며, 이와 함께 칼라 입자의 전하 이동도와 전하량에 영향을 미치는 charge control agent (CCA)양에 따른 특성을 측정 및 최적화하고자 하였다. 확보된 칼라 입자를 화이트 입자와 배합하여 잉크를 제조하고, 제조된 잉크를 필름화하여, 인가되는 전압에 따른 전기 영동 이미지 특성을 확인하였다.

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Synthesis, characterization, and photocatalytic analysis of TiO_2-decorated CNTs

김성필 최현철*

전남대학교 화학과

Recently, photocatalysts have played an important role in the environmental procedures such as air purification, water disinfection and purification. Among them, titanium oxide (TiO_2) has been employed in photocatalyst to decompose many organic and inorganic pollutants under ultraviolet light irradiation. The photocatalytic efficiency of TiO_2 is greatly influenced by crystal structure, particle size, surface area and porosity. One of the methods to improve the photocatalytic efficiency is to increase the surface area of the catalyst. In this study, we prepared TiO2-decorated CNTs using multi-walled carbon nanotubes as a starting material and titanium n-tetrabutoxide as titanium source. The obtained TiO_2-decorated CNTs were characterized by using X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photoactivity of the prepared materials was evaluated by the conversion of methylene blue, methyl orange and rhodamine B in aqueous solution under UV irradiation.

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Effect of sulfur impurities on the catalytic metal of micro-coiled carbon fibers by pyrolysis of acetylene

정순철 강두인 이병윤

(주)창성 연구소

Carbon micro-coils were prepared by the Ni-catalyzed thermal pyrolysis of acetylene containing a small amount of H_2S as impurity, and the preparation condition and morphology of these carbon coils were examined in detail. The coiled carbon grew at the reaction temperature of 760-800℃ and H_2S gas flow rates of 0.15-0.50 sccm. The regularly coiled carbon fibers have generally a 0.1-0.3 micrometer thickness, a 2-8 micrometer coil diameter, and a 0.1-10mm coil length. The coil pitch, coil diameter and coil yield were related to the H_2S gas flow rate and ratio. At the small or high H_2S gas flow, a smaller number of the carbon coils, that have larger coil diameters and larger coil pitch than that obtained at optimum condition of H_2S gas flow.

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Preparation of Charge-Transfer Complex Nanorods via Eutectic Solidification

김주은 서춘희 권태훈 남지혜 강영종[1,*]

한양대학교 화학과 [1]한양대학교 자연과학대학 화학과

Nanomaterials based on charge-transfer (CT) complexes have been widely investigated because of their broad potential applications in various fields of science and technology including sensors, electronics and biology. Among many CT complexes, CT complex formed with tetracyanobenzene (TCNB) and naphthalene is of special interest due to its easy and broad band gap tuning. For example,the band gap of TCNN-naphthalene CT complex can be tuned by doping with small amount of pyrene. Herein, we report preparation and characterizations of TCNB-naphthalene CT complex nanorods by novel eutectic solidification. Unlike other conventional physical vapor deposition or solution methods, eutectic solidification can provide a method for well aligned and patterned nanowires.

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An efficient Heck reaction in water catalyzed by Pd-decorated CNTs

김성필 최현철*

전남대학교 화학과

One of the most important issues in current organic synthesis is the development of new efficient carbon?carbon forming reactions. In this regard, transition metal-based catalysts have generally been used for these reactions. Among them, palladium is an attractive catalyst for the carbon-carbon bond forming reactions. In this study, we prepared Pd-decorated CNTs by modifying thiol groups or amine groups on CNTs surfaces. And the Pd-decorated CNTs as catalyst is used for C-C bond forming reactions (Heck reaction of Ph-I with methyl acrylate in water). Thiol or amine groups were utilized as linkers to secure the Pd nanoparticles without agglomeration. The morphology and structure of Pd-decorated CNTs are also examined by transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS).

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Preparation of $TiO_{2-x}N_y$-coupled Ag-$PbMoO_4$ nanocomposites and their photocatalytic activity under simulated solar light irradiation

<u>김태호</u>

선문대학교 친환경 다기능 나노재료 연구소

The $TiO_{2-x}N_y$-coupled Ag-$PbMoO_4$ nanocomposites have been synthesized by sonochemical synthesis. The as-prepared samples were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), diffuse reflectance UV-vis spectroscopy (UV-vis-DRS), X-ray photoelectron spectroscopy (XPS). The results revealed that the band gap energy absorption edge of $TiO_{2-x}N_y$-coupled Ag-$PbMoO_4$ nanocomposites shifted to longer wavelength as compared to TiO_2, $TiO_{2-x}N_y$, $PbMoO_4$ and Ag-$PbMoO_4$. According to FE-SEM studies, Ag-$PbMoO_4$ gets to be decorated with evenly distributed $TiO_{2-x}N_y$ nanoparticles. The photocatalytic activity of $TiO_{2-x}N_y$-coupled Ag-$PbMoO_4$ nanocomposites for the inactivation of green tide (*Tetraselmis Suecica*) and the degradation of indigo carmine (IC) dyes under simulated solar light was enhanced as compared with $TiO_{2-x}N_y$ and Ag-$PbMoO_4$. The $TiO_{2-x}N_y$-coupled Ag-$PbMoO_4$ nanocomposites may facilitate the charge transfer process more efficiently by inhibiting electron-hole recombination, which enhanced the photocatalytic activity.

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Synthesis and characterization of Pd-Pt bimetallic catalysts supported on thiolated CNTs

이슬기 최현철*

전남대학교 화학과

There have been considerable advances in the development of direct formic acid fuel cells (DFAFCs) which are now considered as promising portable power sources. However, the practical efficiencies, power densities, and energy densities of DFAFC technology are still far below the theoretical limits due to the high electrode overpotentials required for the oxidation of formic acid and reduction of oxygen. Since cathode catalysts for fuel cells are now highly developed, the further development of anode catalysts for formic acid oxidation offers the best prospects for improving DFAFC performance. In this study, carbon nanotubes (CNTs) are chosen as the support materials due to their electrochemical and thermal oxidation stability and relatively high surface areas. The prepared samples were characterized by transmission electrom microscope (TEM), X-ray photoelectron spectroscopy (XPS), and electron probe micro analyzer (EPMA). The electrocatalytic performance to formic acid oxidation was also investigated by cyclic voltammetry (CV).

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Synthesis of ruthenium oxide/poly(3,4-ethylenediothiophene) nanohybrids for energy storage application

여현정 백승민*

경북대학교 화학과

Ruthenium oxide was known to have a very high metallic conductivity and an excellent energy storage performance with high specific capacitance. Therefore, we have tried to fabricate new hybrid materials via restacking of unilamellar ruthenate nanosheet with poly(3,4-ethylenediothiophene) (PEDOT). The exfoliated ruthenate nanosheets were obtained by controlled intercalation of bulky organic cations, and then, these unilamellar nanosheets were randomly restacked with PEDOT polymers. According to X-ray diffraction and transmission electron microscope analysis, ruthenate nanosheets were randomly incorporated into PEDOT matrices. The obtained hybrid materials showed higher specific capacitances than those of starting materials, supporting that this methodology could be extended to fabricate new energy storage materials.

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Preparation of Dion-Jacobson phase perovskite nanosheets

이원재 백승민[1,*]

경북대학교 자연과학대학/화학과 [1]경북대학교 화학과

Lanthanum tantalum oxide[LaTa2O7]- nanosheets were successfully prepared by chemical exfoliation of a layered perovskite (RbLaTa2O7) via ion exchange and two-step intercalation of cationic species. The nanosheets were characterized by powder X-ray diffraction (XRD), Transmission electron microscope (TEM) and Atomic force microscope (AFM) measurement. According to XRD analysis, we found that bulky ammonium cations were intercalated into the interlayer spaces of layered perovskites. Also, TEM and AFM images of nanosheets showed that layered perovskites with Dion-Jacobson phase were exfoliated into very thin nanosheets. The obtained perovskite nanosheets could be applicable as building blocks to fabricate new layered nanostructures.

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Preparation of ZnO2 nanoparticles(NPs) using zinc(Ⅱ) isobutylcarbamate

김경아 공명선

단국대학교 나노바이오의과학과

Zinc peroxide(ZnO2) has been applied in many application including phothcatalyst, rubber technology, cosmetic. Especially, ZnO2 can be used as precursor of zinc oxide(ZnO), because it releases a oxygen atom by thermal heating at low temperature.In this study, ZnO2 nanoparticles(NPs) were synthesized by reacting zinc(Ⅱ) isobutylcarbamate as a precursor with hydrogen peroxide(H2O2). PEG200 was used as a stabilizer, which suppress aggregation of the ZnO2 NPs. Conditions such as concentration of ZnO2-precursor and stabilizer were systematically controlled to determine their effect on the formation of nano-sized ZnO2 NPs. The formation of ZnO2 NPs were confirmed by the UV-vis, TEM(transmission eletron microscope), HR-TEM(high resolution-TEM), and XRD(X-ray diffraction). Finally ZnO NPs were obtained from ZnO2 NPs by heating at 150℃.

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Synthesis of Silica-coated Gold Nanoparticles

유선미 유소라 이충혁 이완인*

인하대학교 화학과

Gold Nanoparticles (NPs) have been intensively studied owing to their unique physical and chemical properties.Gold NPs have absorption visible region based on surface plasmon resonance, which are coherent oscillations of conduction electrons on metal surface excited by electromagnetic radiation at metal-dielectric interfaces.Gold NPs can be further tailored by their surrounding dielectric medium (e.g., silica shell).Silica coated gold NPs can be prepared by oleylamine capped gold NPs in which the hydrolyzation and condensation of tetraethylorthosilicate (TEOS) are catalyzed by ammonium hydroxide in cyclohexane.Silica coating can prevent nanoparticles against aggregation, electron trapping and provide tunable solubility in various solvent.So, the benefit of silica coating is obvious in many application in catalysis, optoelectronics and chemical and biological sensing.

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Sulfobetaine chitosan modified calcium phosphate cements: the effect of the composition of the w-CS and mechanical properties

김효진 이인호 공명선

단국대학교 나노바이오의과학과

Water-soluble sulfobetaine chitosan (w-SC) was newly prepared to obtain neutral water-based chitosan/calcium phosphate cement. w-CS was prepared by reacting chitosan with 1,3-propane sultone at 50 oC, which is freely soluble in neutral water and have viscosity 16400 cPs from 30% water solution at 20 oC. CPC/w-CS composites were prepared by mixing aqueous solution of α-tricalcium phosphate and neutral water solution of w-SC. Bioactivity was investigated by incubating the CPC/w-CS samples containing different ratios of w-CS (0, 0.4, 0.8 and 1.2%) in simulated body fluid (SBF) for 0, 1, 3, 5 and 7 days. The effect of w-CS and formation of bone like apatite was confirmed on CPC surfaces by SEM and XRD analysis. Higher w-CS content of CPC showed faster apatite deposition in SBF and higher mechanical properties such as compressive strength. The in vitro cytotoxicity test with MC3T3-E1 cell derived from mouse osteoblastic cells was investigated for 7 days.

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Enhancements of Performance and Air Stability of Colloidal Quantum Dot Solar Cells

최민재 정연식*

한국과학기술원(KAIST) 신소재공학과

Colloidal quantum dot (CQD) solar cells are of great interest due to their cost-effectiveness and solution-based processability. Lead chalcogenide quantum dots (QDs) have large dielectric constant and strong quantum confinement effect, which provides better carrier transport characteristics and appropriate band gap energy for photovoltaic applications. However, quantum dot solar cells (QDSCs) based on lead chalcogenide materials tend to degrade rapidly in air due to their poor oxidative stability. Therefore, it is necessary to improve the air-stability of CQD solar cells along with performance optimization. We found out that simple air-annealing can dramatically enhance the air stability of QDSCs. While the performances of a pristine QDSC degraded rapidly in several hours, optimally air-annealed devices retained >55% of their initial power conversion efficiency (PCE) even after 500 hours in air. Moreover, the optimized annealing achieved the enhancements of fill factor, open circuit voltage, and PCE by ~200%, ~250%, and ~600%, respectively, compared to the pristine device. This excellent performance and air stability can be mainly attributed to the formation of thin oxide compounds at the top of QD films. We will discuss in detail the effects of proper oxidation on device performances and reliability based on various analysis results.

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Structure-Performance Relationship of Organic Semiconductors in Solution-Processed Small Molecule Organic Solar Cells

이재관

조선대학교 화학교육과

Organic solar cells (OSCs) fabricated by versatile printing methods such as the doctor blade, inkjet, and roll-to-roll methods are inexpensive, lightweight, and highly solution-processable. Over the last few years, considerable effort has been focused on improving the OSC performance, with the aim of achieving a power conversion efficiency (PCE) of 10%. The following strategies have been adopted for this purpose: 1) development of photoactive materials such as pi-conjugated semiconducting polymers and fullerenes, 2) use of functional layers for buffering, charge transport, optical spacing, etc., and 3) tuning the morphology of the photoactive film by post-annealing, solvent drying, or by using processing additives. Particularly considerable research has been recently focused on developing efficient small-molecule organic semiconductors to improve the performance of solution-processed small-molecule OSCs (SMOSCs), with the near-term goal of achieving a PCE comparable to that above 8% in polymer solar cells (PSCs). We have also developed various molecular structures for efficient small-molecule organic semiconductors and reported their unique photovoltaic characteristics in solution-processed SMOSC. Herein, we wish to introduce the research results to figure out the structure-performance relationship for rational molecular design of organic semiconductors in solution-processed SMOSC.

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Flexible Dye-Sensitized Solar Cell Module with Less Volatile Liquid Electrolyte

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부경대학교 화학과

Dye-sensitized solar cell is attractive photo-electricity conversion system, because of its advantages such as low cost, relatively higher light-to-electricity conversion efficiency and easier fabrication process. The electrolyte, I^-/I_3^- in organic solvents, are sealed between two electrodes. One of the critical problems of DSSC is low boiling point of the organic liquid such as an acetonitrile. Such organic solvents cause evaporation of solvent and brokenness of sealing due to expansion of volume of solvent. For this reason, some organic solvents which have boiling point at least 200 ^{o}C were chosen for alternative liquid for DSSC and studied. Composition of electrolyte was simply LiI/I_2 and some additives were also selected to enhance power conversion efficiency. From the results above, selected combination of electrolyte was applied DSSC module with plastic substrate. A flexible DSSC module was fabricated on a sheet of PEN/ITO film. Unit cells with 1 cm by 15 cm were connected at the long side with silver. I-V characteristic of module was measured under irradiation of real sun.

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Studies of GeSbTe Superlattice Nanowires

박기동 정찬수[1] 김한성[1] 임형순[2] 조용재[1] 백승혁[1] 김창현[1] 박정희[1,*]

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We report novel composition-phase-tuned GeSbTe nanowires (NWs), synthesized by a chemical vapor transport method, which guarantees promising applications in the field of nanoscale electric devices. As the Sb content increased, they showed a distinctive rhombohedral-cubic-rhombohedral phase evolution. Remarkable superlattice structures were identified for the $Ge_8Sb_2Te_{11}$, $Ge_3Sb_2Te_6$, $Ge_3Sb_8Te_6$, and $Ge_2Sb_7Te_4$ NWs. The coexisting cubic-rhombohedral phase $Ge_3Sb_2Te_6$ NWs exhibited an exclusively uniform superlattice structure consisting of 2.2 nm period slabs. The rhombohedral phase $Ge_3Sb_8Te_6$ and $Ge_2Sb_7Te_4$ NWs adopted an innovative structure; $3Sb_2$ layers intercalated the $Ge_3Sb_2Te_6$ and $Ge_2Sb_1Te_4$ domains, respectively, producing 3.4 and 2.7 nm period slabs.

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Electrochemical Reduction of Ultrathin Graphene Oxide/Polyaniline Films for Supercapacitors with an Ultrahigh Specific Capacitance

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인천대학교 화학과

In order to develop energy storage devices with high power and energy densities, electrodes should hold well-defined pathways for efficient ionic and electronic transport. In this presentation, we demonstrate ultrathin film supercapacitor composed of polyaniline (PANi) and electrochemically reduced graphene oxide (ERGO) bilayers, which was achieved using layer-by-layer (LBL) assembly method. The supercapacitor comprising the electrodes fabricated using ultrathin PANi-ERGO films (d = 70.2 nm) exhibited a specific capacitance of 1428 F/g (at a current density of 3.0 A/g), and achieved a new record value among carbon-based devices including conducting polymers, to the best of our knowledge. The PANi-ERGO supercapacitor displayed an energy density of 49.6 Wh/kg and a power density of 234.4 kW/kg at an operating potential of 1.0 V in 1 M H2SO4 electrolyte. These values are also among the best values yet achieved using carbon-based materials. This breakthrough energy storage device was made possible by the development of a unique process for preparing the thin film electrodes composed of PANi/GO bilayers that were electrochemically reduced to PANi/ERGO after the assembly of the supercapacitor cells. This technique minimized the morphological damage to the thin film electrodes, and prepared optimal doping and oxidation state of PANi in the multilayer films for achieving excellent electronic conductivities and ionic transport. The LBL-assembly method provides a tool for preparing well-organized homogeneous PANi/ERGO composites.

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Layer-by-Layer Self-Assembled Multilayer Films of Thermoresponsive Block Copolymer Micelles with Photoresponsive Cores

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인천대학교 화학과

Stimuli-responsive polymer materials are increasingly gaining attention owing to their diverse and unique properties such as self-adaption to surrounding environments, transport regulation of ions and molecules, change of wettability, and conversion of chemical and biochemical signals into optical, electrical, thermal and mechanical signals, and drug delivery applications.Herein,we report on the layer-by-layer (LBL) self-assembly of the temperature-responsive diblock copolymer micelles of poly((2-dimethylamino)ethylmethacrylate)-block-poly(diethyleneglycol methyl ether methacrylate) (PDMAEMA-b-PDEGMA) (P363) with a polyanion.The P363 unimers or micelles were included within the multilayer films through LBL-assembly utilizing the electrostatic interactions between the cationic PDMAEMA block and the polyanion.The LBL self-assembly and morphology of the multilayer film was studied as a function of deposition temperature and z-average diameter, using UV/visible spectroscopy, ellipsometry and AFM. Furthermore, the diblock copolymer P363 micelle was also utilized as the building blocks for the incorporation of a hydrophobic photochromic dye (spiropyran SP) into the micellar cores of P363 in the multilayer films via the specific interactions between the SP-dye and the temperature-responsive PDEGMA block of P363 micelle.This method showed a potential use in controlled assembly of stimuli-responsive hydrophobic dyes into LBL multilayer films and could be a promising candidate for the application in separation and sensing.

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Surface Plasmon Induced Enhancement in F?rster Resonance Energy Transfer Based Light Emission in Hybrid QDs-Dye Systems

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이화여자대학교 화학나노과학과

F?rster resonance energy transfer (FRET) is a nonradiative energy transfer from the excited state donor to the ground state acceptor by dipole-dipole interactions. FRET efficiency is strongly influenced by spectral overlap and separation distance between donors and acceptors. Quantum dots (QDs) are considered as very useful donors in FRET due to the simplicity to tune their optical properties by changing their size. Nevertheless, due to the distance dependence on FRET, the efficiency of FRET is limited. Presence of plasmonic metals nanoparticles (NPs) in the vicinity of QDs can enhance the intensity of emission of QDs through plasmonic resonance energy transfer (RET) from metal NPs to QDs and this improved emission energy of donor can be transferred to the acceptor via FRET. Here, we study the RET induced enhancement in FRET between CdSe QDs and Sulforhodamine101 dye by using gold (Au) NPs as a probe to study RET. A core-shell nanostructure was prepared by first coating Au NPs with thin shell of silica followed by decorating the silica surface with CdSe QDs. This core-shell structure was again coated with a second shell of silica, onto which dye is adsorbed. Photoluminescence (PL) spectra and steady-state florescence spectra were used to study the enhanced FRET and change in life time of QDs, respectively. In the first step RET from Au NPs was studied using PL spectra. In the second step concurrent RET and FRET in Au@SiO2@QD@SiO2@Dye nanostructure was studied. This was then compared with the QD@SiO2@Dye core-shell structure. It was observed that efficiency of FRET is significantly improved in the presence of Au NPs, showing the effective transfer of surface plasmon resonance energy from Au NPs to the QDs.

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Molecular Dynamics Simulation on Self-Assembled Layers of C_{60} - Pentapods

유택희

광주과학기술원(GIST) 신소재공학부

Unimolecular rectification behavior of a known amphiphilic fullerene derivative, C_{60}-pentapod (4-$HOC_6H_4)_5HC_{60}$), is reported. The mechanism of unimolecular rectifying using Quantum Mechanical method was already investigated, but adsorption on electrode and packing models in realistic device was not investigated. Therefore, a new force field (FF) was developed and validated against various properties experimentally measured on its component systems such as C_{60}, benzene, phenol, gold, ethane, butane, hexane and their combinations. Using the new FF available to fullerene derivatives, we built and simulated various adsorption unimolecular structures on Au(111). It was found that the side structure is more stable than the upright structure. The results differ from the experiments because the most devices were fabricated by Langmuir-Blodgett (LB) film at the air-water interface. Moreover, molecular dynamics (MD) simulations were performed to understand the structure of a self-assembled monolayer (SAM) of C_{60}-pentapod on Au(111) substrate. The dynamics of SAM were characterized by several analyses. MD simulations with the final FF indicate that the optimum surface density of a monolayer of C_{60}-pentapod corresponds to a footprint of 1.152 nm^2/molecule and that it is more stable when standing upside down than when standing up or lying on the side. In future work, we will apply the bias on SAM on Au electrode and observe the behavior of that.

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A Method for Fabricating Ultrathin Multilayer Film Composed of Poly(p-phenylenevinylene) and Reduced Graphene Oxide on a Plastic Substrate for Flexible Optoelectronic Applications

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인천대학교 화학과

Graphene-based optoelectronics has been a hotbed of research since the experimental isolation and characterization of graphene in 2004. Our current research focus mainly on the photoconductive properties of a uniform ultrathin multilayer film comprising alternating poly(p-phenylene vinylene) PPV and reduced graphene oxide RGO layers, fabricated on a poly(ethylene terephthalate) PET sheet. The assembly of the two electron-rich layer components on the temperature-sensitive substrate was realized using a layer-by-layer-deposition technique under mild conditions and HI/H2O vapor treatment at 100℃. This protocol was established here to simultaneously convert the layer components (the PPV precursor and graphene oxide) to their conjugated counterparts PPV and RGO in the multilayer films. The PET sheets coated with (PPV/RGO)15 films (d = 23 nm) exhibited a photocurrent of 115 μA at an illumination intensity of 1.1 mW and a photoresponsivity of 111.1 mA W-1 at an illumination intensity of 0.5 mW; these are among the best values yet achieved in carbon-based materials. The extraordinary optoelectronic characteristics of the (PPV/RGO) films were ascribed to the charge transfer complex formation of the two PPV and RGO layer components and also to the structural uniformity of the LBL-assembled optoelectronic thin films, which tended to favor the rapid interfacial charge transfer to the electrodes. The establishment of a method for fabricating (PPV/RGO) films on a temperature-sensitive transparent flexible sheet is crucial for the development of organic-based portable electronic devices.

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A Computational Study on the Effects of Oxygen Vacancies on the Electronic Properties of $La_{1-x}Sr_xMnO_3$ for Resistive Switching Memory Application

이노도

광주과학기술원(GIST) 신소재공학부

Resistance random access memory (ReRAM) is promising as a next-generation non-volatile memory device due to its simple capacitor-like structure and ultra-fast speed. $La_{1-x}Sr_xMnO_3$ (LSMO) is an attractive ReRAM material sandwiched between reactive metal. However, the microscopic switching mechanism is still unclear. To reveal the switching mechanism, most studies focused on the redox reaction at the interface region. In a different point of view, we focused on the effect of oxygen vacancies of the LSMO bulk to the change in resistance. The effect of oxygen vacancies on the change in structure, energy, electronic and magnetic properties of the LSMO were investigated by means of the first-principles generalized gradient approximation (GGA) method. Based on the structural and magnetic phase diagrams for the LSMO, we considered four different bulk model systems with different Sr concentration (x=0, 0.25, 0.5, and 1) and investigated their energetics for the oxygen vacancy formation and migration. The results show that the oxygen vacancy formation energy is near linearly decreased with increasing Sr concentration while the migration energy shows an opposite trend. The density of states and the charge density map show that the oxygen vacancy has a significant effect on the electronic structure, especially near the oxygen vacancy sites. For more reliable observations, we will compute the conductance of above systems using a Green's function formalism in these future studies.

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Layer-by-Layer Self-Assembled Ultrathin Multilayer Films Composed of Graphene/Magnetite Bilayers: High-Conductive Electrode Materials for Supercapacitors

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This study describes a simple and facile fabrication of multilayer film comprising magnetite nanoparticle (Fe3O4) and chemically reduced graphene oxide (RGO) on electrodes for supercapacitor application. The thickness of the Fe3O4/GO bilayer was determined using an optical ellipsometer to be 6.53 ± 0.17 nm, which agreed well with the sum of the independently-measured thickness of each layer component; Fe3O4 (5.61 ± 0.14 nm) and GO (0.91 ± 0.1 nm). The results exhibited the uniform and regular deposition of the layer components. The Fe3O4/RGO multilayer film was obtained through the reduction of Fe3O4/GO film using hydrazine, and exhibited the minimum resistance of 1.0 × 104 Ω/sq. (2.8 S/cm), as the bilayer numbers reached to 50. The electrodes fabricated with 30 Fe3O4/RGO bilayers exhibited excellent capacitive performances with a maximum value of specific gravimetric capacitance (151 F/g) at current density of 0.9 A/g.

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Push-Pull Copolymers Based on Bridged Dithiophenes and N-Alkylthienopyrrolediones: Time-dependent Density Functional Theory Study for Photovoltaic Applications

<u>정은환</u>

광주과학기술원(GIST) 신소재공학과

Low-band-gap push-pull copolymers are promising donor materials mixed with fullerene derivative acceptors in bulk heterojunction organic photovoltaic cells. The best push-pull copolymers so far contained benzothiadiazole (BT) pulling units but the BT units have no proper room to accommodate long alkyl side chains that ensure solubility in organic solvents. To overcome the solubility issue, we replace the BT units with N-alkylthienopyrroledione (TPD) which has pyrrole moiety to attach the long alkyl side chains. We investigate the electronic structure of the oligomer models of the copolymers based on bridged dithiophenes and the TPD units with density functional theory and time-dependent density functional theory calculations. We also calculate the binding energy of a stacked pair of the monomers and investigate charge-transfer properties of them. It can be estimated to the first good approximation in Marcus theory that describes the charge-transfer rate between the copolymers calculating the interchain transfer integral and reorganization energy. The results show that the copolymers with TPD have deeper HOMO levels, better charge-transfer properties, and better power conversion efficiencies than copolymers with BT.

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Color Evolution and Phase Transformation Behaviors of Non-toxic Iron Red/yellow Pigments

김유진* 피재환[1]

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In the pigment industry, there is a restricted choice for red/yellow colors because Cd based pigments can effect the environment and human health. The yellow color iron oxy-hydroxides (goethite, α-FeOOH) and red color iron oxides (hematite, α-Fe_2O_3) have attracted much interest owing to their non-toxic, optical properties. Although, nanosized hematite pigment has high red tonality, their colorations at high temperature were changed due to aggregation and oxidation. To minimize coloration change, we proposed ceramic coating systme using silica(SiO_2), zircon($ZrSiO_4$) and study their colorations and thermal behaviors at high temperature. We sythesized nanosized iron oxy-hydroxide, iron oxides pigments and coated with silica, zircon by hydrolysis reaction with TEOS (Tetraethylorthosilicate), Zircon-sulfate as a precursor. Espically, zircon-coated iron oxides were made using double layer systems with silica and zirconia. Silica-coated yellow pigments were transformed to red pigment with high reflectance values. Well designed silica, zircon-coated pigment has high optical properties which are well suited for non-toxic inorganic red/yellow pigments.

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Reversible conversion between polymer nanocapsules and 2D polymers through dynamic covalent self-assembly

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Controlling polymer morphology in nano and mesoscale is important for making functional materials with desired properties. Our group has demonstrated the formation of various polymer morphologies such as capsules, 2D films and toroidal nano and mesostructures by covalent self-assembly of rigid, disk-shaped building blocks via irreversible covalent bond formation reactions including thiol-ene photo-addition, olefin metathesis, and amidation with potential applications. We are now focusing our attention on dynamic covalent assembly using reversible bond formation to control the polymer morphology in a reversible manner. Thus, we have newly synthesized thiol-CB[6], a cucurbit[6]uril (CB[6]) derivative functionalized with twelve thiol groups at the periphery. The thiol-CB[6] formed multiple disulfide bonds with each other to produce (i) 2D polymer films spanning over several micrometers and (ii) nanocapsules with diameters of ca. 100-200 nm. Importantly, we can control and manipulate the polymer morphology by simple solvent exchange. The resulting polymers have been thoroughly characterized by various techniques including SEM, TEM, AFM and DLS.

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Application of TiO2 Sphere in Heterojunction Solar Cells

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Heterojunction solar cell is fabricated with 2~3 nm size of perovskite $(CH_3NH_3)PbI_3$ nanocrystal. Spin-coating of the perovskite precursor solution leads to $(CH_3NH_3)PbI_3$ quantum dots (QDs) on TiO_2 sphere. Here we report on a Perovskite/TiO_2 heterojunction solar cells by using TiO_2 spheres. The pervoskite acts as not only an absorber but also a hole conductor, rendering superfluous the use of an additional p-type material for transporting positive charge carriers. TiO_2 sphere provided a novel hierarchical pore structure with high surface area and large pore diameter. Perovskite is stable in ambient air drying and can be deposited by simple and low cost solution process. This will offer a new way to economical and high efficiency solar cells development.

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Effect of Fluorine Treatment on Electrochemical Performance of Phenol-based Activated Carbons for Supercapacitor

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In this work, we investigated the electrochemical performance of porous Phenol-based activated carbons (P-ACs) by fluorine treatment. The effect of fluorine treatment time on electrochemical performance of the P-ACs was investigated. The textural properties and morphologies of the P-ACs were analyzed by reference to N_2/77 K adsorption isotherms and field emission scanning electron microscope (FE-SEM), respectively. The electrochemical performance of the P-ACs was confirmed by cyclic voltammograms (CV). As results, the electrochemical performance of fluorine treated P-ACs was higher than that of untreated P-ACs. This was suggested that the fluorine functional groups on the P-ACs led to the combination effect of both electric double-layer capacitor and pseudocapacitance in the present system.

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A study on heating value of wood chip composites as cogeneration plant fuel

허지훈 박수진[1,*]

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Polystyrene (PS)/wood chip (WC) composites (PS/WC) were prepared by solution mixing method and the effect of polystyrene on thermal characteristics of WC was investigated with different PS/WC ratios. The heating value of the PS/WC were determined by thermogravimetric analyzer and calorimeter, respectively. From the results, the PS/WC revealed copyrolysis features in the range of 400?470 ^{o}C compared to WC and PS and exhibited high heating value over about 4900 kcal/kg at low PS content (PS/WC = 2/8). These results were attributed to the combination effect by interaction between polystyrene and wood chip.

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Preparation of hydrophilic/hydrophobic functionalized silica mesoporous by controlled concentration of silica and surfactant.

구병진 배재영*

계명대학교 화학과

Hydrophilic/hydrophobic functional groups with silica mesoporous was prepared by sol-gel method. This method is using tri-block copolymer surfactant and CTACl as a template. Preparation of silica mesoporous was by adjusting the molar ratio of the silica and surfactant. Brunauer?Emmett?Teller (BET) method, Transmission electron microscopy (TEM) were used to characterize the preparation of hydrophilic/hydrophobic functionalized silica mesoporous.

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Fabrication of N-doped TiO2 Photoelectrode for Dye-Sensitized Solar Cells Application

박수경 배재영*

계명대학교 화학과

N-doped TiO2 nanoparticles were synthesized through the hydrolysis of TiCl4 in an ammonia water. For comparison, pure TiO2 nanoparticles were synthesized using the same technique without the addition ammonia water. The synthesized N-doped TiO2 were characterized by X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy, UV-vis diffuse reflectance spectroscopy, and N2 sorption techniques. To prepare the N-doped TiO2 electrode, first-layer transparent films were fabricated using Ti-Nanoxide D (Solaronix) paste, and second-layer films were fabricated by N-doped TiO2 paste onto glass substrate coated with transparent conductive oxide (TCO, F-doped SnO2, 8 ~10 Ω/cm2, Solaronix) by the doctor-blade method. For comparison, the pure TiO2 electrode was fabricated using the Ti-Nanoxide D (Solaronix) paste and pure TiO2 paste, respectively. Consequently, we obtained the energy conversion efficiency of the DSSCs based on the N-doped TiO2 electrode is higher than that of the DSSCs based on an pure TiO2 electrode. The DSSCs based on the N-doped TiO2 electrode improved Voc, Jsc, and η, as compared to the pure TiO2 electrode and the Ti-Nanoxide D TiO2 electrode (Solaronix).

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Preparation and characterization of metal and nitrogen doped mesoporous TiO_2

진현탁 배재영

계명대학교 화학과

Metal and Nitrogen doped mesoporous TiO_2 were prepared by a sol-gel process. Nitrogen doped mesoporous TiO_2 were successfully synthesized by the addition of ammonia water. Metal doped mesoporous TiO_2 were prepared by using metal sources (i.e., $SnCl_2$, $NiCl_2$, and $Zn(NO_3)_2$). The resulting materials were characterized by Brunauer- Emmett-Teller method (BET), Transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

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Preparation of inorganic ligand-capped BixSb2-xTe3 nanoparticles and their thermoelectric properties

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Monodispersed BixSb2-xTe3 nanoparticles were synthesized by solution-based procedure with organic ligand in solution. Organic ligands with long hydrocarbon chains on the synthesized BixSb2-xTe3 nanoparticles were replaced with inorganic ligand SnS44- by two-phase transfer reaction. The synthesized organic ligand- and inorganic ligand-capped BixSb2-xTe3 nanoparticles were characterized by using HR-TEM, SEM and XRD analysis. To assess the roles of the ligand on the thermoelectric (TE) properties, we comparatively investigated the organic ligand- and inorganic ligand-capped BixSb2-xTe3 systems. Both types of BixSb2-xTe3 nanoparticles were compacted into nanostructured bulk samples by spark plasma sintering. The densification behavior and microstructure of the sintered samples were characterized and their thermoelectric properties were investigated.

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Water-dispersible photoluminescent nanographitic/nitrogen-doped graphitic hollow shells as a potential candidate for biological applications

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Water-dispersible nanographitic hollow spheres were synthesized using a soft chemical route underhydrothermal conditions by glucose carbonization using a magnetite/silica-encapsulated core-shellsphere as a template. Also nitrogen-doped graphitic spheres were synthesized by a hydrothermal reaction. The graphitic and nitrogen-doped nanographitic hollow spheres show wavelength dependent photoluminescence in 300-600 nm range. The photoluminescence seems to depend on the fraction of the sp^2 domains and N-doping, therefore, tunable PL emission can be achieved by controlling the nature of sp^2 sites. In addition the cellular uptake of the graphitic hollow spheres was evaluated in human HeLa cells, demonstrating its main localization in the cytoplasm. A blue fluorescence signal was the most intensively observed in the cellular uptake process, although some green and red fluorescence was also observed. Since the cores of Fe_3O_4 could be completely or partly eliminated in a controllable way, it can be used as a magnetic resonance imaging agent. In addition, their easily modifiable hydrophilic surfaces for multi-functionality and hydrophobic voids covered by oxidized graphite make them promising candidates for applications in cellular photo-imaging and targeted drug delivery.

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A simple and effective way to fabricate heterophase nanostructured bulk thermoelectric material and their enhanced figure of merit

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이화여자대학교 화학과 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학나노과학부

We show a novel approach to fabricate heterophase nanostructured Bi_2Te_3-based bulk thermoelectric materials and investigate their thermoelectric properties. Highly uniform Bi_2Te_3 nanotubes and Cu doped Bi_2Te_3 nanorods were synthesized through a simple and fast solution process by using ultrathin Te nanowires as templates. Both types of Bi_2Te_3 nanostructures were consolidated into nanostructured bulk using spark plasma sintering (SPS). Unlike pure Bi_2Te_3, Cu doped Bi_2Te_3 nanorods were transformed to Bi_2Te_3/Bi_2O_5Te heterophase nanostructured bulk during the SPS process. Bi_2Te_3/Bi_2O_5Te heterophase nanostructured bulk sample shows drastically reduced thermal conductivity due to the increased phonon scattering by heterophase interface. As a result, the ZT value was significantly enhanced in the Bi_2Te_3/Bi_2O_5Te heterophase nanostructured bulk (ZT ~ 0.68 at 418 K). This approach suggests an easy way to induce heterostructure in the matrix, thus enhancing thermoelectric figure of merit.

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Synergistic effects of biomimetic micropatterns of AgNP-gelatin biocomposites on epidermal wound healings

PRAKASH CHANDRA 이석우*

공주대학교 화학과

Understanding and managing bioburden for generation of scar free skin tissue with appropriate treatments is vital to effective wound healing. In this study, we have applied the microgrooved patches of PDMS coated with AgNPs/gelatin biocomposite over the fibroblast monolayer during in vitro wound healing, which was found to be more efficient compared to gelatin coated microgrooved substrates. This study demonstrates the significant synergistic response in wound healing with application of Gel-AGNPs bionanocomposites and topologically modified surface, ultimately provide a new insight in development of biomimetic scaffold and topical dressing for wound and burn healings.

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Tin oxide/molybdenum sulfide nanohybrids for electrode materials in lithium ion batteries

장지훈 백승민

경북대학교 화학과

New nanoporous SnO2/MoS2 hybrids were successfully synthesized by controlled reassembling of delaminated molybdenum sulfide (MoS2) nanosheets with tin oxide (SnO2) nanoparticles. According to X-ray diffraction and transmission electron microscopy analyses, molybdenum sulfide nanosheets in the present materials were randomly hybridized with tin oxide nanoparticles without any self-restacked phase. Nitrogen adsorption-desorption isotherms clearly shows that the specific surface area of hybrid material was significantly larger than that of self-restacked MoS2. The obtained nanohybrids can be used as electrode materials for lithium ion battery. Discharge capacity of SnO2/MoS2 hybrid was much larger than that of SnO2 nanoparticle after 30 cycles, highlighting the effectiveness of this synthetic route via exfoliation and restacking method.

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Novel Synthesis of Au@Pd/Graphene Nanocomposites and Their Outstanding Electrocatalytic Activity for Oxidation of Ethanol

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We report on Surfactant-free Au@Pd core-shell NPs on the graphene sheets. Our Au@Pd graphene nanocomposites were synthesized from Au, Pd ions and graphene oxide by one-step reduction using ascorbic acid as an eco-friendly reducing agent. The core/shell structures with about 7nm size were observed by XRD, TEM and HAADF-STEM mapping analysis. Prepared Au@Pd/graphene nanocomposites show an excellent elecrocatalytic activity toward ethanol oxidation: If value that was the best for our catalysts is 11573 mAmg-1, which is about 5 times as high as that of the previous catalyst. The data resulted from extremely optimized bimetallic structure of a small Au core and a thin Pd shell. Pd atoms are constantly encouraged by adjacent Au atoms

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Improved air stability of PbS colloidal quantum dots-sensitized solar cells by co-capping of 1-dodecanethiol

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The PbS colloidal quantum dots (CQDs) capped by oleic acid (OA) and 1-dodecanethiol (DT) exhibited much better air stability than the PbS CQDs capped only by OA ligand because the PbS CQDs capped by OA and DT have the S atoms passivated by long alkyl chain of DT molecule on the surface whileas the PbS CQDs capped by OA do not have the passivated S atoms. The unencapsulated senstized solar cell fabricated by the PbS CQDs capped by OA and DT ligand exhibted 3.3 % of power conversion efficiency at 1 sun illumination and showed better device stability with aging time in ambinent condition than the solar cell fabricated by PbS CQDs capped by OA.

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Photo-Induced Cation Exchange Reaction of Germanium Chalcogenide Nanocrystals

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고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자공학

Germanium chalcogenide GeSxSe1-x nanocrystals (NC) were synthesized using a novel gas-phase laser photolysis reaction. The composition of the alloy nanocrystals was simply controlled by the partial pressure of precursors in a closed reactor. Remarkably, these ligand-free NC undertake the photo-induced cation exchange reaction to produce a series of Cd, Zn, Pb, and Ag chalcogenide NC in aqueous solution, which is governed by the thermodynamic driving force based on solubility. This effective synthesisstrategy promises the development of cost-effective excellent optoelectronic devices.

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Fabrication of graphitized carbon nanotubes decorated with gold nanoparticles by conversion of sucrose used template with various size of channel diameter.

이명순 김 돈*

부경대학교 화학과

A facile route for preparation of gold nanoparticles (AuNPs) attached carbon nanotubes (Au@C) through the carbonization of sucrose based on anodic aluminum oxide (AAO) template with various size of channel diameter is described. The AAO template with ordered channel decorated with AuNPs were fabricated by a thermal decomposition of $HAuCl_4$. The diameters of channel inside AAO template were controlled by electrolyte and applied voltage. The channels have within the range of 20~250 nm in diameter. The size of AuNPs obtained from different channel diameter was confirmed by UV-Vis spectrum, TEM images and X-ray diffraction methods. The obtained Au@C is conductive and graphtized carbon nanotubes with a relatively large AuNPs. The degree of crystallization and the size of carbon particle in the graphitized carbon phase were confirmed mirco Raman spectroscopy and field emission current measurements.

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Synthesis and characterization of quaternary Cu2ZnSnSe4 nanocrystals

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공주대학교 화학과 및 GETRC

Copper-based quaternary semiconductor, Cu2ZnSnSe4 (CZTSe) has attracted great attention as low-cost alternatives to conventional solar cell materials due to its direct band gap, as well as a large absorption coefficient ~104 cm-1. Herein, we report the synthesis of Cu2ZnSnSe4 nanoparticles via hot injection method using (Et3Si)2Se as selenium source. Oleic acid and 1-octadecene has been used as coordinating ligand and non coordinating solvent, respectively. The morphology and composition of the products were characterized using SEM, TEM, EDS, XRD and XPS. The nanoparticles were single phase and size in the range 30-50 nm. UV-Vis-NIR absorption measurements showed a band gap of 1.64 eV for the as synthesized Cu2ZnSnSe4 nanoparticles.

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Synthesis and Characterization of Sb2Te3 Nanocrystals from Sb(TeEt)3

LIRICHENG 김진권*

공주대학교 화학과 및 GETRC

Antimony telluride (Sb2Te3), which belongs to the layered semiconductors with tetradymite structure is a promising candidates for near room-temperature thermoelectric applications due to their promising zT values in the temperature range of 300?500 K. Antimony telluride nanostructures with well-de?ned morphologies can be synthesized by gas phase processes such as chemical vapor deposition and vapor transport growth, as well as in solution by hydrothermal processes. We report, a facile solution phase method for the synthesis of crystalline Sb2Te3 nanoplates using Sb(TeEt)3 single source precursor in oleylamine solvent at 300℃. The as synthesized nanoplates are characterized by XRD, SEM and TEM.

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Electrochemical Sensor based on Prussian Blue/ CNT-Graphene Multilayer Electrode for Determination of Hydrogen Peroxide

Yangjiao 조미숙* 이영관*

성균관대학교 화학공학과

AbstractElectrochemical sensor based on Prussian blue (PB) and CNT-graphene multilayer electrode was developed for H2O2 determination. CNT-graphene multilayer electrode was prepared by layer-by-layer assembly on ITO-coated glass: alternatively chemical dipping for CNT layer and electrodeposition for graphene layer. PB was deposited on the CNT-graphene multilayer electrode by self assembles technique. The surface morphology of the PB/CNT-graphene modified electrode was characterized by electron scanning microscopy. The PB/CNT-graphene sensor shows high electrochemical activity and excellent stability for H2O2 sensing in a linear dynamic detection range from 0.05 mM ~ 9.5 mM, and its sensitivity was 382.4 µA mM-1 cm-2. It has good selectivity in the presence of electroactive species such as ascorbic acid, dopamine, glucose, and uric acid.Key words: CNT, graphene, hydrogen peroxide, self-assemble

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Thermally amplified metal-insulator transition of hydro-thermally prepared vanadium dioxide.

박희선 이명순 김 돈*

부경대학교 화학과

Vanadium dioxide (VO_2) was prepared by hydrothermal reaction of mixed acidic (pH_2O_5 and N_2H_4 HCl in the range of 160 - 230°C. The precipitation of the reaction was annealed to complete the formation of VO_2phase at 500°C in Ar for 5 h. The clear metal-insulator (MI) phase transition was observed, in electrical conductivity and differential scanning calorimeter(DSC) measurements and optical images, at around 68°C in the prepared VO_2 samples. The abrupt changes of electrical conductivity at the MI transition were amplified by the number of the thermal cycling (repeated heating and cooling across the MI transition).

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Electrochemical Behaviors of Pt-Ru Nanoparticle Doped on Zeolite-templated Carbon Supports for Direct Methanol Fuel Cells

임태진

인하대학교 화학과

In this work, we prepared zeolite-templated carbon (ZTC) supports for direct methanol fuel cells (DMFCs). We deposited Pt-Ru metals on ZTC with different Pt-Ru amounts. The crystalline and structural features were investigated by X-ray diffraction (XRD). The textural properties of ZTC were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and BJH method. The surface morphology was characterized by scanning electron microscope (SEM) and transmission electron microscopy (TEM). The electrochemical properties of Pt-Ru/ZTCs catalysts were also analyzed by cyclic voltammetry measurements.

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

임태진

인하대학교 화학과

In this work, zeolite-templated carbons (ZTCs) were prepared by a conventional templating method using furfuryl alcohol for catalysts in direct methanol fuel cells (DMFCs). The ZTCs were conducted KOH activation with different activation temperatures. The Pt-Ru metals were deposited onto activated ZTC (A-ZTC) by chemical reduction method. The characteristics of Pt-Ru/A-ZTCs were determined by N2/77 K adsorption analysis, X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM). And the electrochemical properties of Pt-Ru/A-ZTCs catalysts were also analyzed by cyclic voltammetry experiments.

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Three-Dimensional Structure of Helical $Ge_3Sb_2Te_6$ and $Ge_3Bi_2Te_6$ Nanowires Using Electron Tomography

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Recently, interest in 3-dimensional (3D) nanostructures has been steadily increasing, owing to their attractive morphology and mechanical/electrical/optical properties. All of the helical and zigzagged structures in these previous studies were analyzed by examining their 2-dimensional (2D) projections using TEM, which provides a first insight into their size and morphology. There are, however, potentially some cases where important 3D structural information is missed or erroneous information may be obtained when using simply this technique. Electron tomography, which is a method of reconstructing the 3D morphologies from a series of 2D transmission electron microscopy (TEM) images or projections, has been successfully applied to analyze the morphology of various 1D nanostructures. We were synthesized by the thermal evaporation for the $R_2Te_3(GeTe)n$ (R = Sb, Bi) alloy nanowires. Among the nanowires, the $Ge_3Sb_2Te_6$ and $Ge_3Bi_2Te_6$ nanowires consist of a unique helical morphology and superlattice structrures. We employed both electron tomography and high-resolution TEM images to study the 3D structure of helical $Ge_3Sb_2Te_6$ and $Ge_3Bi_2Te_6$ nanowires. Their 3D reconstruction images, acquired from a series of 2D projections, were obtained by high-angle annular dark field (HAADF) scanning TEM (STEM).

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Changing optical properties of InP/ZnS QDs depending on the doping condition

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Semiconducting nanocrystals, or quantum dots (QDs), have been attracting much attention over the last decade due to their outstanding optical properties, including low scattering, tunable bandwidth, high brightness, long-term stability and nm scale size. QDs can be used in various fields such as biomedical fluorophores, biosensor, photovoltaic devices and materials for LEDs. For using the QDs by the LED materials, it has high stability under the thermal and photonic states. The optical properties of QDs are dependent on their individual surface chemistry and chemical environment. However, the connatural stability (photo, thermal so on) of quantum dot has not reached researcher's expectation. QDs have improved their properties through the generation of core/shell CdSe/ZnS structure or core/multishell structures like as CdSe/CdS/ZnS and CdSe/CdS/CdZnS/ZnS. And some groups changed their properties by using the doping materials. Doping material has interband in the quantum dots. The photoexcited electron of QDs transferred to the upper energy level of transition metal and relaxed radiatively to the down energy level. The optical properties of InP QDs can be improved by controlling the doping condition.

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Synthesis and Characterzation of Core-shell ZnO Nano Phosphor

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Zinc oxide (ZnO), is one of important semiconductors with direct band gap of~3.37eV and used in many applications such as drug, carrier and sensor due to their non-toxic, biocompatibility. In addition, doping of transition metals into ZnO is the basic method for controlling the properties of the semiconductor such as band gap or electrical conductivity. 5nm sized ZnO nanoparticles were prepared using hydrolysis by Zn precursors and LiOH. Luminescent properties of ZnO nanoparticles were tunable with various concentrations of Zn acetate and LiOH. The ZnO nanoparticles were coated with silica via a simple sol-gel process in the Stober system and studied their luminescent properties. The samples exhibited an emission peak at 520 nm.

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Quantitative structure-property relationship for predicting the densities of high energetic density materials(HEDMs)

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High energetic density materials(HEDMs) has been applied as explosive, fuels and propellants. Therefore, there is significant interest in the development of novel HEDMs with higher performance. However, the promising candidates requires a great deal of effort such as synthesis, testing, etc. In this study, quantitative structure-property relationship(QSPR) was developed to predict the density of HEDMs provided by ICT-database. A mechanistic interpretable 2D molecular descriptors was selected by wrapper method for population-based forward selection using machine learning method. Machine learning method used multiple linear regression(MLR), support vector machine(SVM). The models were developed and validated for bootstrap method and applicability domain. The each performance was compared between the MLR and SVM using R^2, RMSE(root mean square error), and MAE(mean absolute error). This models will help to screening novel high energy high density materials (HEDMs).

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Polypyrrole/Poly(vinylalcohol-co-ethylene) Solid State Gel Electrolyte for Iodine-Free Dye-Sensitized Solar Cells

정미희

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We presented a solid state gel electrolyte as an alternative to the liquid electrolytes used in dye sensitized solar cells (DSSCs) because the use of liquid electrolyte raises significant technological problems associated with device sealing, long-term stability and corrosive I2. The first solid state gel electrolyte was prepared by using the dimehtylsulfoxide (DMSO) as the solvent, doped polypyrrole (PPy) as the hole-conducting polymer. Then, we introduced block copolymer of poly(vinylalcohol-co-ethylene) (PVA-EL) with low transition temperature into a DMSO-PPy system to change liquid electrolyte into the gel electrolyte. Vinylalcohol (VA) homopolymer can dissolve well in the DMSO electrolyte. The high solubility is attributed to the effect of significant interaction between DMSO and VA. This interaction originates in the OH group of VA and the moiety of the DMSO molecule. Therefore, the high solubility of the PVA-EL in the electrolyte is attributed to the effect of the VA segments, while the EL segments contributes to the following gelation process through the interaction and cross-linking among the EL chains. We have changed EL composition to investigate gelation process. The results show that the diffusivity and conductivity significantly were changed during the gelation period with increasing the ratio of EL segments in the copolymer.

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Epitaxial Growth of Well-defined Rubrene Nanowires by Eutectic Solidification

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One-dimensional (1D) nanomaterials, especially nanorods, are ultimately suitable for the transport of photons, electrons and have been demonstrated as building blocks of optical devices.Organic nanorods having better crystallinity, packing density and assembly in even molecular level usually exhibit better intrinsic properties more exactly. Herein, we present fabrication and characterizations of well-defined rubrene nanowires, which can be applied for patterning and organic field effect transistor.To take an easier way we fabricated nanomaterial that are highly crystalline using epitaxial growth and could control crystallinity and optical properties. The physical properties were characterized by electron and optical microscopies, MALDI-TOF, XRD.

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The synthesis and characterization of $Na_2M_2(PO_3)_3N$ (M=Fe and Co)

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$Na_2M_2(PO_3)_3N$ were synthesized by the thermal nitridation of stoichiometric mixture of $NaPO_3$, $Fe(NO_3)_3{\cdot}9H_2O$ (M = Fe), $Co(NO_3)_2{\cdot}6H_2O$ (M = Co) and $NH_3H_2PO_4$ in flowing ammonia gas. The crystal structure of $Na_2M_2(PO_3)_3N$ was investigated by means of Rietveld refinement based X-ray powder diffraction data. The diffraction patterns showed the cubic symmetry (space group of $P2_13$) with lattice parameters a = 9.3420(17)Å (M = Fe) and a = 9.2633(14)Å (M = Co). In the structure of $Na_2M_2(PO_3)_3N$, phosphorous atom is coordinated to three oxygen atoms and one nitrogen atom to form a PO_3N tetrahedron. The $(PO_3)_3N$ entity is formed by three PO_3N tetrahedra sharing a common corner occupied by nitrogen atom. Na, M (Fe or Co) and N atoms are arranged along [111] direction in the sequence of M1-M2-N-Na1-Na2-M1-M2-…. The $M1O_6$ octahedron is connected to $M2O_6$ octahedron with face-sharing. Hence, the structure of $Na_2M_2(PO_3)_3N$ can be considered as magnetically coupled dimer model. In this work, we discuss the correlation between the structure and magnetic properties of $Na_2M_2(PO_3)_3N$.

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Disorder in crystal structure of $Cu_2ZnSnSe_4$ investigated by powder neutron diffraction method

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$Cu_2ZnSnSe_4$ compound has attracted a considerable amount of attention as an alternative material for $Cu(In,Ga)Se_2$ absorber in thin film solar cells, because its constituents are nontoxic and abundant in the earth's crust. For $Cu_2ZnSnSe_4$, two main tetragonal structure types have been suggested from literature: the kesterite type structure and the stannite type structure. We have performed neutron diffraction analysis on $Cu_2ZnSnSe_4$. Compared to X-ray diffraction, neutron diffraction method provides more precise information on the coordination of constitutive atoms. $Cu_2ZnSnSe_4$ was found to show the kesterite type structure, but with disorder within the Cu-Zn layers at z=1/4 and 3/4. Such as Cu_{Zn} and Zn_{Cu} anti-site defects depends on the sample growth conditions. We found that band gap energy of $Cu_2ZnSnSe_4$ correlates with the degree of order in the Cu-Zn layers.

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Phase transformation mechanism from GdPO4?H2O nanorods to GdPO4 nanoparticle and their multi-funtionalities - optical and magnetic properites

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GdPO4·H2O nanorods with hexagonal phase were synthesized by simple co-precipitation method at relatively low temperature and phase transformation from hexagonal to monoclinic occurred after firing at high temperature. Accordingly, the shape of nanocrystal was also altered from nanorods to nanoparticle. It was revealed that as-prepared GdPO4·H2O nanorods with hexagonal structure were transformed to GdPO4 nanoparticles with monoclinic phase at around 800 C due to the release of zeolitially bound water molecules, which were incorporated in hexagonal crystal lattice. Detailed transformation mechanism was systemically investigated by using XRD, SEM, EDS and TG-DTA in order to check crystallographic phase transformation, morphology transformation, and thermal behavior change. Interestingly, after GdPO4·H2O nanorods transformed to GdPO4 nanoparticle, latter one possessed both intense host lattice UV emission at 315 nm originated from f-f transition of Gd3+ and magnetic property due to presence of f7 electrons from Gd3+. Herein, we presented the multifunctional GdPO4 nanoparticle with optical and magnetic properties and change of multifunctionalities before and after calcination of as-prepared sample. Synthesized GdPO4 nanoparticles with luminescence and magnetic property could be potentially used as MR imaging contrast agent.

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Development of quantitative structure-property relationships(QSPRs) for prediction of impact sensitivity of high energetic density materials(HEDMs)

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An high energetic denisty materials(HEDMs) is a reactive substance that contains a great amount of potential energy. HEDMs, such as military purposes and rocket propellants are used in a variety of fields. In particular, impact sensitivity, denoted as H50%, expresses the sensitivity of materials to a mechanical impact. It is experimentally evaluated by determining the height at which a weight of a defined mass leads to a reaction when falling on a material sample, with a 50% level of probability.Quantitative structure-properties relationship(QSPR) provides a promising way for prediction of HEDMs impact sensitivity. A comparative analysis of multiple linear regression(MLR) and support vector machine(SVM) have been appled to obtain satisfactory QSPR model of impact sensitivity. Forward selection combined with bootstrap-validation procedure was used to select best subset descriptors. The stability and predictive power of these models were further validated by bootstrap-validation and external validation.

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Polymer Sphere directly converted to Mesoporous Graphene ball

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We report a unique and direct route to fabricate a hierarchical graphitic carbon sphere via chemical vapor deposition (CVD) techniques. The synthesis and functionalization of polymer sphere is by emulsion polymerization. The utilization of functionalized polymer sphere is due to the ability to form a homogeneous dispersion with the metal ions derived from the electrostatic interaction between strongly negatively charged groups of polymer sphere and metal ions (M+) in the aqueous solution. Pyrolysis of polymer sphere/metal ions under an argon environment, leads to the creation of hierarchical structure and the reduction process of metal ions. This material has shown great performance as a supercapacitor.

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Photocatalytic Degradation Behaviors of Nitrogen-doped TiO_2

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인하대학교 화학과

In this work, nitrogen-doped TiO_2 nanoparticles (N/TiO_2) have been successfully prepared using tetraisopropyl orthotitanate as a Ti source and urea as a nitrogen source. The surface morphology of N/TiO_2 was examined by scanning electron microscopy (SEM). The structural properties of N/TiO_2 were examined by X-ray diffraction (XRD). The surface properties of the N/TiO_2 were characterized by X-ray photoelectron spectroscopy (XPS). The textural properties of N/TiO_2 were investigated by N_2/77K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. The photocatalytic activities of N/TiO_2 were tested using methylene blue (MB) solution under UV and visible light irradiation. From the result, it was apparent that photocatalytic activities of N/TiO_2 are higher than non-treated TiO_2 due to a wider adsorption wavelength of N/TiO_2.

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Preparation and Characterization of TiO_2 Nanotubes for Adsorption Behaviors of Organic Dye

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In this work, TiO_2 nanotubes were synthesized by a hydrothermal reaction with P25 in an alkaline solution. The adsorption behaviors of methylene blue were studied. The surface morphology of TiO_2 nanotubes was examined by scanning electron microscopy (SEM). The structural properties of TiO_2 nanotubes were examined by X-ray diffraction (XRD). The surface properties of the TiO_2 nanotubes were characterized by X-ray photoelectron spectroscopy (XPS). The specific surface area of TiO_2 nanotubes was investigated by N_2/77K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. From the results, it was found that the adsorption behaviors of methylene blue were strongly influenced by the specific surface area of TiO_2 nanotubes.

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Computational approach for predicting heat of formation by QSPR(Quantitative Structure-Property relationship) modeling

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One of the semi-empirical prediction to the HOF(Heat of formation, ΔHf°) of HEDMs(High Energetic Density Materials) from molecular structure is the QSPR(Quantitative Structure-Property Relationship) method. Generally, HEDMs should have high performance related to HOF, density, oxygen balance, and so on. The QSPR method for designing HEDM are not only simple but also more potentially faster than quantum chemical approach. In this study, we tried to make QSPR models for predicting HOF of HEDMs. We collected HOFs of gas-state energetic material data from ICT database. The HOF of HEDMs is calculated on the basis of functional descriptors defined from specific atom and bond types groups and the other simple descriptors. Linear and non-linear method are applied to develop the best subset equations. These descriptors reflected the chemical environment, such as chemical interactions or explosive properties.

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Controlling the aspect ratio of lead selenide nanorods

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Lead selenide nanocrystal quantum dots (PbSe NQDs) have received considerable attention because of several characteristics: PbSe has narrow bulk band gap (0.26 eV), large exciton Bohr radius (46 nm), and tunability over infra-red region in absorption. Multiple exciton generation (MEG) has been shown to be possible in PbSe NQDs. Advantages exist in PbSe nanorods (PbSe NRs) shaped crystals for improved MEG efficiencies *via* reduced Auger recombination. Also, improvement in electrical performance is expected based on better alignments. However, monodispersed rod conformation of small aspect ratio is hard in colloidal system. Until now, structure of PbSe NRs showed a low uniformity.In this work, we synthesized highly uniform PbSe NRs by controlling reaction parameters, such as ligand concentration, injection temperature, growth temperature/time and precursor concentration. Precise control over different aspect ratio was obtained. The PbSe NRs were characterized by high-resolution transmission electron microscopy (HR-TEM) and absorption spectroscopy.

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Ligand exchange of lead sulfide nanocrystal quantum dots using boron triiodide

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Nanocrystal quantum dots (NQDs) has been drawn much attention for optoelectronic device applications because of their confinement-based optical and electrical properties. Among the NQDs, the lead chalcogenides are highly attractive materials owing to their large exciton Bohr radius (46 nm for PbSe, 23 nm for PbS) and possible use in solar cell. To use lead chalcogenides in solar cell device, long chain ligands upon synthesis have to be changed to shorter ligands. Several approaches in obtaining ligand-exchanged NQDs for optoelec-tronic device have been reported previously.In this work, we prepared BI3 capped PbS NQDs from oleate passivated PbS NQDs. BI3 passivated PbS NQDs were characterized using optical measurement, ultra violet absorption spectra (UV) and Fourier-transform infrared spectroscopy (FTIR). Additionally, the surface charges and corresponding conductivities were investigated with zeta potential measurement (ELS-Z). Finally, we fabricated QD array field effect transistor to study the charge transport characteristics.

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Synthesis of 3D-Graphene Nano-structure for Supercapacitor via Chemical Vapor Deposition(CVD)

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We demonstrate simple way to synthesize a 3D-Graphene. Base on Fe-C phase diagram, we synthesize 3D-Graphene by a chemical vapor deposition (CVD) technique using FeCl3/PVA(carbon source). We confirmed the quality of 3D-Graphene by Raman spectrum, SEM, TEM. And then we have fabricated 3D-Graphene based electrochemical double-layer capacitors (EDLC). EDLC using 3D-Graphene have superior supercapacitor performance with a specific capacitance greater than 200 F/g and 90% retention after 1000 cycles due to its outstanding conductivity and large surface area.

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Hexagonal pyramid manganese-doped ZnO nanoparticles using controlled decomposition rate of metal precursors

배두리 이계행*

한국기초과학지원연구원

We propose the solvothermal synthesis and characterization of Mn^{2+} doped ZnO nanostructures and their formation mechanism. The Mn^{2+} doped ZnO particles have various shapes from quasi-spheres to hexagonal pyramids and irregular shapes. It is possible to dope Mn^{2+} ions up to 11% into ZnO lattices, and this is the highest amount of $Zn_{1-x}Mn_xO$ nanocrystals reported to date. The XRD, EDX, and EPR data indicate the successful incorporation of Mn^{2+} into the tetrahedral site in the host ZnO. The UV/vis spectra were obtained in order to examine degree of the interaction between the metal complex and surfactant, which is significantly related to the decomposition rate of the metal precursors. Based on the UV/vis results, we discovered that the decomposition rate of the metal precursors is a critical factor in controlling introduction of a dopant into a host lattice: it is the first time that this has been reported. In addition to the Mn^{2+} doping into the ZnO material, this proposed synthetic system allows for the incorporation of Fe^{2+} and Co^{2+} ions into host ZnO lattices.

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Effects of Oxyfluorination on the Adhesion Forces between Carbon Fibers and Epoxy Resins

배경민 박수진*

인하대학교 화학과

In this study, the influence of oxyfluorinated conditions on the interfacial shear strength (IFSS) of carbon fibers/epoxy composites was investigated. A single fiber pull-out test was performed to investigate the basic characteristics of the single carbon fiber/epoxy resins interface. Based on Greszczuk's geometrical model, the debonding force for pull-out of the fiber from the resins was discussed. As a result, the IFSS of the carbon fiber/epoxy resins composites was enhanced by oxyfluorination. It was that the oxyfluorination produced the functional groups on carbon fiber surface which caused increasing the adhesion forces between carbon fiber and epoxy resins.

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Influence of Hydroxyl Groups on Elemental Mercury Adsorption Behaviors of Nanoporous Carbons

배경민 박수진*

인하대학교 화학과

In this work, a series of nanoporous carbon was synthesized by self-assembly of polymeric carbon precursors and block copolymer template under acidic conditions. Resorcinol, phloroglucinol, and formaldehyde were used as carbon precursors, and poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) tri-block copolymer was employed as a soft template. The pore structures and total pore volumes of the nanoporous carbons were analyzed by reference to N_2/77 K adsorption isotherms. The porosity and elemental mercury adsorption of nanoporous carbons were increased. It could be concluded that elemental mercury adsorption ability of nanoporous depends on the textural properties.

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One-pot synthesis of superparamagnetic nanoblackberries using bioligands.

김봉준

연세대학교 일반대학원 화공생명공학과

Novel properties and potential applications have been emerged from monodisperse nanomaterials. Thus, the artificial synthesis of nanoparticleshas attracted great interest. Especially, magnetic nanoparticles have become important area of research because of the potential applications such as electronic devices, information storage, magnetic resonance imaging, and drug-delivery technology. Most of these approaches were focused on the synthesis of single nanoparticles. However, recent efforts have shifted to secondary structure manipulation to upgrade the properties of individual nanoparticles based on interactions between their subunits.Herein we report a novel one-pot synthetic method for the fabrication of superparamagnetic nanoblackberries (SPNBs). SPNBs are composed of assembled individual magnetic nanoparticles (MNPs) and coated with L-lysine amino acid. SPNBs were synthesized by thermal decomposition method using controlled reduction reaction between iron(III) acetylacetonate (Fe(acac)3) and diethylene glycol (DEG). L-lysine assisted the DEG mediated reduction of Fe(acac)3 to Fe3O4 and clustering of individual MNPs to SPNBs. The size, crystalline structure, and magnetic properties of the SPNBs were tunable by controlling the amount of L-lysine and reaction time. Monodisperse and single-crystalline structure of SPNBs were characterized by TEM and XRD. Superparamagnetic properties of SPNBs were investigated with a vibrating sample magnetometer. As a proof of our concept, we modified the SPNBs surface with dextran and applied to T2 contrast agent for MRI. Dextran coated SPNBs showed higher sensitivity than individual MNPs with no cytotoxicity. From this novel strategy, advanced designs and development of magnetic nanomaterials will be possible.

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Ultra-clean Transfer of Graphene on Various Substrates using Self-adhesive Films

김상진

서울대학교 화학부

As graphene is known for its outstanding mechanical, chemical and physical properties, people have endeavored to obtain high-quality graphene using ME, CE and CVD methods. Nevertheless, it has been a great challenge for researchers to transfer graphene to desired substrates without any impurities or defects. Here, we transferred graphene to various substrates including mica, BN and PET using self-adhesive film. Note that thermal or mechanical stress was not introduced during the process. Through the analyses of Raman, AFM and SEM data, we could confirm that self-adhesive film was indeed effective in transferring graphene to substrates without much residue. Moreover, electronic property analysis showed that the graphene transferred using self-adhesive film showed higher mobility than those transferred using PMMA or TRT

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The Surface Modification of Magnetite (Fe_3O_4) Nanoparticles by Silica (SiO_2) and Polyethyleneglycol (PEG) for Intracellular Uptake

이동헌 정 현*

동국대학교 화학과

Magnetic nanoparticles (MNPs) have been developed for a wide range of biomedical applications, such as magnetic resonance imaging (MRI) contrast-enhancement agents, drug delivery carriers and biosensors. However, most of synthetic routes for MNPs give to unsuitable for practical using due to their poor dispersibility in aqueous media, which is derived from their hydrophobic nature limited by preparing process. Therefore, surface modification is necessary to make them water-dispersible and to enhance their intracellular uptake efficiency. In this study, oleate and oleylamine capped superparamagnetic magnetite (Fe_3O_4) nanoparticles were synthesized by the thermal decomposition method as a core material. The resulting these MNPs were then coated with silica (SiO_2) and polyethyleneglycol (PEG) derivatized phospholipid ligands to endow them with biocompatibility. The obtained products were characterized by measurements of X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HR-TEM), Fourier transform infrared spectroscopy (FT-IR), and dynamic light scattering (DLS). Also, these surface modified MNPs were treated in bone marrow mesenchymal stem cells (BM-MSCs) and the cytotoxicity of them was measured by MTT assay (cell viability test). After that, these surface modified MNPs were measured Fe concentrations within cells by inductively coupled plasma-atomic emission spectrometry (ICP-AES) analysis for comparison of their uptake efficiency in cell lines depending upon the nature of coated materials and surface property.

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Physico-chemical dimension control of manganese oxide by top-down approach

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We successfully control dimension and phase of manganese oxide by physico-chemical top-down method. The pristine layered $K_{0.5}MnO_2$ was prepared byconventional solid state reaction of K_2CO_3 and Mn_2O_3 at 800 ℃. Unilamellarmanganese dioxide (MnO_2) nanosheets (two-dimensional) were obtained byintercalation and exfoliation reaction of the protonic manganese dioxide withtetrabutylammonium (TBA) cation. Because the suitable amount content of protonand organic material have key role in this physico-chemical top-down method,well-dispersed MnO_2 nanosheets were adjusted to pH 6 by addition of 1M HCl andremoved excess TBA cation by washing. The phase transformation of layered MnO_2nanosheets to Mn_3O_4 nanocrystals was successfully carried out by heat-treatmenteven at 150 ℃. And dimension of obtained particles was controlled as nanorods(one-dimensional) or nanoparticles (zero-dimensional) depending upon applied heattemperature (from 150 ℃ to 300 ℃). These nanocrystals have higher capacitanceproperties than that of the reference bulk Mn_3O_4 (Sigma Aldrich) powder dueto their nano-size effect. Physicochemical characterization and transformationmechanism study were performed by using X-ray diffraction (XRD) and X-rayabsorption spectroscopy (XAS). Dimensions of Mn_3O_4 nanocrystals were confirmedby high-resolution transmission electron microscopy (HR-TEM). The componentand organic content of the sample were measured by Fourier transform infrared(FT-IR) spectroscopy, elemental analysis (EA) and thermal analysis, includingthermogravimetry (TG) and differential thermal analysis (DTA). The capacitanceproperties of Mn_3O_4 nanocrystals investigated in 1M Na_2SO_4electrolyte showedmaximum capacitance of 160 F/g at scan rate 2 mV/s.

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Synthesis and characterization of silica-coated gold nanorods (GNR@SiO_2) core-shell structure for phototherapeutic application

안지아 정 현*

동국대학교 화학과

Core-shell nanoparticles have received tremendous attention due to their extensive electronic, catalytic, optical and phototherapeutic application. Gold nanostructures are mainly used as a core because of their unique optical properties called surface plasmon resonance (SPR). However, gold nanostructures have an insufficient structural and optical stabilities in aqueous media. Therefore surface treatment is unavoidable to preserve an initial structural and optical properties. In this research, CTAB ($(C_{16}H_{33})N(CH_3)_3Br$, cetyltrimethylammonium bromide, hexadecyltrimethylammonium bromide) -capped gold nanorods (GNRs) were simply coated with silica by an improved St?ber method. The UV/Vis spectroscopy and TEM imaging were used to characterize the morphology and the optical properties of GNRs or silica coated gold nanorods (GNR@SiO_2). The formation of Si-O-Si linkages was attested by IR spectroscopy. The thermogravimetric analysis (TGA) confirms contents of GNR@SiO_2.

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Fabrication of fluorescent $[Eu(Phen)_2]^{3+}$-laponite polymer nanocomposite with superhydrophobic surface

김아란 정 현*

동국대학교 화학과

Fluorescent nanohybrid materials, europium(III) complex ($[EuCl_2(Phen)_2(H_2O)_2]Cl \cdot H_2O$) intercalated hectorite clay (laponite XLG), were obtained through ion exchange reaction of interlayer sodium cation with europium complex ion. The intercalated complex maintains a characteristic red $^5D_0$-$^7F_2$ emission at wavelength 617 nm, which is comparable to the free complex. To increasing the processing ability such as adhesion, flexibility and hydrophobicity of fluorescent clay nanohybrid, the obtained particle is coated with polypropylene polymer (M.W. = 250,000). Structural and morphological characterizations were done using powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM). The component and thermal stability of the product were measured by Fourier transform infrared (FT-IR) spectroscopy, thermal analysis (TG-DTA), elemental analysis (CHN/ICP-AES). Optical and hydrophobicity of the obtained nano-composite were studied with UV-vis and fluorescence (PL) spectroscopies along with water contact angle measurement.

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Study on the effect of gold nanoparticle in liquid-crystalline blue phases

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동국대학교 화학과

Cholesteric blue phases exhibit unique properties for applications as a display or sensor. However, in only single component systems, they show very narrow temperature range between the isotropic and the chiral nematic phase. This behavior significantly hinders their applications. In order to widening of the temperature range of blue phase, we introduce surface modified gold nanoparticles with thiol or ammonium ions in blue phase of liquid crystal (mixture of 4-cyano-4’ pentylbiphenyl, JC-1041XX and 7.5 wt% of chiral dopant). The monodispersed and nonaggreated pristine gold nanoparticle can be easily obtained by ‘Brust’ two-phase method from aqueous solution of hydrogen tetrachloroaurate in the presence of tetraoctylammonium bromide (TOAB). After reduction of gold ions, surface of gold nanoparticle further functionalized by ligand exchange reaction with 4’-(10-mercaptodecyloxy)biphenyl-4-carbonitrile (HS10OCB). These multi-component liquid crystal mixtures shows enhanced thermal stability due to addition of gold nanoparticle in the lattice disclinations of cholesteric blue phases.

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Graphene Oxide-Coated Polymer Sulfur Materials for Lithium Sulfur Batteries

문준희

서울대학교 화학과

Sulfur has a high specific capacity of 1672 mAh/g as one of the promising lithium secondary battery cathode materials than traditional metal oxides/phosphates cathodes. However, it has been faced with the rapid capacity fading due to the dissolution of polysulfides and the precipitation of lithium polysulfides. To make up for the weak points in lithium sulfur batteries, many researchers have studied various methods of overcoming these problems, controlling of carbon coating and electrolyte. In this study, the graphene oxide-coated polymer sulfur composites have an important role in accommodating volume expansion of the coated sulfur particles during discharge, trapping soluble polysulfide intermediates, and rendering the sulfur particles electrically conducting. The resulting these materials showed high specific capacity and good cycle ability up to ~ 700 mAh/g over more than 100 cycles. Moreover, the introduction of LiNO3 additive seems to have improved the coulombic efficiency over 95% at 0.2 C.

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Ultra-Thin Gas Barrier using Graphene Films

최경준

서울대학교 화학부

Monolayer graphene is not permeable to any gas including helium.[1] By developing chemical vapor deposition(CVD), we can make large scale graphene about 30inch. Graphene has many exotic properties such as electrical, chemical and mechanical characteristics [2]. Among them, the lattice constant of graphene is smaller than water vapor or oxygen molecule. Here, we demonstrate the performance of gas barrier using few layer graphene, only ~10nm thickness. We measure the water vapor transmittance rate (WVTR) of graphene which is about 0.48g/m2/day. Therefore, graphene, flexibility, transparency and barrier properties, is suitable candidate for a variety packing applications.

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Stimulation of Cardiomyogenic Gene Expression of Mesenchymal Stem Cells Cultured on Graphene

박수범

서울대학교 화학부

Cardiomyogenic gene expressions of bone marrow-derived mesenchymal stem cells (MSCs) are enhanced when MSCs are cultured on graphene as compared to MSCs cultured on coverslips. Diverse substrates have been utilized for MSCs culture to induce their commitments toward specific tissue lineages. Recently, graphene has been suggested as a promising substrate for stem cell culture. Graphene has potential to promote specific stem cell differentiation. Herein, we showed the specifically activated cell signaling pathways that can enhance cardiomyogenic differentiation of MSCs when the cells were grown on graphene. The cell signaling pathways may have affected actin filament recruitment, cytoskeletal dynamics, and cardiomyogenic gene expression in MSCs. As a consequence, extracellular matrix (ECM) gene and cardiomyogenic lineage specific protein expression of MSCs cultured on graphene were significantly enhanced as compared to those of MSCs cultured on coverslips. Our results demonstrate the potential of graphene for stem cell research.

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양성자 빔 조사를 통한 Pt나노입자의 합성

이윤지 송재희*

순천대학교 화학과

이 실험에서는 용액 상태인 백금이온을 양성자 빔 조사를 통해 백금 나노입자로 합성하였다. 계면활성제로는 CTAB 와 SDS 를 가지고 사용하였다. 계면활성제와 백금이온의 몰비를 바꾸어 가며, 그리고 IPA 을 첨가하면서 다양한 빔 전류와 조사시간을 통해 백금나노입자의 크기와 모양을 조절하였다. 합성된 Pt 나노입자는 UV-VIS 와 TEM 분석을 통해 확인되었다.

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A Hybrid Ink of Binary Nanoparticles and Precursor Solution for CIGS Solar Cell Absorber and its Photovoltaic Performance

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한국에너지기술연구원 태양에너지연구단 [1]한국과학기술원(KAIST) 화학과

Cu(In,Ga)Se2 (CIGS) chalcopyrites have known as one of the most promising materials in solar cell research and production area due to their high light absorption coefficient (~10^5 cm^-1) and a tunable direct band gap (1.0~2.4 eV) by changing the In/Ga and Se/S ratio. Owing to their original characters, thin layers (1~2 μm) are enough to be used as an absorber in CIGS solar cell compared to well-known 100~300 μm thickness of crystalline Si solar cell on the market. Until now, electro-photonic stable CIGS solar cell has already reported around 20 % conversion efficiency with high vacuum process. In this study, a newly developed hybrid ink of binary nanoparticles and precursor solution was prepared to form a Cu(InGa)Se2 (CIGS) thin film. Deposition using hybrid ink offers advantages including the provision of stress-relief and crack-deflection centers by pure material based nanoparticles and effective binding with the nanoparticles by precursor solutions without other organic binders. Here, we demonstrate several types of binary nanoparticles to make different hybrid inks. A precursor solution was prepared by using a non-toxic chelating agent to disperse the In component stably. Synthesized absorber thin films were characterized through X-ray diffraction (XRD), Energy Dispersive Spectroscopy (EDS), and their photovoltaic performances were analyzed by I-V and external quantum efficiency (EQE) measurements.

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Synthesis and Structure of a New Mixed-metal Phosphate, $V_{0.2}Nb_{1.8}(PO_4)_3$

선주빈

아주대학교 에너지시스템학부/응용화학과

The new quandary phosphate, $V_{0.2}Nb_{1.8}(PO_4)_3$ has been synthesized with the reactive halide flux and structurally characterized by single-crystal X-ray diffraction techniques. $V_{0.2}Nb_{1.8}(PO_4)_3$ crystallizes in the space group R3 ?c of the rhombohedral system with twelve formula unit in a cell of dimensions, a=8.7028(8) Å, c=22.1484(20) Å, and V= 1452.76(2) $Å^3$. The host structure is built up by $[MO_6]$ octahedra and $[PO_4]$ tetrahedra. In this compound, these polyhedra are connected by sharing oxygen atoms to form a three-dimensinal framework. The classical charge balance of the title compound can be represented as $[V^{4+}]_{0.2}[Nb^{5+}]_{1.8}[PO_4^{3-}]_3$.

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The new Palladium Tetrathiophosphate of β-$Pd_3P_2S_8$

임윤미

아주대학교 화학과

In the middle of searching for new alkali metal thiophosphate using the reactive halide-flux technique, we have found new Palladium Tetrathiophosphate. The crystal structure of the compound was determined by single-crystal X-ray diffraction. The $Pd_3P_2S_8$ cluster is composed of square planar [PdS_4] and tetrahedral [PS_4]. Six [PdS_4] is bonded with [PdS_4] sharing four corners. One of [PS_4] is linked with three [PdS_4] by sharing three edges. And then one cluster has almost tetraheral shape on the whole. While products previously synthesized the reactive halide-flux technique consist of cluster, chain, layer and framework separated by alkali metal, these clusters have weak packing by only molecular interaction. But this compound has a different structure found in the previously reported α-$Pd_3P_2S_8$. While α-structure crystal has hard hexagonal plate of dark wine color, β-structure crystal has soft plate of bright red color. The classical charge balance of the compound can be represented as $[Pd^{2+}]_3[P^{5+}]_2\ [S^{2-}]_8$.

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The Synthesis and Characterization of the New Thiogermanates, $Cs_2CuGe_3S_8$

윤우진

아주대학교 에너지시스템학부 응용화학과

A new two-dimensional thiogermanate, $Cs_2CuGe_3S_8$has been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. The title compound crystallizes in the space group *Pnma* of the orthorhombic system with four formula units in a cell dimensions, a=16.89000(6) ?, b=7.2387(2) ?, c=12.4334(4) ?, and V=1520.13(1) ?^{3}. Cu and Ge atoms are surrounded by four sulfur atoms in a tetrahedral fashion. One of the Ge sites are partially replaced by Cu. These tetrahedra are connected through sharing corners along the a-axis, forming infinite chains which are linked together with GeS_4 tetrahedra along the c-axis. The Cs^+ ions stay between the layers. The classical charge valence of the title compound can be described as $[Cs^+]_2[Cu^{2+}]\ [Ge^{4+}]_3[S^{2-}]_8$.

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Effect of Conformational Transition on Biodegradability in Electrospun Silk Nanofibrous Mat

김종욱 진종성*

한국기초과학지원연구원 부산센터

The biodegradable properties, is one of the most important parameters for the biomaterials applications, of silk fibroin (SF) are could control of diverse range of times depending on conditions of alcohol treatment. In this study, SF nanofibrous mat was fabricated by electrospun and teated with different alcohol mixtures for controlling secondary structure of SF. The various properties that morphological structure, conformational transition and etc. of SF mat, treated with various conditions was observed by SEM, FT-IR, TGA and NMR. And the observation of feasibility of biodegradability control was evaluated by enzymatic degradation method in vitro.This work was supported by the grant No. R0001026 from the Ministry of Knowledge and Economy and Busan Metropolitan City, Korea.

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The Synthesis, Structure and Solublization of the 1-D Alkali Metal Thiophosphates $APdPS_4$(A=K, Rb, Cs)

김필수

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In the middle of searching for new soluble inorganic polymers using the reactive halide-flux technique, we have found new various phases, $APdPS_4$ (A= alkali metals). The crystal structures of the compounds vary depending on the synthetic conditions. All of the compounds in this family adopt one-dimensional structures. Although square planar Pd and tetrahedral P atoms are common in the structure two different linear chains, $^{1}_{\infty}[PdPS_4]$ chains are found. In these phases, the one-dimensional $^{1}_{\infty}[PdPS_4]$ chains are separated by the A^+ ions. The classical charge balance of the compounds can be represented as $[A^+][Pd^{2+}]$ $[P^{5+}]$ $[S^{2-}]_4$. When exposed to polar solvent such as NMF and DMSO, $APdPS_4$ phases can be dissolved. Using UV-Vis and TEM, we show that some of these solutions contain individual $^{1}_{\infty}[PdPS_4]$ chain. UV-Vis spectrum of the solution along with the solid state reflectance spectrum will be presented. We expect to synthesize new compound by using an ion-exchange reaction.

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Efficient decomposition of organic compounds with $FeWO_4/TiO_2$ heterojunction under visible light irradiation

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인하대학교 화학과

Dark brown color $FeWO_4$ nanoparticles of average size 50-70 nm was prepared by hydrothermal method. $FeWO_4$ showed a profound absorption over the entire visible range which is the promising criteria for a visible light sensitizer. A heterojunction between $FeWO_4$ and TiO_2 was made by sol-gel method. This heterojunction shows notably high visible light photocatalytic activity in decomposing Isopropanol (IP) in gas phase. It was found that the hetero composite shows greater CO_2 evolution than N-doped TiO_2 which is a well known visible light Photocatalyst. The valence band (VB) position of $FeWO_4$ is lower than that of TiO_2. The unusually high photocatalytic efficiency of the $FeWO_4/TiO_2$ composite was therefore deduced to be caused by hole transfer from VB of $FeWO_4$ to VB of TiO_2.

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Narrowing the emission spectrum of a green pc-LEDs with a band-pass filter

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In this study, we characterized the highly efficient and pure green monochromatic phosphor-converted light-emitting diode (pc-LED) capped with a band-pass filter (BPF). The BPFs, which are combined both long-pass dichroic-filters (LPDFs) and short-pass dichoric-filters (SPDFs), narrow the emission spectrum by reflecting the bluish and reddish green spectrum. In this experiment, blue LED (445 nm) and a series of orthosilicate green phosphors were used for the fabrication of the various-color green monochromatic pc-LEDs. The BPF-capped green monochromatic pc-LEDs provide a high luminous efficacy (134 lm/W at 60 mA), and pure green color with 1931 Commission Internationale d'Eclairage (CIE; CIEx, CIEy) color coordinates (0.24, 0.66) owing to the narrowed emission spectrum.

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Synthesis and characterization of type I and quasi-type II CdSe/CdS quantum rods

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The type I and quasi-type II CdSe/CdS quantum rods (QRs) were prepared by a seed growth technique that preceded a two step method. These nanoparticles were easily synthesized by controlling core diameters with different injection temperatures and growth time. These showed a tendency wherein with increasing temperature and growth time the band gap decreased, which meant core size decreased. We compared the optical properties of type I CdSe/CdS QRs with quasi-type II QRs using decay time and row temperature PL. Structural information of QRs were observed by UV-vis spectroscopy, PL spectroscopy, X-ray diffraction (XRD) and transmission electron microscopy (TEM).

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Superhydrophobic/superhydrophilic ITO nanorods with self-cleaning and anti-fogging

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ITO nanorods were fabricated on glass substrate via radio frequency (RF)-magnetron sputtering deposition with changing the growth time. The ITO nanorods with different growth times have superhydrophilic property due to increase of high surface roughness. The superhydrophilic ITO nanorods can become superhydrophobic by coating their surfaces with perfluorodecyltrichlorosilane (PFS) under a liquid phase. In addition to superhydrophilic/phobic properties of ITO nanorods on glass substrate, anti-fogging and self-cleaning properties of ITO nanorods measured. In order to demonstrate superhydrophilicity/phobicity of ITO nanorods, static contact angles of ITO nanorods with different growth times were measured by a contact angle analyzer. The structural, morphological, and optical properties of ITO nanorods were investigated by performing scanning electron microscopy (SEM) and UV-Vis transmittance.

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Pore Structure and Size Controlled Nitrogen-Doped Mesoporous Carbon Thin Films with Electrochemical Properties.

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성균관대학교 나노과학기술학과 [1]성균관대학교 화학과

In our previous study, nitrogen-doped mesoporous carbon thin films (MCTFs) with worm-like structure were synthesized and their electrochemical properties were studied. Herein, we diversified structures of hard-templates, mesoporous silica thin films (MSTFs), by using different surfactants (F-127, F-68) and use of the varied ratio of surfactants to ethanol, TEOS, acid. Because the MCTFs were formed by replication method, pore structures and sizes of the MCTFs could be controlled. The MSTFs were characterized by small angle X-ray diffraction (XRD), and the MCTFs were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and elemental analyzer (EA, CHON). The capacitances of MCTFs were obtained by electrochemical measurement. As a result, we confirmed that the capacity properties depend on the pore structures and sizes of MCTFs.

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Fabrication of Au Nanoparticles use MSTF for Organic Photovoltaic Solar Cell.

권아현 권영욱*

성균관대학교 화학과

The Au nanoparticles and nanofilms with strong localized surface plasmon resonances (LSPRs) have attracted great interests in fields such as nanoscale photonics, biological sensing, surface-enhanced Raman scattering (SERS), photocatalytic and photoelectrochemical processes, and plasmonic absorption enhancement in solar cells. We have recently studied a relatively simple approach in fabricating uniform gold nanocparticle on mesoporous silica thin film by electrodeposition. The Au nanoparticles were characterized by SEM, TEM, XRD and UV-visible. The Au nanoparticles on indium tin oxide (ITO) glass substrates, the blend films PCBM doped with PTB7 and PEDOT:PSS on Au with ITO glass substrates, and we measured PEC performance. It obtained much better efficiency than commercial Au nanoparticle on ITO sample because of our sample without capping agent.

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Synthesis of Alkyl-substituted Thiophene derivates based on Anthracene for Organic Thin-Film Transistor.(OTFTs).

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경상대학교 자연과학대학 화학과 [1]경상대학교 화학과 [2]경상대학교 나노신소재공학부

We synthesized small molecules as OTFT material in Flexible display because its have much advantages. The advantages of easy manufacturing and processing make them suitable for selected commercial applications. Produced solution processibility OTFT device for printing process, both solution process ability and air stability of organic semiconductors can achieve low cost OTFTs. Our new candy shape molecules can tune the electronic properties of small fused anthracene by electron donating ability. We expect derivates alkyl-subsituted Thiophene is a good oxidation stability. Therefore, we expect this small molecules can high electrical properties and low cost material of Organic Thin-Film Transistor (OTFTs).

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Synthesis and characterization of Quantum dots into Silica beads for DNA sensor applications

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Bead-based assays have been increasingly used for detecting and screening toxic, biological molecules, cells, and pathogens. Compared to organic dyes, semiconductor quantum dots (QDs) have better properties such as broad absorption coupled to narrow tunable photoluminescent emissions and exceptional resistance to both photobleaching and chemical degradation. In this study, we have synthesized and characterized the silica microbeads incorporated with QDs for detecting target DNA with high sensitivity. Target DNA are analysed by the sandwich assay using microbeads surface-modified and linked to DNA probes. Based on fluorescence microscopic image analysis, the sub-picomolar concentration of target DNA can be detected using silica beads incorporated with QDs. Furthermore, optical properties and the sensitivity of the microbeads were characterized using transmission electron microscopy(TEM), scanning electron microscopy(SEM), UV-Vis, fluorescence microscopy and PL spectroscopy, respectively.

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Synthesis and Characterization of Eu(TTA)3Phen in a Poly(Ethylene Oxide) Matrix as a Fluorescent Probe for Detecting Traces of Water

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To realize flexible organic light emitting diodes, theses require the availability of robust, lightweight, portable and rollable function. One of them is the water vapor transmission rate (WVTR) which is limited to 10-6g/m2/day for flexible organic light emitting diodes. However, it is difficult to measure permeability as low as 10-6g/m2/day with current commercial testing methods like calcium test, mocon test etc. To address this need, a developed optochemical method which is extremely sensitive to oxygen or water shows potential. In this study, an Eu-complex is synthesized and characterized as a fluorescent probe for detecting traces of water molecules. The Eu-complex film dispersed in poly(ethylene oxide) has strong red fluorescence that is easily quenched by a trace of water. Based on the photoluminescence (PL) spectra, the detection limit of the film to water appears to be below 1.0x10-9 g/cc. This suggests that the Eu-complex film can be used as a film sensor to measure WVTRs below 10-6g/day/m2.

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Synthesis and Characterization of Polymerizable Chiral Dopant for Switchable Broadband IR-Reflector Based on Cholesteric LC

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콜레스테릭 액정(cholesteric liquid crystal CLC)은 네마틱 액정에 주기적인 나선구조를 유도하는 chiral 성분의 물질이 더해진 액정 혼합물로, 네마틱 액정이 꼬여서 돌아가는 나선구조의 회전방향과 액정의 방향자가 나선 축 방향으로 360°회전한 거리인 피치(pitch)에 따라 구분된다. CLC 의 나선 축 방향이 기판 표면에 수직으로 균일하게 배열된 planar 구조일 때, CLC 는 나선의 회전방향과 동일하며 피치에 상응하는 빛은 반사하고 나머지 빛들은 투과하게 된다. 피치를 다양하게 가지는 CLC 를 제조하면 반사되는 빛의 파장영역을 넓힐 수 있다. 적외선은 가시광선이나 자외선에 비해 강한 열 작용을 가지고 있는 것이 특징이며, 이 때문에 열선이라고도 한다. CLC 의 반사되는 빛의 파장영역이 적외선 전체영역이 되면 열 차단을 기대할 수 있다. 본 발표는 다양한 피치를 가지는 CLC 를 제조하기 위해 중합 가능한 Chiral dopant 를 합성하고 이를 사용한 CLC 박막을 제조하는 방법과 그 특성에 대해 보고한다.

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Incorporation of nicotinic acid into the interlayer of layered double hydroxide for controlled release

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이화여자대학교 화학.나노과학과

The nicotinic acid are a part of the vitamin B_3, which have a variety of pharmaceutical and dermatological functions such as effective skin whitening, anti-inflammatory and anti-anxiety properties. However, since high dose of vitamin B_3 in the body is considered to be a toxic drug, it is necessary to develop the delivery system with controlled release property. Therefore, we have incorporated nicotinic acid into layered double hydroxide (LDH) for the sustained release property. We could immobilize the nicotinic acid in the interlayer of Mg/Al-LDH by conventional co-precipitation reaction at pH 10 with varying the molar ratio of Mg/Al. According to the x-ray diffraction pattern, the basal spacing of nicotinic acid incorporated LDH was determined to be ~ 0.86 nm, indicating that nicotinate anions were incorporated into the interlayer with the structure of pyridium ring of nictontinate parallel to the ab plane of LDH. The content of nicotinic acid in LDH could be controlled in the range of 28 ~ 39 wt% with the layer charge density of LDH. The release profiles would be systematically discussed depending on the layer charge density.

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Photocatalytic activity of TiO_2-pillared titanniobate prepared from 6-aminocarproic acid intercalated titanoniobate

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Porous TiO_2-pillared titanoniobate with high photocatalytic activity on hydrogen evolution were synthesized from 6-aminocarproic acid intercalated titanoniobate. Since it is very difficult to directly incorporate the positively charged nanoparticles into the titanoniobate due to its high layer charge density, in order to incorporate TiO_2 nanoparticles into the interlayer of layered titanoniobate, at first, we have intercalated the 6-aminocarproic acid into layered titanoniobate, And then we could incorporate TiO_2 nanoparticles into the aminoacid-intercalated titanoniobate via ion-exchange reaction. According to x-ray diffraction analysis, the basal spacing was expanded to ~ 4.7 nm depending on reaction temperature and molar ratio of Ti/Nb, indicating that the titania nanoparticles were successfully intercalated into the layered titanoniobate. N_2 adsorption-desorption isotherm analysis showed that thus prepared titania intercalated titanoniobate had a high specific surface area with 150 ~ 270 m^2/g. Thus prepared titania pillared titanoniobate showed the high photocatalytic activity for hydrogen evolution from water under UV light irradiation compared to the pristine proton-type titanoniobate, which would be ascribed to its large surface area and the quantum size effect of pillared titania particle.

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Thermal Stability of Poly(Ethylene Vinyl Acetate) Nanocomposites Containing Organoclays

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이화여자대학교 화학.나노과학과

In order to improve thermal stability of poly(ethylene vinyl acetate) (EVA), we prepared various nanocomposites of EVA with organo-clay depending on the kind of organic modification, and the content of organo-clay and kind of host clay by solution blending method. However, intact clays are not compatible with the hydrophobic polymer matrix due to their hydrophilic property. Therefore we modified the surface of clays such as Kunipia F, fluorine mica (ME), and laponite to be hydrophobic by intercalating the long chain alkylammonium surfactant such as dimethyldistearyl ammonium (DMDSA+) and cetyltrimethylammonium (CTA+) with different structure, which were confirmed the expansion of basal spacing. We synthesized EVA/organo-clay nanocomposites by mixing the organoclays dispersed in toluene with EVA solution dissolved in toluene and evaporating the solvent. According to X-ray diffraction (XRD) analysis, the sharp peaks corresponding to the organoclay were diminished, indicating that organoclays in the EVA were predominantly exfoliated. Thermogravimetric analysis (TGA) show that EVA/CTA-clays nanocomposites have more improved thermal stability than EVA/DMDSA-clays. In case of EVA/CTA-ME, the decomposition temperature of EVA was proportionally improved by 44 K compared to pure EVA increasing the content of CTA-ME in EVA.

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High Conductive Single-Crystal Poly(3,4-ethylenedioxythiopene) Nanowires

조보람 성명모*

한양대학교 화학과

We develop high conductive single-crystal poly(3,4-ethylenedioxythiopene nanowires using liquid-bridge-mediated nanotransfer molding (LB-nTM) via vapor phase polymerization (VPP). LB-nTM method can simultaneously enable the synthesis, alignment and patterning of the nanowires from molecular ink solutions. Two- or three-dimensional complex structures of various single-crystal organic nanowires were directly fabricated over a large area using many types of molecular inks. VPP method is a versatile technique that can be used to obtain highly conducting coatings of conjugated polymer on both conducting and nonconducting substrates. The PEDOT nanowires by LB-nTM and VPP have confirmed single-crystalline from X-ray diffraction pattern and select-area diffraction patterns. Also, the PEDOT nanowries have tremendously high conductivity compared commercial PEDOT:PSS. We used the PEDOT nanowires as electrodes of field-effect transistors of 6,13-bis(triisopropyl-silylethynyl)pentacene (TIPS-PEN) nanowire.

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Fabrication of transparent electrodes with silver nanowires by using a direct printing process.

백장미 성명모*

한양대학교 화학과

We report the transparent electrodes fabricated by a direct printing process with silver nanowires. The silver inks were filled into the mold by wetting and dewetting process and the silver inks in mold were transferred onto poly(3,4-ethylenedioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS) conductive polymers. We investigated the formation of silver nanowire array by SEM and transmittance of the transparent silver nanowire based electrodes. We also measured the sheet resistivity of silver nanowire based electrodes to confirm the potential of our approach.

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Fabrication of Crossed Organic Single Crystal Nanowires Diode by Liquid-bridge-mediated Nanotransfer Molding Method

이기석 성명모

한양대학교 화학과

Recently, we developed a direct printing method named liquid bridge mediated nanotransfer molding(LB-nTM) for make well-aligned nanoscale structures. Furthermore, we can make multi-layering nanostructures using LB-nTM without other special skills. Using this method, we can produce organic single-crystal nanowires like 6,13-Bis(triisopropylsilylethynyl)pentacene(TIPS-PEN), fullerene(C60) and Poly(3-hexylthiophene)(P3HT). As a result, the heterojunction can be formed easily by the above-mentioned three kinds of organic materials. P-N heterojunction diodes are basic components of integrated circuits which require the hybridization of p- and n-type semiconducting materials. We implemented the procedure of cross multi-layer patterning of organic single crystal nanowires. TIPS-PEN/C60 nanowires crossed diode was working like rectifier. In addition, P3HT/C60 nanowire crossed diode current was increased by light.

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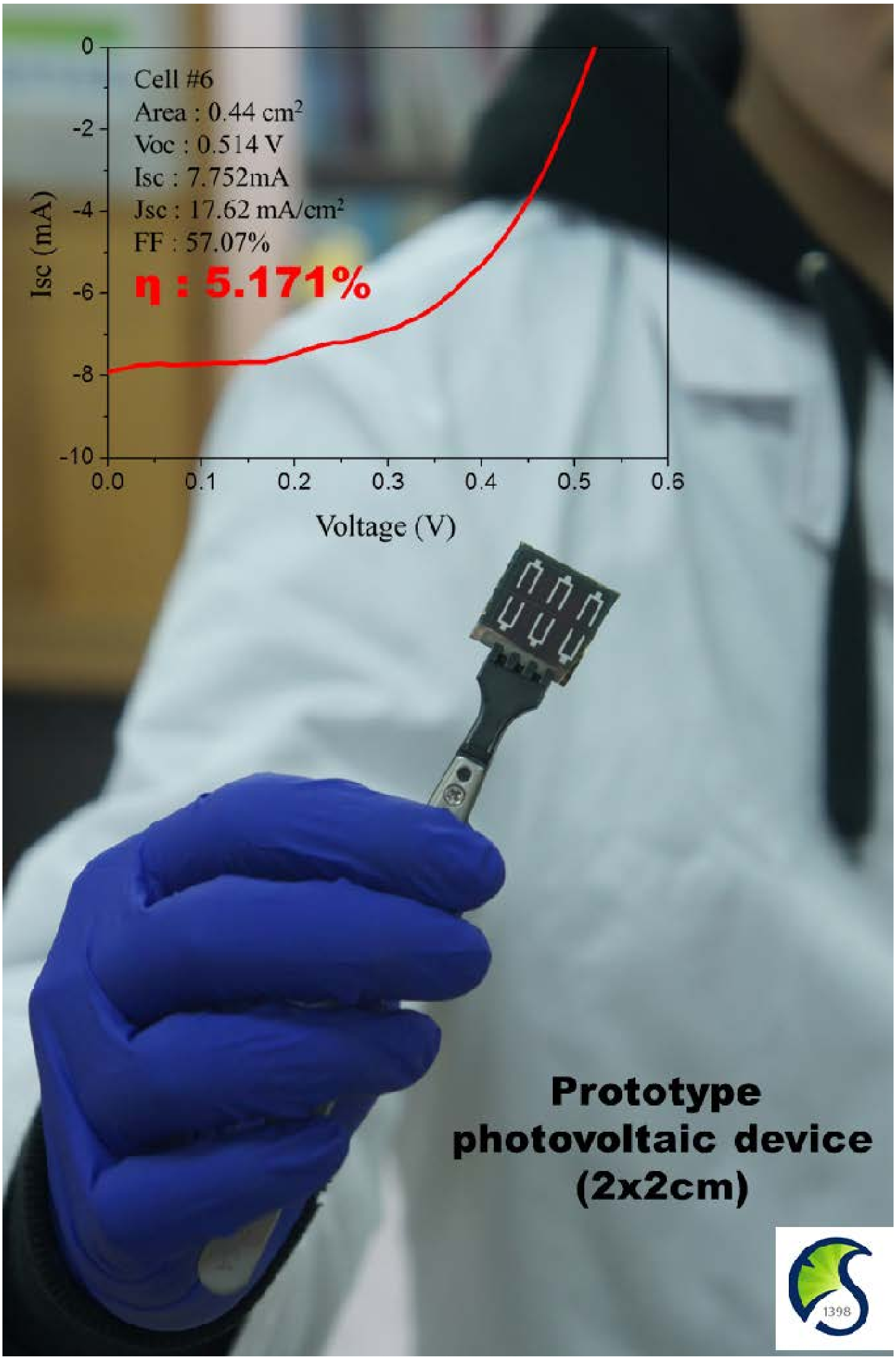
Structural and compositional analysis of Cu(In,Ga)Se_2 nanoparticles and their photovoltaic applications

차지현 정덕영*

성균관대학교 화학과

We synthesized Cu(In,Ga)Se_2(CIGSe) absorber layer for thin film photovoltaics by using nano-inks solution in which zinc-blend structure CIGSe nanoparticles were synthesized by sonochemical methods. Influence of reaction medium toward chemical composition and phase transformation by annealing process were investigated for synthesized nanoparticles as precursors of ink solution. The amount of amines in reaction medium play an important role in the sonochemical synthesis of CIGSe, especially the gallium contents of the products. The annealing process in inert atmosphere transformed the as-prepared nanoparticles into high-crystallinity chalcopyrite CIGSe without any other tetragonal structures, Cu-Au and Cu-Pt systems. Eventually, we could obtain the chalcopyrite structure CIGSe with adjusted In/Ga ratio and pure phase, as confirmed by X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray fluorescence (XRF), and Raman spectroscopy. The CIGSe thin absorber layer, formed on molybdenum coated soda-lime glass, was completed to pass through with spin coating process and annealing step. The photovoltaic devices yield 5.17% conversion efficiency under AM 1.5 illumination with the use of glass/Mo/CIGSe/CdS/i-ZnO/AZO/Ni:Al device structure.



Prototype photovoltaic device (2x2cm)

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Fluorescence origin of GQD and its optical, electrical properties

박명진

서울대학교 화학부

Graphene is composed of sp2 bonded carbon atoms densely arranged in 2D honeycomb lattice. As demonstrated from the fact that ambipolar electric field effect is valid even under ambient condition, graphene exhibits excellent mobility and conductivity. Such notable properties support graphene to become a great replacement for currently existing conducting materials. In addition, its flexibility and optical transparency have gained graphene much attention in the field of electronics. Given that graphene has zero band gap, however, its applications in optics and semiconductor have been hindered despite the outstanding properties. According to recent studies, 1D nanoribbon and 0D graphene quantum dot (GQD) could overcome such restriction because electron density is confined as the sizes of the materials decrease. These noble findings enabled SET (single electron transistor) to become feasible and it is highly possible that people could discover more in the field of optics based on these. Noticeably, industrially applied GO-based GQDs are environmentally harmless. Moreover, its well-dispersed character could possibly be the key to solve various deposition problems occurring upon OLED and OPV fabrications. When oxidized GQD is converted to reduced GQD through hydrothermal reduction process, graphene's electrical properties can be reacquired due to the increased number of sp2 domain sites. Here, we synthesized GO-based GQDs cleaved into small pieces and were able to determine the excitation site by observing anomalous PLE (photoluminescence excitation), correlated with hydrothermal reduction. After fabricating OPV from two different types of GQDs, we could figure out that Jsc and FF used in characteristic evaluation are indeed controllable.

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Interlayer structure study on amino acid intercalated layered double hydroxide depending on the structure of amino acid

박가영 양재훈 최진호*

이화여자대학교 화학.나노과학과

We have successfully prepared two different kinds of Amino Acid such as Phenylalanine (Phe) and Glutamic acid (Glu) into layered double hydroxide (LDH) *via* ion exchange reaction. At first, we synthesized Mg_2Al-(NO_3)-LDH at pH10 *via* coprecipitation. Since amino acids have different charge depending on the pH of the reaction solution, we carried out the ion-exchange reaction in the pH range of deprotonating the carboxylic acid group of amino acid, 7 ~ 10 for Phe and 7 ~ 11 for Glu. According to X-ray diffraction analysis, Phe is not intercalated into LDH at pH7, but Phe is successfully intercalated into LDH at pH 10, which is higher than pK_{a2} of Phe (9.32) and the basal spacing was expanded to 1.8 nm compared to that of the pristine LDH (0.88 nm), indicating that Phe lattice with bilayer structure. On the other hand, Glu is intercalated into LDH at the range of pH 7 ~ 11, and the basal spacing is ~0.95 nm regardless of pH, since dicarboxylic acid group in Glu were completely deprotonated above pH 6 to be negatively charged. The difference of basal spacing between Phe-LDH and Glu-LDH nanohybrid was caused by the different interlayer structure of amino acid through the different total net charge,indicating that Phe is incorporated into LDH with paraffin-type interdigited bi-layer structure, but Glu is intercalated into LDH with parallel mono layer structure to the ab plane of LDH.

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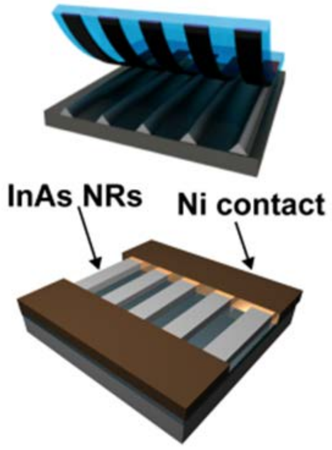
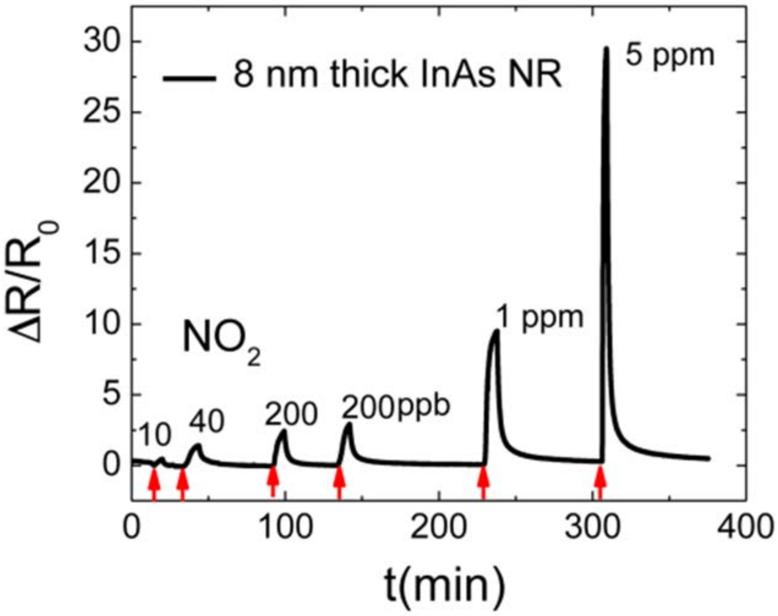
Ultra-sensitive NO_2 Gas Sensor using Ultrathin InAs Nanoribbons

__이민형__

경희대학교 응용화학과

This work presents the fabrication and characterization of NO_2 gas sensors by using ultrathin 2-D semiconductor nanoribbon (NR) membranes. The sensor employs the 8 nm-thick InAs NRs, transferred on a Si/SiO_2 substrate, as a sensing element. Using a conventional CMOS fabrication process, the sensor devices were fabricated. The sensor demonstrated the responses down to parts-per-billion (ppb) level at room temperature and the predominant reaction to NO_2 exposures. Furthermore, a 4-fold higher sensor response was observed in the 8 nm-thick InAs NR sensor compared with the one with the 18 nm-thick InAs NRs, indicating the improved size effects by scaling down to quantization limits.





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Alpha lipoic acid / layered metal hydroxide nanohybrids with controlled release property

이지희 김가인 양재훈 최진호*

이화여자대학교 화학.나노과학과

Alpha lipoic acid (ALA) is powerful antioxidant that can directly scavenge free radicals and protect cell from oxidative damage. However, ALA is photochemically unstable due to the distorted dithiolane ring which absorbs light around 330 nm. In order to solve this problem, we attempted to incorporate ALA into the interlayer of zinc based layered metal hydroxies with different layer charge density via co-precipitation and ion-exchange reaction. According to x-ray diffraction analysis, the basal spacings of the nanohybrids were expanded to ~ 2.5 nm for ZBS and ~ 2.2 nm for LDHs, which is similar regardless of synthetic methods (coprecipitation and ion-exchange). Infrared spectra show that ALA molecules in anionic form were incorporated into the interlayer space of ZBS and LDH through electrostatic interaction without any structural change. According to the thermogravimetric analysis, the thermal stability of nanohybrid was fairly improved compared to the ALA itself. UV-vis spectra of intact ALA and ALA obtained from the nanohybrids show similar shape, indicating that ALA is safely encapsulated in to the layered metal hydroxides. According to the UV-vis spectroscopic analysis and HPLC analysis, the content of ALA in nanohybrids was determined to be 28 ~ 46 wt% depending on the layer charge density of host layers. The release property and stability would be systematically discussed depending on the charge density of the inorganic host layer.

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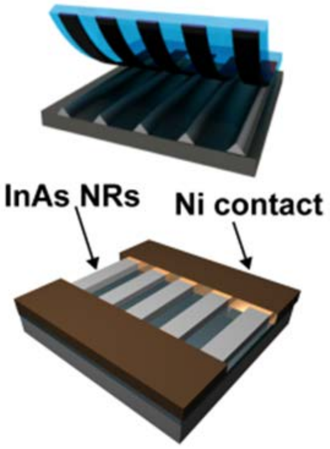
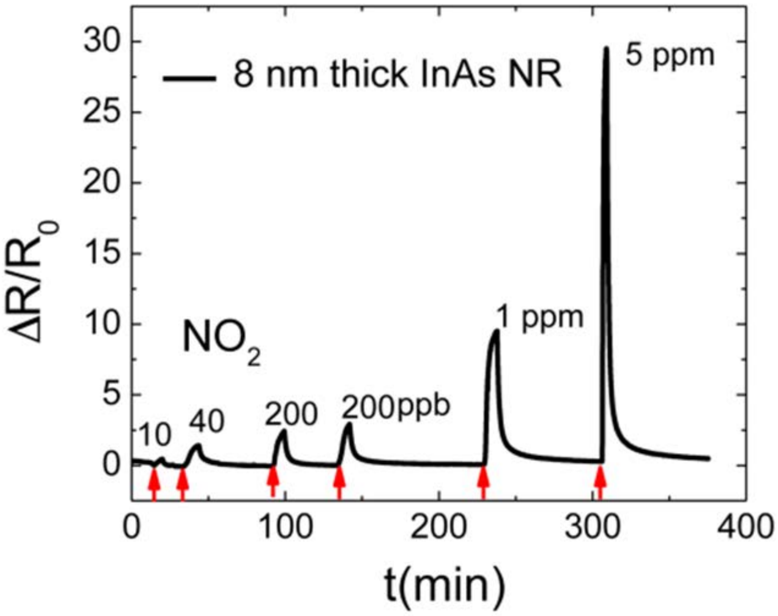
Ultra-sensitive NO_2 Gas Sensor using Ultrathin InAs Nanoribbons

<u>고우리</u> 이정은 이현주 전충섭 이민형*

경희대학교 응용화학과

This work presents the fabrication and characterization of NO_2 gas sensors by using ultrathin 2-D semiconductor nanoribbon (NR) membranes. The sensor employs the 8 nm-thick InAs NRs, transferred on a Si/SiO_2 substrate, as a sensing element. Using a conventional CMOS fabrication process, the sensor devices were fabricated. The sensor demonstrated the responses down to parts-per-billion (ppb) level at room temperature and the predominant reaction to NO_2 exposures. Furthermore, a 4-fold higher sensor response was observed in the 8 nm-thick InAs NR sensor compared with the one with the 18 nm-thick InAs NRs, indicating the improved size effects by scaling down to quantization limits.





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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Olivine $LiCoPO_4$ Nanoparticles

Hung-Cuong Dinh 여인형[1] 강영구[2] 모선일

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과 [2]한국화학연구원 화학소재연구단 1팀

As new class of intercalation compounds, phosphates with olivine structure rather than oxides, has emerged that overcome many of the weaknesses inherent to earlier cathode candidates. While $LiFePO_4$ and $LiMnPO_4$ olivine structure have already used in commercial Li-ion cathode batteries, there is a strong increasing demand for the counterparts with other transition metals in olivine family, in particular on the Co-based compound due to its higher cell voltage of 4.8V vs. Li/Li^+, high theoretical capacity of 170 $mAhg^{-1}$, and thus enhanced energy density. However, the very low electronic conductivity is preventing high rate performance of the $LiCoPO_4$ cathode. To improve electrochemical characteristic of $LiCoPO_4$, various strategies have been developed as optimizing particle size to nano-scale that is necessary owing to its high specific surface area, short diffusion lengths for Li-ion, carbon coating, and substitution of exotic ions. In this work, various morphologies of well-crystallized $LiCoPO_4$ nanoparticles were prepared by a simple hydrothermal method. To improve battery performance of $LiCoPO_4$, the carbon was coated on $LiCoPO_4$ surface by a simple method. The structure, morphology and electrochemical properties, carbon content were analyzed by the X-ray powder diffraction (RXD) patterns, scanning electron microscopic (SEM) images, Raman spectrometer, and thermal gravimetric analyzer (TGA). The lithium batteries with the C-coated $LiCoPO_4$ particles cathode were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled galvanostatically a potential range of 3.0-5.0V using a multichannel battery test mode.

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Mixtures of $LiMnO_2$ and Li_2MnO_3 Cathodes for Lithium ion Batteries

유다연 여인형[1] 모선일[*]

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과

Monoclinic-layered Li_2MnO_3 has shown to be one of cathode material for rechargeable lithium ion batteries because of the relatively lower cost, less toxicity, environment-friendly property, and high theoretical capacity. However, it has disadvantages such as lower conductivity and shorter cycle life with severe capacity fading in comparison to the other layered structure materials. Forming composite phase of Li_2MnO_3 with other polymorphs of lithium metal oxides is also of great interest. $LiMO_2$(M = Mn, Co, Ni, Cr, etc.)-Li_2MnO_3 composite electrode materials were reported on previous work that the Li_2MnO_3 in the composite can stabilize the orthorhombic of monoclinic structure of $LiMO_2$ upon cycling.In this work, $LiMnO_2$-Li_2MnO_3 composite powder was synthesized by using a hydrothermal method with different ratio LiOH to γ-MnOOH; solution of LiOH is mixed with γ-MnOOH particles pre-synthesized with $KMnO_4$ and P123 as a surfactant. From this experimental, synthesized $LiMnO_2$-Li_2MnO_3 can be shown improved cycling performances. The characteristics of Li_2MnO_3 as a cathode have been investigated by scanning electron microcopy (SEM), X-ray powder diffraction (XRD), and battery performance with multichannel battery test mode.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of C-coated Li_2FeSiO_4 nano particle Cathodes

이정진 **Hung-Cuong Dinh** 여인형[1] 모선일[*]

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과

A new class of polyoxyanion cathodes based on the orthosilicates,Li_2FeSiO_4, have been attracting significant attention, due to high theoretical capacity(~332 $mAhg^{-1}$, it can be extracted more than one Li^+ ion per formula unit). These orthosilicates have advantages as low cost, environmentally friendly and stable. However, Li_2FeSiO_4 has a poor electronic and ionic conductivity restricts the possibility of using orthosilicates in practical cells. To improve electrochemical characteristic of Li_2FeSiO_4, optimizing particle size to nano-scale is necessary owing to its high specific surface area, short diffusion lengths for Li-ion and increased electronic conductivity by using conductive materials as carbon. In this work, nanostructured Li_2FeSiO_4 particles were prepared by a hydrothermal method using different of Li^+, Fe^{+2}, Si-ion sources. In order to improve conductivity of Li_2FeSiO_4 crystals materials, the various amounts of conductive carbon was coated on Li_2FeSiO_4 particles surface by pyrolyzing glucose; The Li_2FeSiO_4 particles were well dispersed in glucose solution, dry in vacuum, and heated in N_2 atmosphere. The structure, morphology, and C-coated amount were analyzed by the X-ray powder diffraction (XRD) patterns, scanning electron microscopic (SEM) images and thermal gravimetric analyzer (TGA). The lithium batteries with the C-coated Li_2FeSiO_4 nanoparticles cathode were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled galvanostatically a potential range of 1.5-4.6 V using a multichannel battery test mode.

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Nano-spheres of Silica-$LiMn_2O_4$ Core-Shell Structure Cathodes for Li-ion batteries

이종문 모선일* 여인형[1]

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과

The spinel-structured $LiMn_2O_4$ has many intrinsic advantages of the structural characteristics with the 3-D path of lithium ion, high operating voltages, moderate theoretical capacities, low material cost, and acceptable environmental friendliness. For these reason, spinel-structured $LiMn_2O_4$became one of the most promising material for rechargeable Li-ion batteries. The Spinel $LiMn_2O_4$ has a problem of poor cycling efficiency for long life operating, especially at high temperature, which was caused by the dissolution of manganese ions and the structural instability. The silica- $LiMn_2O_4$ composite with core-shell structure can improve cycle performance, because the silica has a structural stability role in composite. In this study, silica-$LiMn_2O_4$ was prepared by combination of precipitation and heat treatment method. For the preparation of spherical size controlled silica nanoparticles, NH_4OH was added into mixture of ethanol and TEOS under magnetic stirring. After the synthesis of silica, the silica-$MnCO_3$ composite was prepared by precipitation at high temperature with silica nanoparticle dispersed solution including $MnCl_2$, CTAB, urea. Then, silica-$LiMn_2O_4$ was prepared from the silica-MnO_2, product of heating silica-$MnCO_3$, by heat treatments with Li salts added. The lithium batteries were assembled in a coin-type (CR2032) cell in a dry room and the batteries were cycled using multichannel battery test mode. Crystalline structures and morphology were analyzed by X-ray diffraction (RigakuD/max 2700V/VP) and scanning electron microscope (JEOL JSM-6380).

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Noble Nanoinjector-based Electrochemical Gene Delivery into a Single Cell Nucleus

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한국과학기술원(KAIST) 화학과 [1]한국과학기술원(KAIST) 생명화학공학과

Delivery of bioactive materials into a cell is highly important in the study of cell biology and medical treatments. Ideal delivery devices should be able to deliver biomaterials with high spatial resolution while causing minimum cell damage. We developed a noble nanoinjector using metal nanowire of cylindrical geometry with very small diameter as well as optimum mechanical properties, minimizing cell damage. The nanoinjector enables precisely timed and efficient electrochemical release of DNA molecules attached on a nanowire surface. Both linear DNA and plasmid DNA were delivered separately, and showed successful expression. The nanoinjector would find important biomedical applications in the fields such as gene therapy, DNA vaccination, targeted drug delivery, and probe/control of cell signaling events.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic activity of nanoporous black gold surfaces fabricated by cathodic anodization

복영웅 김종원*

충북대학교 화학과

본 연구에서는 양극 산화반응을 통해 검은색의 나노다공성 금 (nanoporous black gold, NPBG)를 형성하여 표면적의 변화 및 결정구조에 따른 전기화학적 촉매활성의 변화 양상을 관찰하였다. Nanoporous gold (이하 NPG) 구조의 특징은 매우 큰 표면적을 가진다는 것이다. 이러한 특징을 이용해 전기화학적 센서부터 연료전지까지 여러 분야에 걸쳐 연구가 진행되고 있다. 이번 연구에서는 NPG 를 만드는 몇 가지의 방법 중 비교적 단순한 방법인 양극 산화반응을 통해 NPBG 를 형성하였다. 양극 산화반응은 높은 전압을 걸어주어 전극 표면에서 산화반응을 일으키는 방법이다. 이때 산화반응시간을 조절하여 표면적의 변화를 주었고, 메탄올, 글루코오스, 그리고 산소의 산화/환원 반응에 대해 NPBG 의 표면적에 따른 촉매적 활성을 살펴보았다. 양극 산화반응에서 반응시간이 길어짐에 따라 표면적은 선형적으로 증가하였다. 이것을 토대로 산소와 글루코오스의 산화/환원에 대해 살펴 보았을 때, 표면적이 증가함에 따라 봉우리 전위는 변하였지만, 봉우리 전류의 경우 큰 변화를 보이지 않았다. 메탄올 산화의 경우 동일한 농도에서 표면적이 증가함에 따라 봉우리 전류가 증가하는 것을 확인하였다. 그리고 동일한 표면적일 때, 메탄올의 농도가 증가함에 따라 봉우리 전위가 변하는 것 또한 확인하였다. 이와 같이 봉우리 전위/전류의 변화를 설명하기 위해 UPD 방법으로 NPBG 의 표면 결정구조를 확인 하였으며, 확인된 표면 결정구조의 비율을 통해 전기화학적 촉매 활성을 설명하였다.[본 연구는 교육과학기술부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임.]

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Borate 완충용액에서 니켈의 부식에 대한 대류와 산소 및 염화이온의 영향

남진아 김연규*

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변전위법과 전기화학 임피던스 측정법을 이용하여 borate 완충용액에서 Ni 의 부식과 부동화에 대한 대류와 산소 그리고 염화이온의 영향을 조사하였다. 용액에 녹아 있는 염화이온은 산화피막 파괴에 크게 영향을 끼쳤으나 전극 회전 속도가 3000 rpm 이하일 경우 부식전위와 부식전류의 대류-확산 의존성은 없었다. Ni 전극 표면에 OH^-의 흡착-탈착 과정이 전극의 부식과 부동화에 관여하며, 부동화 피막은 $Ni(OH)_2$ 가 생성되었다가 열역학적으로 더 안정한 NiO 로 변화됨을 알 수 있었다.

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Electrodeposition of Triangular Rod Pd Nanostructures and Their Electrocatalytic and SERS activities

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충북대학교 화학과

전기화학적 석출 방법을 이용하여 형성된 팔라듐 나노 구조와 전기화학적 촉매 현상 및 표면증강 라만 분광 (Surface Enhanced Raman Spectroscopy, SERS) 활성에 대한 연구를 수행하였다. 주사 전자 현미경(Scanning Electron Microscopy, SEM) 과 투과 전자 현미경(Transmission electron microscope, TEM) 을 통해 삼각 봉 형태를 지니는 독특한 형태의 팔라듐 나노 표면 구조를 확인하였다. 팔라듐 삼각 봉 나노 구조는 산소 환원 반응과 포름산 산화 반응에 우수한 전기화학 촉매적 활성을 나타내는 것으로 확인 되었다. 산소 환원 반응의 경우, 팔라듐 삼각 봉 구조는 변형되지 않은 평평한 팔라듐 전극에 비해 200 mV 정도 양의 방향으로 이동된 환원 봉우리를 나타내었는데, 이는 평평한 백금 전극보다도 약간 더 우수한 촉매활성에 해당한다. 포름산 산화 반응에서는 변형되지 않은 평평한 팔라듐 전극 표면보다 큰 산화 봉우리 전류와 산화 봉우리의 이동을 보였다. 팔라듐 삼각 봉 구조는 SERS 활성도 크게 나타나는 것으로 관찰이 되었는데, 기존에 널리 활용된 전기화학적으로 거칠게 형성된 표면에 비해 약 2 배 정도 높은 활성을 나타내었다. 팔라듐 삼각 봉 나노구조의 우수한 전기화학적 및 SERS 활성의 원인에 대하여 나노구조의 크기 및 모양, 그리고 결정면 정보를 활용하여 설명하였다. 또한 변형되지 않은 평평한 팔라듐 전극과 비교하여 효과적인 SERS 활성을 보여준다. [본 연구는 교육과학기술부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임]

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Study of I^- substitution on carbon free cathode bimetallic olivine material for Li battery

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울산대학교 화학과

There has been considerable interest in olivine struc-ture as a cathode active material for Li rechargeable battery due to its strong phosphate-oxygen covalent bond, environmental benign, and structural stability. The iodine anion substituted $LiFeMnPO_4$ composites have been prepared by solid state reaction without carbon coating and additional carbon retreatment. The XRD and XPS results of composite indicate iodine anions have been successfully substituted to PO_4 sites without structural modification. Electrochemical analysis has been also performed with various C-rates and cycleability.

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Compositional Analysis of Electrodeposited Cu-Se Compound Semiconductor Thin Films Using Flow-Electrochemical Quartz Crystal Microgravimetry

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건국대학교 응용화학과 [1]고려대학교 신소재화학과

A novel method for the compositional analysis of electrodeposited Cu-Se semiconductor films was developed using a combined voltammetry and flow-electrochemical quartz crystal microgravimetry (Flow-EQCM). Cu-Se semiconductor films containing free Se, Cu_2Se and free Cu depending on the electrodeposition potential were electrosynthesized on the Au electrode and their composition was analyzed by Flow-EQCM. Concomitant frequency changes during the selective stripping steps facilitated compositional assay of films. Amount of free Se and Se in Cu_2Se were obtained at constant potentials of -0.8 V and -1.3 V, respectively. Potential steps to -0.8 V and -1.3 V were employed to reduce free Se to Se^{2-} and Cu_2Se to $Cu+Se^{2-}$, respectively. Resultant total Cu was stripped at +0.8 V and free Cu contents were calculated using the frequency changes observed during the stripping of total Cu and Se in Cu_2Se. The results showed that composition of electrodeposited Cu-Se films was sensitive to the deposition potentials as well as thickness.

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Electrodeposition of Bismuth Oxide: Voltammetric and Electrochemical Quartz Crystal Microgravimetric Study

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Combined voltammetry and electrochemical quartz crystal microgravimetry (EQCM) were employed for the investigation of electrodeposition and compositional analysis of bismuth oxide (Bi_2O_3) thin films. Electrodeposited thin films contain Bi and Bi_2O_3 depending on the electrodeposition potential. First, Bi_2O_3 films containing Bi were electrodeposited at several potentials on the polycrystalline gold electrode in 0.1M KNO_3 containing 1 mM $Bi(NO_3)_3$ and 0.01 M EDTA. Contents of Bi_2O_3 and Bi were determined using reduction peak of Bi_2O_3 to Bi and oxidation peak Bi to Bi^{3+}, respectively. The results show that composition was very sensitive to the electrodeposition potential. Electrodeposited films were also characterized with XRD, SEM and EDX. Their photocatalytic activities and photoelectrochemical properties were measured.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Graphite Oxide in Carbon Paper on the Electrical Properties for Gas Diffusion Layer

이지한 박수진*

인하대학교 화학과

In this work, we studied the gas diffusion layers (GDLs) made from carbon fiber papers for using gas diffusion matrix (GDM) in polymer electrolyte membrane fuel cells (PEMFCs) by wet processing. Graphite oxide (GO) was added in carbon paper during impregnating phenol resin to investigate the effect of GO on the electrical properties of carbon paper. GO was prepared by Hummer’s method. We used 0.1 g of 6 ㎜ chopped carbon fibers for making carbon paper preform with 5 x 5 ㎠ size. Various contents of GO was added and estimated. The properties of GO was characterized by X-ray diffraction (XRD). The dispersion states of carbon fibers were investigated by scanning electron spectroscopy (SEM) and the electric resistivity of carbon paper was measured using two probe techniques.

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Influence of Carbonization Temperatures on the Properties of Nitrogen doped Microporous Carbon/Carbon Nanotube for EDLCs

이지한 박수진*

인하대학교 화학과

In this work, the electrochemical properties of nitrogen doped microporous carbon/CNTs (N/C-MWCNTs) were investigated for electrodes in electric double-layer capacitors (EDLC). MWCNTs were used after purification with acids. To coat the nitrogen onto CNTs, melamine was used as nitrogen source and the N-coated CNTs were carbonized with different temperatures. Each N/C-MWCNTs were activated with KOH at the same conditions. The crystalline and structural features were investigated by X-ray diffraction (XRD). The surface properties of the N/C-MWCNTs and Activated-N/C-MWCNTs were characterized by X-ray photoelectron spectroscopy (XPS). The textural properties of N/C-MWCNTs and A-N/C-MWCNTs were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. And their electrochemical behaviors were confirmed by cyclic voltammetry (CV).

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Effect of Different Pretreatments on Indium-Tin Oxide Electrodes

정진교 양해식*

부산대학교 화학과

The effect of pretreatment on indium-tin oxide (ITO) electrodes has been rarely studied, although that on metal and carbon electrodes has been enormously done. The electrochemical and surface properties of ITO electrodes are investigated after 6 different pretreatments. The electrochemical behaviors for oxygen reduction, $Ru(NH_3)_6^{3+}$ reduction, $Fe(CN)_6^{3-}$ reduction, and p-hydroquinone oxidation are compared, and the surface roughness, hydrophilicity, and surface chemical composition are also compared. Oxygen reduction, $Fe(CN)_6^{3-}$ reduction, and p-hydroquinone oxidation are highly affected by the type of the pretreatment, whereas $Ru(NH_3)_6^{3+}$ reduction is almost independent of it. Interestingly, oxygen reduction is significantly suppressed by the treatment in an HCl solution. The changes in surface roughness and composition are not high after each pretreatment, but the change in contact angle is substantial in some pretreatments.

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Hydroquinone Diphosphate as a Phosphatase Substrate in Enzymatic Amplification Combined with Electrochemical-Chemical-Chemical Redox Cycling for the Detection of E. coli O157:H7

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부산대학교 화학과

Signal amplification by enzyme labels in enzyme-linked immunosorbent assays (ELISAs) is not sufficient for detecting a low number of bacterial pathogens. It is useful to employ approaches that involve multiple signal amplification such as enzymatic amplification plus redox cycling. An advantageous combination of an enzyme product [for fast electrochemical-chemical-chemical (ECC) redox cycling that involves the product] and an enzyme substrate (for slow side reactions and ECC redox cycling that involve the substrate) has been developed to obtain a low detection limit for E. coli O157:H7 in an electrochemical ELISA that employs redox cycling. In our search for an alkaline phosphatase substrate / product couple that is better than the most common couple of 4-aminophenyl phosphate (APP) / 4-aminophenol (AP), we compared five couples: APP / AP, hydroquinone diphosphate (HQDP) / hydroquinone(HQ), L-ascorbicacid 2-phosphate / L-ascorbic acid, 4-amino-1-naphthyl phosphate / 4-amino-1-naphthol, and 1-naphthyl phosphate / 1-naphthol. In particular, we examined signal-to-background ratios in ECC redox cycling using $Ru(NH_3)_6^{3+}$ and tris(2-carboxyethyl)phosphine as an oxidant and a reductant, respectively. The ECC redox cycling that involves HQ is faster than the cycling that involves AP, whereas the side reactions and ECC redox cycling that involve HQDP are negligible compared to the APP case. These results seem to be due to the fact that the formal potential of HQ is lower than that of AP and that the formal potential of HQDP is higher than that of APP. Enzymatic amplification plus ECC redox cycling based on a HQDP / HQ couple allows us to detect E. coli O157:H7 in a wide range of concentrations from 103 to108 colony-forming units / mL.

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Electrochemical oxidation of glucose at nanoporous gold surfaces prepared by cathodic anodization in carboxylic acids

노성진 정화경 이금섭 김민주 김종원*

충북대학교 화학과

세 가지 다른 카르복실산 용액 하에서 양극 산화반응을 통해 형성된 nanoporous gold (NPG) 의 형성 과정을 관찰하였다. 포름산, 아세트산, 그리고 프로피온산 용액 하에서 NPG 를 형성시킨 결과 step time 이 늘어날수록 표면적이 증가하는 경향을 보였지만, 포름산의 경우 가장 효과적으로 표면적이 큰 NPG 구조를 만들 수 있었다. 세 가지 용액 하에서 형성시킨 NPG 의 글루코오스 산화는 염소 이온이 없을 때 표면적이 증가가 전류 밀도에 큰 영향을 주지 않지만, 염소 이온이 있는 경우 표면적 증가에 따라 전류 밀도가 일정하게 증가하는 경향을 보였고, 포름산이 동일한 step time 에서 글루코오스 산화에서 가장 높은 전류 밀도를 보이는 NPG 구조임을 확인하였다. 포름산 용액 하에서 생성시킨 NPG 의 최대 표면적 및 글루코오스 산화에서 전류밀도를 확인하기 위해 양극 산화반응 조건인 step potential, step time 을 최적화하였으며, 주사 전자 현미경(Scanning Electron Microscope, SEM) 을 통한 표면 구조 및 전류법 검출에서 민감도의 증가를 확인하였다. [본 연구는 교육과학기술부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임.]

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Formation of CIGS by Electrochemical ALD(Atomic Layer Deposition) at Au(111).

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Au(111)의 원자층 증착(Atomic Layer Deposition)은 원소를 주기적으로 바꿔주는 공정 때문에 증착속도가 느리다는 단점이 있다. 하지만 박막의 두께를 수 Å단위로 정밀하게 제어 할 수 있어 다음과 같은 장점이 있다. 단차피복성이 우수하여 복잡한 구조도 균일하게 증착이 가능하고, 박막의 두께와 조성을 정밀하게 조정 할 수 있다. 또한, 불순물이 적으며, 결함이 없는 박막제조에도 유리하다.

박막태양전지 중에서 높은 변환효율을 가지고 있는 CIGS 계 태양전지는 일반적인 유리나 고분자 또는 스테인레스스틸을 기판으로 하는 태양전지로 태양광을 흡수하는 광 흡수층이 CIGS 다 성분계로 이루어진 태양전지이다. 특히 이 CIGS 광흡수계수는 효율이 가장 높아 두께 1 ~ 2㎛ 박막으로도 고효율의 태양전지 제조가 가능하다.

본 실험은 Au(111)를 작업전극(Working Electrode)으로 사용하여 산화전극(Counter Electrode)과 환원전극(Reference Electrode)은 각각 백금과 Ag/AgCl 로 하여 Copper, Indium, Gallium, Selenium 각각의 원소의 UPD(Under Potential Deposition) 되는 Potential 을 찾고, Step by Step UPD 방식으로 Ar 기체 상태에서 전착 시켰다. 그 후 전착시킨 원소를 Cleaning Cycle 로 제거하여 Current 를 비교해 보았다.

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백금 전극 표면에서 회전속도 변화에 따른 개미산 촉매독과 산화 전류량에 대한 연구

신동완 오성훈 이충균*

충남대학교 화학과

Rotating Disk Electrode(RDE)는 전극을 회전시킴으로서 전극표면과 용액사이의 diffusion layer 를 감소시켜 mass transfer 를 원활하게 함으로서 전극에서의 반응이 잘 이루어지도록 하는 역할을 한다. 그러나 개미산에서는 RDE 의 회전 속도가 증가할 수록 산화 전류량과 촉매독 양이 감소하는 것을 관찰하였다. RDE 의 회전 속도가 증가할수록 개미산 분자가 백금 전극의 반응점에 흡착하여 산화되기 전에 빠르게 지나가게 되어 흡착량이 감소되고 결과적으로 산화 전류의 감소와, 촉매독이 감소한다는 가설을 가지고 실험을 계획하였다. 본 연구에서는 개미산이 산화하는 여러 전압에서 RDE 의 회전속도를 다르게 하였고, 대시간전류법을 이용하여 일정한 시간이 지난 후의 개미산 산화 전류와 촉매독을 측정하였다. 일정 시간이후의 개미산 산화와 촉매독이 생성되는 것을 방지하기 위해서 Iodine 을 이용하였다.

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Enzyme functionalized gold nanoparticles for the electrochemical detection of 1,4-dioxane

이상혁 이혜진*

경북대학교 화학과

This poster demonstrates a novel electrochemical detection method for 1,4 dioxane using enzyme functionalized gold nanoparitcles immobilized on a carbon working electrode. A self-assembled monolayer of 3-mercaptopropionic acid (MPA) was first attached on to gold nanoparticle surfaces. The MPA modified Au NPs were then reacted with 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and N-hydroxysulfosuccinimide (NHSS) followed by the reaction of the monooxgenase, (e.g. cytochrome P450). The enzymatically functionalized nanoparticles was then encapsulated in a Nafion matrix combined to a carbon electrode. The electrode was finally reacted with 1,4-dioxane to produce 1,4-dioxane-2-ol, which was further reduced to 1,4-dioxane-2,5-one. The electrochemical characteristics of the enzymatically modified electrode for the detection of 1,4 dioxane was studied using cyclic voltammetry and differential pulse voltammtery.

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Amperometric phenol biosensor based on covalent immobilization of tyrosinase on a polypyrrole/Au-nanoparticle modified screen printed carbon electrode

Karim Md. Nurul 이혜진*

경북대학교 화학과

In this poster, we demonstrate an amperometric biosensor for the highly selective detection of phenol based on the covalent immobilization of the tyrosinase onto a polypyrrole/Au-nanoparticle modified screen printed carbon electrode. Polypyrrole and gold nanoparticles were first electrochemically deposited onto a carbon electrode by scanning cyclic voltammetry. Gold nanoparticles were then modified with 3-mercaptopropionic acid followed by the covalent immobilization of tyrosinase using 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide and N-hydroxysulfosuccinimide (EDC/NHSS) cross-linking chemistry. The immobilized tyrosinase assisted the hydroxylation of the phenol to form catechol molecules which was then oxidized to produce quinone. It was found that an amperometric signal upon the subsequent reduction of quinone increased linearly as a function of the phenol concentration.

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Ion separation with facial fabricated conducting polymer modified membrane by electrochemical method

PIAOHUSHAN 손용근*

성균관대학교 화학과

A lot of membrane separation methods were introduced in recent years. However, not many micro/nano separation methods of fast separation with low energy and low cost. In this study, we went to perform an ion separation with conducting polymer modified membrane by applying potentials easily. First, gold was sputtered on the PC(polycarbonate) membrane and then a polypyrrole layer was electrochemically deposited on the Au surface in aqueous solution until the pores were covered perfectly. Then ion transport was performed with various potential conditions. If the ions have different size, charge and different specific interaction with the Ppy, the transport velocity and mechanism are different. So, the ions could be separated by applying potentials to the Ppy modified membrane. This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Knowledge Economy(No. 2010501010002B)

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Thrombin detection using graphene oxide as an electrochemical indicator

최동철 김규원

인천대학교 화학과

Graphene oxide, an insulating and disordered analog of highly conducting graphene has been widely used in electrochemical sensor due to their versatility and excellent properties as platforms for biosensing. In this presentation, we report an electrochemical detection for thrombin using graphene oxide employed as an indicator. The changes in the interfacial properties of the electrode surface before and after its exposure to a solution of thrombin and graphene oxide were monitored using cyclic voltammetry and electrochemical impedance spectroscopy. We optimized the pH of the solution of graphene oxide to maximize the interaction between graphene oxide and thrombin. We demonstrate also that graphene oxide can be a good electrochemical indicator for sensitive and selective detection of thrombin

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Preparation of bio-recognition surface by using a novel diazonium compound as a linker molecule.

Md Mohibul Islam Khan 김규원

인천대학교 화학과

A new electroactive linker molecule with cyclic disulfide as an end functional group was synthesized and electrodeposited on the indium tin oxide (ITO) surfaces. Cyclic disulfide tethered diazonium (CDSD) modified surfaces were characterized by cyclic voltammetry and X-ray photoelectron spectroscopy (XPS). Electrochemical oxidation of CDSD modified electrode was done to activate disulfide functionality for surface immobilization reaction. It has been established that the activated surface contains thiosulfonate or thiosulfinate, which has been displayed by electrochemistry, XPS and fluorescence microscopy. Selective detection of multi-antigen on ITO micro electrode array was performed by the sandwich immunoassay based on fluorescence.

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Influence of amine surfaces on electrocatalytic activity of electrochemically reduced graphene oxide for uric acid oxidation

박수미 유희선 김규원

인천대학교 화학과

Employing an efficient linker molecule for immobilizing nanomaterials being used in biosensor application is important for enhancing sensitivity and selectivity of the detection results of biosensor. In this presentation, we report the influences of amine linker molecules attached on electrode surfaces on the electrocatalytic activity of electrochemically reduced graphene oxide (ERGO) for uric acid oxidation. Various amine linker molecules were attached onto indium-tin oxide electrode surfaces with different ways. Graphene oxide was immobilized on the amine liker layer through electrostatic interaction, and then reduced electrochemically with cyclic voltammetry. We observed the electrocatalytic activity for the oxidation of uric acid on the ERGO-modified electrode surface with differential pulse voltammetry. The activity was dependent upon the kind of amine and attachment method of amine.

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Prussian blue-cobalt hexacyanoferrate electrochromic device with a K+-doped gel electrolyte

정영희 김영일

부경대학교 화학과

Prussian blue(PB, iron(Ⅲ) hexacyanoferrate(Ⅱ)) and prussian blue analogue(Co-PBA,cobalt (II)hexacyanoferrate(III)) are a well-known electrochromic materials. They have a zeolitic structure which show K+ selectivity based on size-selective inter/deintercalation. For high performance and long-term stability of EC device, one of the most important elements is electrolyte. In most EC system, Li salts are used to electrolyte due to noticeable advantages. However they are expensive and Stoke’s radius of Li+ is lager than that of K+ in electrolyte solution(solvated ions). The polymer gel electrolyte was prepared from polyvinyl butyral doped with KPF6 to accommodate the conduction of K ions. The PB and Co-PBA films were prepared on ITO/PEN substrate by bar-coating and the flexible electrochromic film devices were fabricated by the combination of the PB and Co-PBA electrodes with a K+ -doped gel electrolyte. PB/Co-PBA devices(PEN/ITO, 10cm2) showed electrochromic color change between blue and yellow, response time was 6.5s(bleaching) and 3.3s(coloring). EC devices were maintained high contrast ratio during 1,000 cycles and more.

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ELECTROCHEMICAL DEPOSITION OF CIGS ON MO/GLASS

최익호

고려대학교 신소재화학과

최근 환경오염 문제와 화석 에너지 고갈로 차세대 청정에너지 개발에 대한 중요성이 증대되고 있다. 그 중에 태양전지는 공해가 적고, 자원이 무한적이며 반 영구적인 수명을 가지고 있어 미래 에너지 문제를 해결할 수 있는 에너지원으로 기대되고 있다. Cu, In, Ga, Se 의 4 가지 원소로 구성된 Cu(InGa)Se2 (이하 CIGS) 박막태양전지는 105cm-1 이상의 높은 광흡수계수로 인하여 두께 ~1µm 의 박막으로도 고효율의 태양전지제조가 가능하고 또 한 장기적으로 전기적?광학적 안정성이 우수한 특성을 지니고 있다. 또한 비 실리콘 계열 태양전지 중 가장 높은 에너지 변환 효율, 유연성이 좋으며 공정비용과 재료비용이 저렴하다는 장점이 있다. Electro deposition 방법으로 CIGS thin film 을 제작하여 selenization 공정 후 CdS 전착 후 SEM, EDX, XRD 를 통해 각 시료를 분석하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical characteristics of hexachloroplatinate and its electrocatalytic effects for the redox reaction of hydrogen peroxide

김경태 장승철[1] 박덕수[2,*]

부산대학교 바이오센서연구소/분자과학기술 [1]부산대학교 바이오피지오센서연구소 [2]부산대학교 바이오피지오연구소

The electrochemical characteristics and electrocatalytic effects of hexachloroplatinate ions were studied by cyclic voltammetry and amperometry at different pH, concentrations and potential range. The grassy carbon and screen-printed carbon electrode were used as working electrodes, Ag/AgCl electrode and Pt wire were used as reference and counter electrode. Hexachloroplatinate ions modified electrodes could be showed electrocatalytic effect on the redox reaction of H_2O_2. Which indicated a sensitive and rapid detection of H_2O_2. The hexachloroplatinate modified electrodes were fabricated by electrochemical deposition or entrapment in the polymer matrix on the electrode surface. Electroanalytical conditions for amperometric detection of H_2O_2 by using the electrode modified with hexachloroplatinate were investigated. Based on the results for the electrocatalytic effect on the redox reaction of H_2O_2, the biosensor performance was evaluated in connection with glucose oxidase or cholesterol oxidase using hexachloroplatinate modified electrodes.

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A Zinc Porphyrin Sensitizer Modified with Donor and Acceptor Groups for Dye-Sensitized Solar Cells

이시우 홍종달*

인천대학교 화학과

In view of the limited availability of fossil fuels and the disastrous environmental issues related with their combustion, it is imperative to develop renewable energy resources for the increasing global energy demand. The dye-sensitized solar cell (DSSCs) has attracted considerable attention as a promising technology for low-cost photovoltaic cells due to its high efficiency. Significant efforts are now being focused on the development of new sensitizer dyes to improve performance and commercial viability. Porphyrins have been intensively developed for efficient dye candidate in use of DSSCs over 12 years. For instance, an 11% solar-to-electric power conversion efficiency was achieved from a judiciously tailored porphyrin dye under standard condition. The cell efficiency was comparable to that of other organic dyes developed recently. Porphyrins are especially attractive dyes for DSSC application, due to their large absorption coefficients in the visible-near IR region, tunable redox and photophysical properties. In the poster, we focused on illustrating the influence of dye structure on sensitizer performance in DSSC. The synthetic route to the dye was summarized here along with the analytical data of the chemical structure of the dye. The physical properties of the dye were investigated using UV/visible spectroscopy and IPCE.

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Effect of the incorporation of carboxylated carbon nanotubes onto the wired-bilirubin oxidase cathode for the electrocatalytic reduction of oxygen

강찬* 신효설 정혜란

전북대학교 화학과

The BOD cathode constructed with the carboxylated CNTs (CNT-COOHs) and a redox hydrogel film made from a copolymer of polyacrylamide and poly (N-vinylimidazole) complexed with [Os(4,4’-dichloro-2,2’-bipyridine)2Cl]+/2+ (PAA-PVI-[Os(dCl-bpy)2Cl]+/2+) wiring bilirubin oxidase (BOD) enzymes was employed for the electrocatalytic O2 reduction. The performance was compared with that of the same BOD cathode but with no CNT-COOHs incorporated. The CNT-COOH incorporated BOD cathode showed a large increase in the O2 reduction current density in a 0.15 M NaCl buffer at pH 7.4 and a better stability when a potential of 0.1 V vs. Ag/AgCl was applied to the cathode being rotated with a 200 rpm speed for 8000 s. At a BOD cathode with no CNT-COOHs incorporated, the current decreased by 22 % with 0.9 M NaCl added, and 27 % with 0.9 M KBr added, but, with CNT-COOHs incorporated, only 6 % and 5 % current decays were measured, respectively.

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Electrocatalytic oxidation of glutamate at an electrode modified with a composite of redox polymer and carbon nanotube.

강찬* <u>이현아</u> 신효설

전북대학교 화학과

Glutamate is the major excitatory neurotransmitter in the central nervous system. Glutamate dehydrogenase(GlDH) enzyme based electrode with a composite of redox polymer and carbon nanotube is used for the amperometric detection of glutamate. β-Nicotinamide adenine dinucleotide (NADH) is involved as a cofactor with glutamte dehydrogenase (GlDH) in the glutamate oxidation reaction. The electrodes was prepared by coating a mixture of oxidatively treated carbon nanotubes, GlDH, poly(ethylene glycol) diglycidyl ether (PEGDGE) as a cross-linker, and redox polymer (polyacryamide and poly(N-vinylimidazole) complexed with [Os(4,4'-dimethyl-2,2'-bipyridine)2Cl]+/2+). Effects depending on various parameters such as NADH concentration and the amount of CNT mixtures were examined. The GlDH/CNT electrode is expected to be used for a potential application as an efficient amperometric glutamate biosensor.

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The Study about Effect of Reducing Agent and Modification of a Copper Surface for Bonding of Cu-PPS Resin

정은혁 정의덕*

한국기초과학지원연구원 하이테크소재연구부

Various surface modifications has been applied to improve adhesion properties of bivalent metal such as copper and aluminum for electrodes terminal application and sealing for Li ion batteries. Copper oxide layer is very effective in improving the bonding strength. However, a copper oxide is readily hydrolyzed and dissolved upon contact with an acid. In this study, we have investigated the method of forming cupric oxide on the surface of copper and improved acid resistance by reducing the cupric oxide to cuprous oxide. Also, we have tried to find the effective condition on the polymerization of a triazine thiol on modified copper surfaces. We evaluated the effect of time, temperature of solution condition for the adhesion of polymeric film on copper. Characterization of the polymerized film on copper was explored by SEM, XPS and SIMS. SEM results reveal that the meaningful roughness was formed on the copper surface by chemical oxidation. SIMS results represent that the peel strength was found to depend on film thickness and the composition of adhesion layer. As a result, Cu/polymer assemblies developed in this study have superior adhesion property. Therefore, these assemblies might be a viable candidate as a sealing technique for Li ion batteries, and will be beneficial in reducing the process cost and increasing the safety of Li ion batteries.

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Synthesis of FeF_3/Ordered Mesoporous Carbon (OMC) Nanocomposites and Their Enhanced Electrochemical Performance as a Cathode Material of Lithium Ion Batteries

정혜윤 신지현 김용경 김종식

동아대학교 화학과

FeF_3 is of great interest as a potential candidate of cathode materials because of their low cost, safety and environmental friendliness. FeF_3 has a theoretical capacity of 237.51 $mAhg^{-1}$ at the voltage range of 2.0 - 4.5 V, which is higher than that of $LiCoO_2$ (≈140 $mAhg^{-1}$). However, FeF_3 has a low intrinsic electrical conductivity, slow diffusion of lithium ions, and poor cycle stability. These issues of FeF_3should be improved for the applications in lithium ion battery systems. In this study, pristine FeF_3 showed an initial discharge capacity of 117 $mAhg^{-1}$ at 0.1 C (23.7 mAg^{-1}) with voltage range of 2.0 - 4.5 V at room temperature with poor cyclability. The electrochemical performance of FeF_3 was successfully improved via forming FeF_3/ordered mesoporous carbon (OMC) nanocomposites, e.g. higher capacity, capacity retention, and rate performance.

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Synthesis of Carbon-Coated V_2O_5 for Enhancing Electrochemical Performance as a Cathode Material for Secondary Li-ion Batteries

신지현 정혜윤 정혜인 김종식

동아대학교 화학과

Vanadium pentoxide (V_2O_5) is considered to be a promising candidate as a cathode material for Li-ion batteries (LIBs) because of their low cost, abundance, and high theoretical capacity. V_2O_5 has theoretical capacities of 441 mAhg^{-1} at 1.5-4.0 V and 294 mAhg^{-1} at 2.0-4.0 V, corresponding to redox reactions with three and two lithium ions, respectively. However, V_2O_5 has disadvantages of low electrical conductivity and lithium ion diffusion, resulting in poor cycling stability and rate performance. In this study, in situ carbon-coated V_2O_5 was synthesized via an incipient wetness impregnation technique with a carbon form as both a hard template for the synthesis of V_2O_5 and a carbon source for the formation of the carbon layer on the surface of V_2O_5. The carbon-coated V_2O_5 showed enhanced energy efficiency and rate capability, compared to those of nano-sized V_2O_5.

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Electrochemical detection of heavy metal ions with gold nanoparticle modified carbon fiber electrodes

권나현 한송이 차유정 윤장희*

한국기초과학지원연구원 부산센터

In this study, carbon fiber electrodes having different gold nano-particle levels were tested for the simultaneous detection of heavy metal ions (Pb, Cu, Hg and Zn) using the electrochemical method (anodic stripping voltammetry, ASV and differential pulse anodic stripping voltammetry, DPASV). Various experimental parameters that affect on response, such as electrolytes concentration (0.1, 0.5, 1M HCl, 0.1M KCl), deposition time (1~6 min) and Au nano-paticle level (2~5 min) were carefully optimized with the carbon fiber electrodes. The structural of carbon fiber electrodes were characterized by Scanning Electron Microscope (SEM).

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8000 ppm-Boron Doped Diamond Electrode for Detection of Trace Level Metal Ions Using Anodic Stripping Voltammetry

한송이 권나현 차유정 윤장희*

한국기초과학지원연구원 부산센터

Anodic stripping voltammetry (ASV) is a powerful technique for the determination of trace metals in aqueous solutions. The 8000ppm-Boron doped diamond(BDD) electrode was tested for the simultaneous detection of heavy metal ions (Pb, Cu, Cd, Hg, Cr and Zn) using the electrochemical method (anodic stripping voltammetry, ASV and differential pulse anodic stripping voltammetry, DPASV). Various experimental parameters that affect on response, such as deposition time, deposition potential, and electrolytes concentration were carefully optimized with the BDD electrodes. The deposition time screened only within a range of 1-5min. The experiment was conducted within electrolytes concentration range of 0.1~1M. The best result was obtained at a deposition potential of -1.5V. With the improved conditions, a final detection limit of below 5ppb was accomplished.

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Study on the relationship between the outer Helmholtz plane potential and the supporting electrolyte concentration

남광모 장병용

부경대학교 화학과

Electrochemical reactions are activated by the potential difference between the electrode and the solution. Normally, the potential difference is defined by the potential at the outer Helmholtz plane (OHP) because the supporting electrolyte of high concentration deforms the electric field to eliminate the potential drop outside of the OHP. Sometimes, the measurement of electrochemical information under such conditions can make distorted results. Here, we studied the effect of the supporting electrolyte concentration on the electrochemical information. We measured the electron transfer rates of $Fe(CN)_6^{3-}$ reduction at different concentrations of the supporting electrolytes using the Fourier transform electrochemical impedance spectroscopy method. From the results, we calculated k0 values and fitted them to the Frumkin effect equation in order to evaluate the potential of the OHP. Finally, we correlated the OHP potential to the concentration of the supporting electrolyte

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Influence of Pore Characteristics on Electrochemical Performance of Nickel oxide for Pseudocapacitor Applications

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Three types of mesoporous nickel oxide (NiO) with different pore characteristics and shapes have been synthesized via sol-gel method. Nanoflower-, nanoslice- and nanopariticle- shaped NiO with different features such as pore size and pore distribution were achieved. From measurement of pore size, pore distribution and electrochemical properties, the relationship between the capacitances and their pore characteristics was discussed in this study. The nanoflower-shaped NiO has higher pore volume, larger pore size as well as shorter distance between pores, which help to foam a distinctive three-dimensional (3D) pore network. As a result, nanoflower-shaped NiO shows outstanding electrochemical capacitance than other structures with smaller pores and pore volume because not only many mesopores in flower-shaped nanostructures improve the contact and transport of the electrolyte but also the 3D nanochannels in NiO structures developed by larger pore volume and pore size provide longer electron pathways.

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Synthesis and electrochemical properties of ReO_3 nanorods grown on W microwires

하예진 김명화[1] 이영미*

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Nanorods (NRs) of ReO_3, the only stable trioxide among the Group 7 elements, were successfully synthesized by employing the chemical vapor deposition (CVD) method. Inexpensive but conductive metal, W microwires were used as substrates for the growth of ReO_3 NRs. In the initial growth period, cube shaped ReO_3 crystals were formed and then some of those cubes were transformed to ReO_3 NRs on W microwires. Morphology of ReO_3 NRs on W microwires was characterized with scanning electron microscopy (SEM). As-prepared ReO_3 NRs on W microwires were also electrochemically characterized. Using the technique cyclic voltammetry (CV) in acidic media, electrical capacitance and electrocatalytic activity were examined. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2012-0005422).

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Development and Application of an Electrochemical Dual Microsensor for Simultaneous CO and NO Measurements.

나지선 하예진 이영미*

이화여자대학교 화학나노과학과

Endogenously produced carbon monoxide (CO) and nitric oxide (NO) gases have similar biological functions such as vasodilation and neurotransmission. For years, studies have suggested that two gases do not work independently, but rather corregulate each other. Nevertheless, researchers still can’t reveal their interactions clearly due to the lack of proper analysis techniques. In this presentation, we present the development of an electrochemical dual CO/NO sensor and its biological application. The sensor is made up of a dual platinum working electrode (WE) and a Ag/AgCl counter/reference electrode. The dual WE possessing two platinum disks (WE1 and WE2, 76 and 25 μm in diameter, respectively) is etched to form mircopore-shaped electrode and then electrodeposited with porous platinum layer. The larger WE1 is additionally modified with electrochemical deposition of tin. Modifications of two sensing disks different in their size as well as in their disk surface treatments give apparently different selectivity of CO at WE1 and NO at WE2. For the sensor application, we employ the CO/NO dual microsensor for simultaneous measurements of CO and NO on cerebral cortex of rat. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2012-0003779).

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Synthesis and Electrocatalytic Activity of Ir Nanoparticles Self-assembled on Graphene

김지언 심준호[1] 이종목[2] 이영미*

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One of the most important challenges for the ultimate commercialization of fuel cells is the preparation of active, robust, and low-cost electrocatalysts. In particular, better electrocatalysts for the fuel cell cathode, where oxygen reduction reaction (ORR) requiring a high overpotential occurs, are needed to improve the efficiency and to lower the cost of fuel cells. In this respect, various nanostructured materials are of interest and have been studied for their catalytic activities. Since graphene was first discovered, it has been studied extensively and received great attention by scientists because of its low cost and advantageous characteristics over graphite, such as high electron mobility and intensity. Considering the high stability of Ir in acidic condition Ir is a good catalyst candidate for acidic fuel cell cathode.In this presentation, graphene coated with Ir nanoparticles is synthesized via self-assembly and characterized for its catalytic activity toward ORR. The structure, morphology and electrocatalytic activity of this product is characterized by scanning electron microscopy (SEM) and rotating disk electrode (RDE) voltammetry.

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2012-0005422).

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Fabrication of Dual Microsensor for Simultaneous Nitric Oxide and Potassium Ion

김미선 심준호[1] 이영미[2,*]

이화여자대학교 화학나노과학부 [1]대구대학교 화학·응용화학과 [2]이화여자대학교 화학나노과학과

Nitric oxide is known to be closely to potassium ion (K^+) in biological system. For instance, NO/cGMP (guanosine 3’,5’-cylic monophosphate)/K^+ channel pathways have been reported to be involved in many biological processes including vasodilation. A technique, which could analyze NO and K^+ simultaneously, would be able to provide more information to understand biological processes mediated by NO/cGMP/K^+ pathway more clearly.In this presentation, we demonstrate the development of a dual microsensor for simultaneous measurements of NO and K^+ ion. A sensor possesses two microdisks: one disk is used for amperometric NO measurement and the other is used for potentiometric K^+ measurement. Sensor performances such as sensitivity, selectivity, are characterized. As-prepared sensor is applied for the measurements at biological organ tissues. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2012-0003779).

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Synthesis and Electrochemical Characterization of Pd Nanoparticles on Reduced Graphene Oxide

조윤빈 이종목[1] 이영미*

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과

Nowadays, researchers are trying to find effective oxygen-reducing electrode materials. The best material today is platinum which still shows slow reaction rate and high overpotential. In addition, because of platinum's high price and limited supply, there are studies underway to develop alternative electrode materials. One of the most intensively studied alternative materials is palladium. In this study, reduced graphene oxide sheets (RGO) were introduced to support palladium nanoparticles (Pd NPs), providing not only high conductivity but also large surface for the immobilization. Pd nanoparticles loaded on reduced graphene oxide (Pd NPs/RGO) were prepared by reduction of metal salts and reduced graphene oxide with ethylene glycol. The morphology and electrocatalytic activity of Pd NPs/RGO for the oxygen reduction reaction (ORR) are characterized by scanning electron microscopy (SEM) and rotating disk electrode (RDE) voltammetry. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2012-0005422).

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Single Crystalline RuO_2 Nanorods Grown on a Carbon Fiber Microelectrode for NO Sensing

김수진 이종목[1] 김명화[2] 이영미*

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과 [2]이화여자대학교 화학 나노과학과

Single crystalline ruthenium oxide nanorods (RuO_2 NRs) were successfully grown on a single carbon fiber (CF, diameter = 5~10 μm) by simple thermal annealing. The morphology and structure of RuO2 NRs on CF were characterized by FE-SEM. According to the current study, RuO_2 is a good catalyst for nitric oxide (NO) oxidation. Nitric oxide is well known for its crucial physiological functions as a vasodilator, neurotransmitter, mediator of anti-tumor activities, etc. Therefore, the as-prepared CF decorated with RuO_2 NRs is tested for its feasibility as an amperometric NO microsensor. The sensor is composed of a RuO_2 NRs on CF working electrode and a Ag/AgCl counter/reference electrode. Electrochemical activities of these materials are characterized by Linear sweep voltammetry (LSV), amperometric experiments (i-t). In addition, the sensor is applied for real-time NO measurements of living organ tissues. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2012-0005422).

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Synthesis and Characteristics of PAA-PVI-Fe(CN)$_5$ Polymer and its application to Glucose Biosensor

최영봉 김기훈 이수정 김혁한*

단국대학교 화학과

A series of novel, electro-active PAA-PVI polymer of pentacyanoamminferrate ($Fe(CN)_5NH_3$) were prepared and then characterized using UV-vis spectroscopy and electrochemical techniques. The redox mediators presented here are described in shorthand as [$Fe(CN)_5$(poly(acrylicacid-4-vinylimidazole) (PAA-PVI))]$^{3-/2-}$ which were immobilized on the ITO Electrodes without or with gold nanoparticles (AuNP). The electrical signals were measured by voltammetry technique. Also, catalytical current was amplified by GOx which is electrically mediated by new iron redox film, converting the film into an electro catalysts for the electron reduction of oxidation of glucose. The resulting catalytical current was linearly related with the concentration of glucose.

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Development of Biofuel Cells using New Redox Polymer under Physiological Conditions.

이정민 조남현 박햇님 최영봉 김혁한

단국대학교 화학과

Biofuel cells have a tremendous opportunity to provide much higher energy densities and smaller footprints than batteries for powering implantable medical devices, leading to less intrusive implantable devices with longer lifetimes. The biofuel cell in this works is composed with a glucose electro-oxidizing anode and an dioxygen(O_2) electro-reducing cathode. The anodic electrocatalyst comprised the electrostatic adduct of glucose oxidase(GOx) at physiological pH(pH 7.4, 0.1 M NaCl, 37.5 °C), and the redox polymer of poly(acrylicacid-4-vinylimidazole -acrylamide) (PAA-PVI-PAA) complexed with [Os(dimethoxy-bipyrideine)$_2$Cl$_2$]$^{2+/3+}$. The cathodic electrocatalyst was electrostaic adduct of bilirubin oxidase(BOD) from Myrothecium verrucaria. also physiological pH, and the redox polymer of poly(acrylic acid-4-vinylpyridine-acrylamide) (PAA-PVP-PAA) complexed [Os(dicarboxylicacid -bipyridine)$_2$Cl$_2$]$^{2+/3+}$. And both electrodes are cross-linked on screen printed carbon electrodes(SPCEs). We have investigated the enzymatic biofuel cells that have the high potential to achieve better current densities and longer stability in physiological condition.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Nanoparticle ensemble electrode prepared on metal surface by selective passivation

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한국과학기술원(KAIST) Chemistry [1]한국과학기술원(KAIST) 화학과

Electrochemistry through nanoscale electrode achieves investigations of ultrafast kinetic reactions and useful analysis in microenvironment. Platinum nanoparticles were absorbed on gold electrode surface and gold surface has been selectively insulated by electrochemical polyphenol passivation method. Pt nanoparticle has not passivated due to slightly higher oxidation potential of phenol on Pt than on Au. Through a number of Pt nanoparticles, electron transfer reaction is possible and electrochemical reaction on this nanoparticle ensemble electrode shows similar aspect with that on nanoelectrode array.

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Dopamine And Ascorbic Acid Detection Using poly(dopamine) Formation on Indium-Tin Oxide Electrode

김병권 곽주현*

한국과학기술원(KAIST) 화학과

Dopamine is neurotransmitters which is important and widely investigated for the several decades. A deficiency of dopamine is associated with some physiological problems such as Parkinsonism, schizophrenia, and HIV infection. Therefore, the determination of the dopamine concentration is essential for disease diagnosis and for the study of physiological mechanisms. In this study, we have developed a sensitive dopamine and ascorbic acid detection method on bare indium-tin oxide (ITO) electrodes. The anodic peaks of dopamine and ascorbic acid were separated by scan rate. In case of high scan rate (5 V/s), the peaks of dopamine and ascorbic acid were effectively separated. 1 nM dopamine can be detected in the presence of 0.1 mM AA: this detection limit is very low compared to previously reported methods including those involving surface modified electrodes. Moreover, bare ITO electrodes can simultaneously detect 0.1 mM AA

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Development of new electron transfer mediator for an enzyme-based glucose sensor

김동민 **S.subba reddy** 김민영 심윤보*

부산대학교 화학과

A novel electron transfer mediator, Fe-PhenTPy was synthesized through the Paal-Knorr condensation reaction. FT-IR, 1H-NMR, 13C-NMR, and mass spectroscopy were used to analyze the structure of Fe-PhenTPy. The new Fe-PhenTPy evaluated for the potential application as an enzyme based glucose sensor. An amperometric enzymatic glucose sensor was constructed on a screen printed carbon electrode (SPCE) employing NAD-dependant glucose dehydrogenase (NAD-GDH) as a catalytic subunit and Fe-PhenTPy as an electron transfer mediator. The stability of the sensor was investigated in terms of the pH, temperature, and humidity toward glucose detection. The proposed glucose sensor exhibited a good linear range between 30 mg/dL and 400 mg/dL.

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Sponge-like Nanoporous Pd and Pd/Au Structures: Facile Synthesis and Enhanced Electrocatalysts

손정우 심준호*

대구대학교 화학·응용화학과

Palladium and palladium/gold based nanocatalysts have been investigated extensively as a key component for a variety of research fields such as environmental protection, electrochemical sensors, and fuel cells. In this study, sponge-like nanoporous Pd (snPd) and Pd/Au (snPd/Au) were prepared by a galvanic replacement reaction between a hierarchical Co nanostructure, which was fabricated on the glassy carbon substrate by cyclic voltammetric deposition of Co^{2+} ions, and K_2PdCl_4 (or $HAuCl_4$). The electrocatalytic activities of the prepared films were evaluated for oxygen reduction reaction (ORR) using rotating disk electrode (RDE) experiments in alkaline (0.1 M NaOH) conditions. Due to the increased active surface area, the nanoporous catalysts exhibited superior ORR activity (i.e., more positive onset and half-wave potentials, higher current density and greater number of electrons transferred) than commercial catalysts. This research was supported by the Daegu University Research Grant, 2012.

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Electrochemical Synthesis and Electrocatalytic Activity of Gold Nanoporous Thin Films

조승기 심준호*

대구대학교 화학·응용화학과

Gold noble metal nanocrystals have received increasing interest in various fields of chemistry due to their important roles in different branches of science, such as chemical catalysis, nanomedicines, and nanoelectronics. The intrinsic properties of a gold nanomaterial strongly depend on its size, shape, composition, crystallinity, structure, and morphology. In this presentation, we investigated the electrodeposition of gold nanoporous thin films assisted by poly(N-vinylpyrrolidone) (PVP) surfactant in different concentrations and obtained nanoporous gold (npAu) films. The npAu electrode shows possible applicability for electrochemical biosensors, enabling the efficient, ultrasensitive detection of biologically important molecules. The structure, morphology and electrocatalytic activity of the npAu films are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electrochemical analyzer. This research was supported by the Daegu University Research Grant, 2012.

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Synthesis of Pd and Pt-on-Pd Nanochain Networks for Oxygen Reduction Reaction

정인택 심준호*

대구대학교 화학·응용화학과

Development of low-Pt content cathode electrocatalyst in fuel cell has been recognized recently as one of the most important issues due to its high cost and limited supply. In particular, some approach to minimize the Pt content of electrodes has focused on the formation of small nanoparticles. In this presentation, we demonstrate a facile wet chemical strategy for preparing Pd based nanochain networks (PdNNs) and Pt decorated PdNN (Pt-on-PdNNs). The PdNNs were synthesized by simply mixing PdCl2 aqueous solution and poly(vinylpyrrolidone) (PVP) at pH = 7, followed by hydrazine hydrate reduction. For Pt-on-PdNNs, Pt was deposited spontaneously on the surface of the PdNNs. The prepared Pd based nanocatalysts, especially the Pt-on-PdNNs decorated with a very low amount of Pt, exhibited significant electrocatalytic activity and stability for the oxygen reduction reaction (ORR). This research was supported by the Daegu University Research Grant, 2012.

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Facile Synthesis and Electrocatalytic Activity of Asymmetric Core-Satellite Nanostructures

노성민 심준호*

대구대학교 화학·응용화학과

Noble metal nanoparticles are used widely in a range of electrochemical applications, such as electrocatalysis, electrochemical analysis, electrochemical synthesis, etc., due to their catalytic properties and inertness. The electrocatalytic activity of the metal nanoparticles is of great interest, particularly in the field of fuel cells. In this presentation, we demonstrate the synthesis and characterization of asymmetric Au nanoparticles (AuNPs) core-AuPd nanoparticles (AuPdNPs) satellites nanocomposites. The asymmetric core-satellite (CS) nanoassemblies exhibited significantly enhanced catalytic activity toward the ORR as well as the biologically important molecules. This research was supported by the Daegu University Research Grant, 2012.

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Impedimetric analysis of Graphene and its applications at different platforms

AKHTARMAHMOODHASSAN **K.Sudhakara Prasad** 김동민
MALENAHALLIHALAPPANAVEEN 심윤보*

부산대학교 화학과

Graphene, which is an allotrope of carbon having 2D crystal structure, has been successfully synthesized with the modified Hummer`s method. UV, FT-IR, TEM and AFM study showed good quality of synthesized material. Due to the valence and conduction bands touch in two independent points called K and K`; graphene acts as zero-band gap semiconductor and has good electrical conductivity merit attention. Even though at zero-level carrier’s density, its conductivity does not vanish linearly. Considering this aspect, we investigated its electrical behavior in terms of impedance. Under different circumstances, with sonication method, it showed more optimized characteristics which have further applicability in sensing.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Voltammetric Detection of Neurotransmitters with Nano-structured Iridium Oxide

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One of the most important neurotransmitter in brain is dopamine because its deficiency can cause neurological disorder such as Parkinson's disease. Epinephrine is another important neurotransmitter and has many roles in sympathetic and parasympathetic nerve regulating blood vessel and heart rate. Dopamine and epinephrine detector using nano-structured Iridium oxide was thus studied. Nano-structured Iridium oxide on gold microwire (d = 25 μm) (IrO_2-Au) was synthesized by chemical vapor deposition (CVD) and morphology was characterized by field emission scanning electron microscope (FE-SEM). Differential pulse voltammetrys (DPVs) experiments showed successfully that IrO_2-Au responded selectively to dopamine (DA) and epinephrine (EP) against ascorbic acid (AA) which is major interferent for sensing neurotransmitters. Calibration plot of DA and EP in presence of AA showed sensitivity of DA and EP were 90.2 μA mM^{-1} and 19.3 μA mM^{-1}, repectively.

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Nonenzymatic Glucose Detection with Hollow Gold Nanoparticles

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Recently importance of nonenzymatic glucose detection applying nano-structured material increases to supplement drawbacks of enzymatic sensor, e.g., complexity of device and instability with change of pH and temperature. To match this goal, in present study, hollow gold nanoparticles (hAuNPs) were synthesized in aqueous system containing Co and Au precursor and applied to electrochemical glucose detection. The morphology of hAuNPs was characterized by field emission scanning electron microscope (FE-SEM) and high-resolution transmission electron microscope (HR-TEM). Cyclic voltammetrys (CVs) in acidic condition show that real surface area (RSA) of hAuNPs was enlarged by 40 times at least compared with that of bulk Au electrode. Rotating disk electrode (RDE) voltammetry was performed to find the appropriate potential for glucose oxidation. In amperometric i-t curves at Eapp (applied potential) of -0.1 V, the sensitivity of glucose was 3.86 ?A mM-1 which is much higher than interferent signals such as ascorbic acid (AA), acetamidophenol (AP) and dopamine (DA).

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Synthesis and physio-chemical characterization of terthiophene biphenyl acid

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A novel terthiophene biphenyl acid (TTBPA) was synthesized and characterized by FT- IR, 1H & 13C NMR, mass spectroscopy, and elemental analysis. The synthetic route involves three steps including hydroboration, Suzuki coupling, and a cyano group was converted into carboxylic acid through the alkaline hydrolysis to get the title compound (TTBPA). The monomer was electrochemically polymerized on the GC and Pt electrodes, then poly-TTBPA film was characterized by voltammetry, impedance spectrometry, and in situ UV- Visible spectroscopy.

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Preparation of gold nanoparticles based electrode for the determinaion of piroxicam and pyridoxine

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This work describes the first electrochemical separation of piroxicam (PX) and pyridoxine (PY) using the gold nanoparticles (AuNPs) modified glassy carbon (GC) electrode. The synthesized AuNPs were characterized by UV-Visible and TEM and were fabricated on the GC surface. The cyclic voltammogram and impedance analyses show that the electron transfer reaction was more facile at the AuNPs based electrode. Hence, AuNPs based electrode was used for the voltammetric separation of PX and PY.

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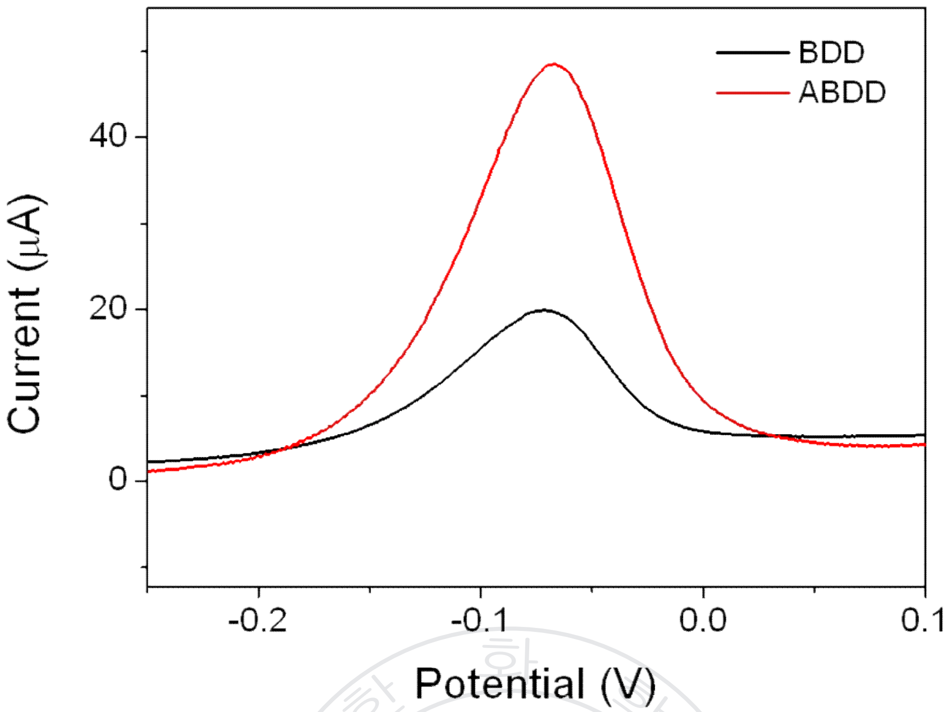
Electrical and structural properties of the electrode was deposited gold nanoparticles on BDD

차유정 한송이 권나현 윤장희

한국기초과학지원연구원 부산센터

Au nanoparticle modified boron-doped diamond (ABDD) electrodes were prepared by simple sputtering method. Au electrode is highly sensitive and has low resistivity. However, It has narrow potential window and unstable baseline. In addition, Au is very expensive. Boron-doped diamond(BDD) thin film is new electrode material that has received great attention recently because it possesses several technologically important characteristics such as an inert surface with low adsorption properties, remarkable corrosion stability, even in strong acidic media, and an extremely wide potential window in aqueous and non-aqueous electrolytes. Therefore, the electrodes were made by combining the advantages of Au and BDD. ABDD electrodes were showing wide potential window and clear peak of detection of heavy metal ion. ABDD electrodes have high detection sensitivity and intensity than BDD electrodes.


BDD
ABDD
Current (μA)
0
20
40
-0.2
-0.1
0.0
0.1
Potential (V)

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Adlayer structures of the Trimesic acids on Au(111) depend on potentials

오성훈 신동완 이충균*

충남대학교 화학과

The TMA ad-structures on Au(111) strongly depend on the potential. At -0.1 V, TMA adsorbs molecularly and forms a nanoporous network of (6×6). Without potential control (i.e., at OCP), the TMA adlayer is most likely to be a contoured nanoporous network of crown-like primary hexagons made up of six non-flat-lying TMAs in a (5√3×5√3)R30° arrangement. One carboxylic acid of each TMA in the primary structure is de-protonated to anchor on Au(111) via anionic adsorption. The existence of such carboxylate anions in the network of (5√3×5√3)R30° is supported by the selective adsorption of Cu2+ ions and thiols into the nanoporous network. Furthermore, the contoured network explains the various observed properties distinguishing from those of the (6×6) honeycomb structure of flat-lying TMA. The potential shift to a higher potential like 0.25 V induces further de-protonation of TMA adsorbates to the arrays of anionic dimers without nanopores.

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Direct electrochemistry of glucose oxises based on aminothiophenol-Pd bonded to electrochemically reduced graphene oxide

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A glucose biosensor was prepared by glucose oxidase and electrochemically reduced graphene oxide (ERGO) grafted with aminothiophenol (ATP), and covalently bonded to palladium (Pd) nanoparticles (NPs) on to glassy caron electrode (GCE). The Nafion/ GOx/ ERGO-ATP-Pd/GCE was easily prepared in a rapid and simple procedure, and its application is improved the sensitive of glucose determination. It's activity and exhibited a suface controlled, two-proton and two-electron transfer reaction with a fast heterogeneous electron transfer rate constant (k_s) of 3.82 s^{-1}. Meanwhile, the results obtained from each cyclic voltammetry (CV) and amperometric methods for glucose determination were comparable. Result of the amperometric method, the line of regression equation was obtained even at the low concentration region of 10 μM. The proposed glucose biosensor exhibited a wide linear response range of 10 μM ? 5 mM during amperometric testing using an applied potential of -0.45 V (*vs* Ag/AgCl) in pH 7.4 PBS buffer, with a low detection limit of 1.07 μM (S/N =3). The Michaelis-Menten constant (K_M) was calculated to 0.94 mM. The biosensor was showed good stability and selective is able to include by AA and UA. These results indicate that the Nafion/GOx/ERGO-ATP-Pd/GCE have application of glucose detection.

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Electrochemical biosensor based on electrochemical reduction of GO-FeP/GCE for determination of Dopamine

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It is reports the synthesis of graphene using a modified Hummer's method and its application for the electrochemical detection of dopamine. GO-FeP reacted with hydroxyl groups grafted onto the surface of GO and amino group of FeP. The amide bonding formed by combining the amino group of FeP and graphene oxide. The GO-FeP has characterized by FT-IR, UV-Vis spectroscopy and XPS. The electrochemical reduction (ECR) GO-FeP is possibilities for employing to electrochemical detection of dopamine. It is important to develop sensitive sensor for the determination of dopamine without the interference by ascorbic acid. Electrocatalytic activities are verified to CV and DPV in 0.1 M phosphate buffer solution (PBS). And then, it is carried out about the influence on the amount of ECR GO-FeP, solution pH (4.08~9.0) on the electrocatalytic oxidation of DA and interference experiments interfering substances such as serotonin, UA, glucose, hydrogen peroxide. The electrochemical results at DPV are showed detection limit of DA 6.23×10^{-2}μM, detection limit of UA 10.8×10^{-2} μM (where s/n = 3), detection range 1.0~400 μM at the ECR GO-FeP modified glassy carbon electrode (GCE).

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Synthesis of thiophene-functionalized graphene and its application to sensor and electrochromism

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Graphene oxide (GO) was functionalized with thiophene derivatives. The GO-thiophene was electrochemically reduced to thiophene-functionalized graphene(TFG) at a potential range of 0 ~ -1.5 V and used in electrochemical biosensing for dopamine and serotonin. The TFG-modified electrode showed the advantages of excellent electrocatalytic activity toward dopamine and serotonin simultaneously. The TFG was characterized by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS) and electrochemical impedance spectroscopy (EIS), UV-vis, IR, Raman spectroscopy. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used to characterize the biosensors' performance. The proposed biosensor exhibited a wide linear range and a low detection limit with a fast response time. Meanwhile, electropolymerization of TFG gives efficient electrochromic materials.

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Electrochemistry of quinone-functionalized graphene and its application to molecular sensing

윤미라 전승원

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Graphene oxide (GO) functionalized with quinone derivatives. The GO-quinone was electrochemically reduced to quinine-functionalized graphene (QFG) at a potential range of 0 ~ -1.5 V and used in electrochemical biosensing for superoxide and hydrogen peroxide(H2O2). The QFG-modified electrode showed the advantages of excellent electrocatalytic activity toward H2O2 in PBS solution. The QFG was characterized by UV-vis, IR, Raman spectroscopy, transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), energy dispersiveX-ray spectroscopy (EDS) and electrochemical impedance spectroscopy (EIS). Cyclic voltammetry (CV) and chronoamperometry (CA) were used to characterize the biosensors' performance. The proposed H2O2 biosensor exhibited a wide linear range and a low detection limit with a fast response time. The biosensor therefore demonstrated excellent capability as a candidate for superoxide and H2O2 analysis.

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Nonenzymatic glucose sensors based on thiolated cabon material bonded to Pt nanoparticles

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A nonenzymatic glucose biosensor based on thiolated multiwall carbon nanotube bonded to Pt nanoparticles (MWCNTs-Pt) was developed. The MWCNTs-Pt was characterized by transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS). Nafion/MWCNTs-Pt/GCE was simply and quickly prepared; it showed improved sensitivity of glucose determination. Cyclic voltammetry (CV) and chronoamperometry (CA) were used to characterize the biosensors' performance. Amperometric testing demonstrated the sensor's fast responses with linear regression observed even at very low concentrations below 1.0 mM. Linear responses to glucose were observed between 1mM and 20 mM at an applied potential of 0.0 V. The sensor demonstrated fast responses and good stability.

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수은 전극(Mercury electrode)을 이용한 퍼클로레이트(Perchlorate)의 전기적 환원 분해

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연세대학교 화학과 [1]건국대학교 응용화학과

전기화학적인 방법을 이용한 분해는 전처리과정이 비교적 간단하여 필요한 시간을 단축시킬 수 있으며 산화, 환원 반응 (Redox reaction)을 쉽게 조절함으로써 활용가치가 매우 높은 기술이라고 할 수 있다. 퍼클로레이트 (Perchlorate)는 갑상선 암을 유발하는 위험요인이고, 미국 기준치가 강화되고 있는 만큼 한국에서도 이를 대비하는 분해 기술이 필요하다. 그 중 암모늄 퍼클로레이트 (Ammonium perchlorate)는 공업적으로 가장 많이 제조 되고 있는 퍼클로레이트솔트 (Perchlorate salt)로 이를 분해하는 연구를 진행 하였다. 지금까지 전기적 방법을 이용한 연구는 많이 진행되었으나 효율적으로 제거한 경우는 많지 않다. 따라서 계속해서 새로운 전극을 개발하고 분해조건을 최적화하여 효율성을 높이는 연구가 필요하다. 본 연구에서는 3 전극 시스템을 사용하였고, 수소 과전압이 큰 수은 작업 전극 (Mercury working electrode)을 작업전극으로 사용함으로써, 다른 물질의 환원 반응을 방해하지 않도록 하였다. 작업 전극으로 사용하였다. 기준전극(Reference electrode)은 Ag/AgCl (sat.NaCl)을 사용했고, 상대전극 (Counter electrode)은 백금 (Platinum)을 사용하였다. 순환전압전류법 (Cyclic voltammography)을 사용하여 환원전위 (Reduction potential)를 확인하고, 시간대 전류법 (Chronoamperomety)을 사용하여 퍼클로레이트를 전기적으로 환원 분해 (Electrochemical reduction)하였다. 또한 용액의 종류와 농도, pH, 온도 조건을 최적화하여 분해연구를 실행하였다.

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Graphite oxides for anode materials in secondary Ion batteries

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Addressing the challenge to produce new materials for lithium ion batteries (LIB) anode, which can simultaneously achieve high power, high energy capacity and stability, we present a facile route to synthesize a graphite oxide (GTO)-SnO_2 nanocomposite (SGT). SGT was developed in a one-step process by reacting GTO in a mixture of DMSO/H2O and Sn^{4+}(at different weight ratios), followed by subsequent thermal reduction (r-SGT). The r-SGT (SnO_2=80wt%) is proven as a promising anode for high capacity anode materials. The r-SGT delivers a very high reversible capacity of ca. 761 $mAh.g^{-1}$ (76 % retention) at the end of 50 cycles at a charge/discharge current density of 100 $mA.g^{-1}$, in performance in contrast to SG nanocomposite (graphene oxide/SnO_2 nanocomposite) which showed a lower capacity (ca. 535 $mAh.g^{-1}$) and faster fade (48 % retention). The high Li storage capability of the r-SGT nanocomposite is based on the fact that nanometric SnO_2 particles, dimensionally confined by an optimized ratio of partially exfoliated graphitic layers, can substantially relieve the mechanical strain upon lithiation, create pore channels for Li diffusion, thereby leading to near theoretical specific capacity.

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전자빔을 이용한 TiO_2의 합성 및 전기화학적 특성 분석

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충남대학교 녹색에너지기술전문대학원

리튬이온 전지의 음극소재 중에서 $Li_4Ti_5O_{12}$(LTO)를 비롯한 Ti 계 소재는 탄소계 음극에 비해 작동전압이 높아 전해질 분해반응이 일어나지 않아 SEI(Solid Electrolyte Interface)가 형성되지 않는 특성이 있다. 이로 인해 초기 충방전 효율이 100%에 가깝고, SEI 에 의한 저항성분이 없어 탄소계 음극에 비해 우수한 충방전 출력 특성을 나타내므로 고출력용 음극소재로의 적용이 기대되는 물질이다. 또한 LTO 의 고출력화를 위해 리튬이온의 확산경로를 줄이기 위한 나노크기의 합성법도 고려되어야한다. 이에 본 연구는 전자빔을 이용하여 LTO 의 전구체인 TiO_2 를 나노 크기로 합성하고 이 소재의 전기화학적인 특성을 분석하였다. 다음 단계로는 전자빔 조사법을 이용하여 전기화학 반응없이 LTO 를 합성하고자 한다.

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Enhanced ECL of $Ru(bpy)_3^{2+}$ at ITO modified with Pt DENs

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우리는 이번 연구에서 Indium tin oxide (ITO) 전극의 투명하다는 장점을 유지하면서 향상된 Electrogenerated chemiluminescence (ECL) signal을 얻기 위하여 ITO 전극 표면을 Pt Dendrimer encapsulated nanoparticles (Pt DENs) 으로 고정화 하였다. Pt DENs 은 amine-terminated polyamidoamine (PAMAM) dendrimer 를 이용하여 합성하였다. 합성된 Pt DENs 은 electrografting 방법으로 ITO 전극 표면에 고정화하였으며 이 경우 PAMAM dendrimer의 아민 말단기를 이용하여 PAMAM dendrimer를 ITO 전극 표면에 고정화함으로써 Pt nanoparticles를 비교적 간단한 방법으로 ITO 전극 표면에 고정화할 수 있다. Ruthenium Tris(2,2')bipyridyl ($Ru(bpy)_3^{2+}$)/Tripropylamine (TPrA) system 에서 Pt DENs 이 고정화된 ITO 전극은 PAMAM dendrimer 가 고정화되어 있는 ITO 전극이나 bare ITO 전극과 비교해보았을 때, 눈에 띄게 향상된 ECL signal 을 방출하였다. 이 결과는 Pt DENs 에 의해 $Ru(bpy)_3^{2+}$와 TPrA 의 산화가 촉진되었기 때문이다.

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Self-assembled SnO_2/graphene nanocomposites with alternating oxide and amine layers as advanced anode material for Li ion batteries

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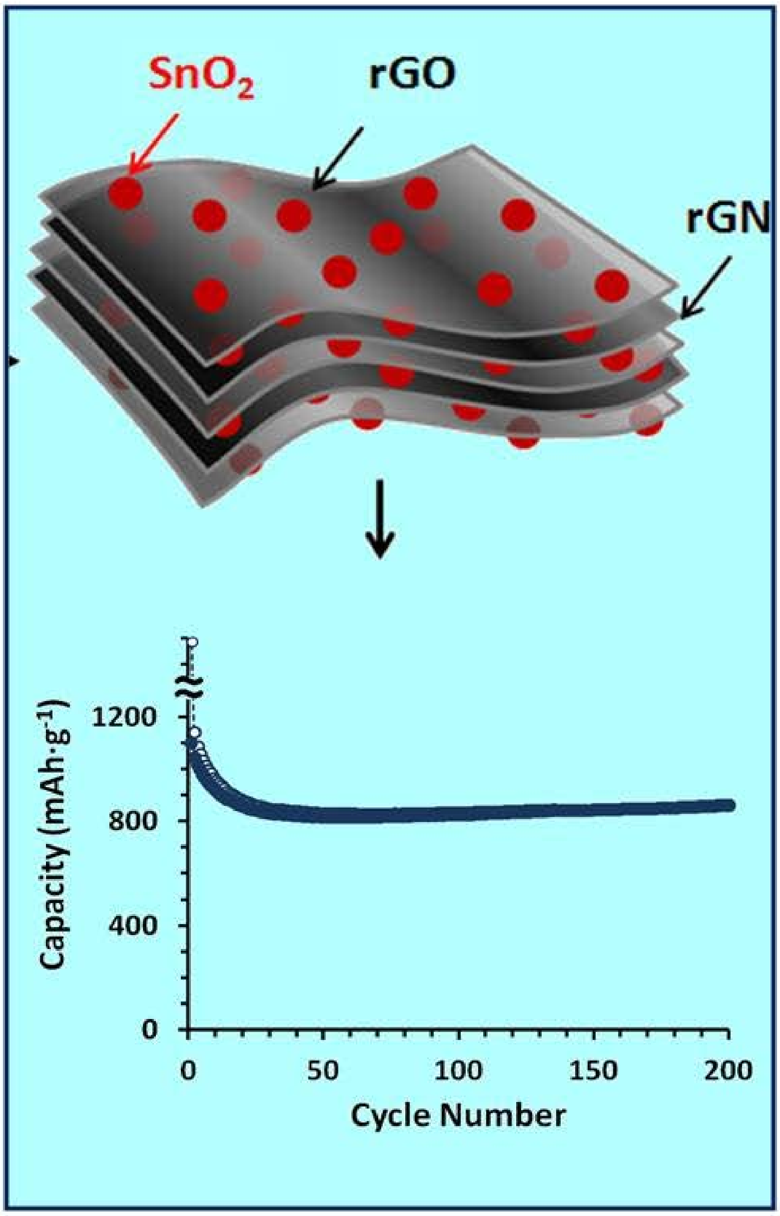
Self-assembled nanostructures with well-controlled architecture involving multiphase building blocks for the synthesis of layered nanocomposites consisting graphene and metal oxides as electrodes for energy storage have been dealt with limited success. We report a new layered nanocomposite r(SG/GN) consisting alternating layers of graphene and SnO_2 nanoparticles by performing a self-assembly of oppositely charged Sn^{2+} anchored graphene oxide (GO) and amine-functionalized graphene (GN) in solution without the aid of additional hybridization with charged nanomaterials. The simple synthetic procedure, results in well-organized, well-ordered, highly stable and densely stacked layered structure (driven by the electrostatic pre-aligning of GO and GN and strong π-π stacking interactions between graphene layers), which were confirmed through cross-sectional SEM, HR-TEM, Raman and BET studies. We investigate the Li-ion insertion properties of the r(SG/GN), which can achieve near theoretical specific capacity (870 $mAh \cdot g^{-1}$ after 200 cycles at a rate of 100 $mA \cdot g^{-1}$.), enhanced cyclic performance at very high rate charge and discharge conditions, remarkable capacity increase with extended cycling (unlike the expected fade observed with graphene supported SnO_2 composites) and large suppression in electrode volume change and pulverization.


SnO₂
rGO
rGN
Capacity (mAh·g⁻¹)
1200
800
400
0
0
50
100
150
200
Cycle Number

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발표종류: 포스터, 발표일시: 수 16:00~19:00

N-Doped Graphene Nanosheets as Anode Materials for Sodium Ion Batteries

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순천대학교 인쇄전자공학과 [1]순천대학교 화학과

Sodium ion batteries (SIB) have recently gained identification as a fascinating alternative to lithium ion batteries mainly due to their low cost and reliable electrochemical energy storage applications[1]. Nitrogen doped graphene nanosheets have concerned extensive interest in the field of energy storage applications. In the N-doped carbon, N-doping can generate extrinsic defects, and hence enhance the reactivity and electronic conductivity and can adsorb Na ions and hence improve the sodium storage performance. The doping levels of N in reduced graphene oxide (N-rGO) was varied and optimized by changing factors such as temperature and doping conditions. The doping levels were compared with pristine reduced graphene oxide (rGO) by XPS, FTIR and Raman techniques.In this work, we have synthesized N-rGO and investigated their electrochemical performance of Na intercalation properties compared to rGO. In lieu of the advantage of N doping, a higher storage capacity of Na^+ is expected in N-rGO. The higher conductivity and disorder structure created in the stacking of graphene by N doping and sintering conditions are also expected to contribute to the enhanced electrochemical performance.*Reference*1. V. Palomares, P. Sarras, I.Villaluenga, K.B. Huseo, J. Carretero-Gonzalez, T.Rojo, Energy. Environ. Sci., 2012, 5, 5884.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Surface Modification of Indium Tin Oxide Electrode with Dendrimer-Encapsulated Nanoparticles

이순보 주영원 김여주 김주훈*

경희대학교 화학과

이번 발표에서는 electrografting 을 이용하여 indium tin oxide (ITO) 전극에 선택적으로 dendrimer-encapsulated nanoparticles (DENs)를 고정화하고, 전극에 형성된 amine 작용기를 이용하여 biologically active material 을 전극에 도입하는 과정을 소개한다. 약 2 nm 이하의 크기를 갖는 DENs 를 합성하여 ITO 전극에 고정화하였고, 전기화학적 방법, X-ray photoelectron spectroscopy 그리고 optical microscope 이미지를 통해 electrografting 이 physisorption 보다 5 - 10 배 DENs 의 고정화에 효과적임을 확인하였다. 그리고 전극에 형성된 amine 작용기를 이용하여 biologically active material 을 고정할 수 있음을 확인하였다. 이번 연구의 결과로 ITO 전극을 다양한 nanoparticles 와 biologically active material 로 functionalization 할 수 있음을 확인하였고, electrochemical bioanalysis 에 응용될 수 있을 것이라 기대한다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

고등학교 화학Ⅱ 교과서에 제시된 화학평형이동 실험분석과 Microscale Gas Chemistry에 기초한 실험 개선

조은희 최병순[1]

인천해송고등학교 녹색과학부 [1]한국교원대학교 화학교육과

이 연구는 고등학교 화학Ⅱ 교과서에 제시된 화학평형이동 단원의 실험을 수행하여 문제점을 분석하고 주사기 과학을 적용한 개선된 실험방안을 모색한 것이다. 분석한 교과서 모두 화학평형이동 실험으로 이산화질소와 사산화이질소의 가역반응을 제시하였으며, 한 교과서에서만 반응물질의 양을 정확히 제시했다. 실험 과정을 분석한 결과, 이산화질소와 사산화이질소의 가역반응 실험은 기체발생 실험과정과 발생된 기체의 포집 과정에서 기체 압력에 의한 폭발의 위험과 독성기체의 다량 배출 등의 위험이 있어 학생 조별 실험 시 많은 주의와 환기가 필요했다. 따라서 이러한 문제를 극복하기 위해 Microscale Gas Chemistry 에 기초하여 개선된 실험을 개발하고, 이를 인문계 고등학교 3 학년 학생 134 명을 연구대상으로 개선된 실험을 적용한 수업과 전통적인 교과서 실험수업을 비교하였다. 학생들은 개선된 기체발생 실험 장치는 전통적 실험 장치보다 안전성면에서 매우 긍정적이라고 응답하였으며, 실험이 원활히 진행되어 재현성 있는 결과를 얻을 수 있어서 실험과정에서 생기는 의문점등을 잘 해결할 수 있었다고 응답했다. 이러한 연구결과는 Microscale Gas Chemistry 적용 실험수업을 현장에서 활용하기 위하여 교사 대상 실험연수 기회가 확대될 필요가 있음을 시사한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램의 영향

양찬호 노태희*

서울대학교 화학교육과

이 연구에서는 과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램을 개발하고 적용하여 그 영향을 과학 탐구의 본성을 직접 가르치지 않은 암시적 탐구 수업과 비교하였다. 또한, 개발된 탐구 학습 프로그램에 대한 학생들의 인식을 조사하였다.

과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램은 중학교 2 학년 '물질의 특성' 단원 중 밀도 개념을 목표 개념으로, Schwartz 등(2008)이 정의한 '과학적 탐구 방법의 다양성', '자료에 대한 타당한 해석의 다양성', '자료와 증거의 차이', '과학 탐구의 목적'을 과학 탐구의 본성으로 선정하여 개발하였다. 탐구 학습 프로그램은 Bybee(2000)의 과학 탐구 교수의 세 가지 요소를 바탕으로 학생들이 과학 탐구를 직접 수행하고 이와 관련된 과학 탐구의 본성 측면을 함께 학습하도록 하며, 소집단 토론을 통해 과학 탐구의 본성을 명시적-반성적으로 학습하도록 구성하였다.

서울시에 소재한 중학교의 2 학년 학생들을 두 집단에 배치하였다. 사전 검사로 과학 수업에 대한 즐거움 검사를 실시하였다. 총 5 차시 동안 수업 처치를 실시하였다. 처치 집단에서는 과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램을 실시하였고, 비교 집단에서는 과학 탐구의 본성과 관련된 내용을 제외하고 처치 집단과 동일한 탐구 활동을 사용한 수업을 실시하였다. 사후 검사로 과학 탐구에 대한 인식론적 견해, 과학 성취도, 과학 수업에 대한 즐거움, 수업에 대한 인식 검사를 실시하였다. 또한, 처치 집단의 학생 중 임의로 10 명을 선정하여 반구조화된 면담을 실시하였다.

연구 결과, 과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램이 암시적 탐구 수업보다 학생들의 과학 탐구에 대한 인식론적 견해를 향상시키는데 효과적인 것으로

나타났다. 또한, 처치 집단의 수업에서 탐구 활동 및 개념 학습의 비중이 상대적으로 적었음에도 비교 집단과 과학 성취도가 유사한 것으로 나타났다. 그러나 과학 수업에 대한 즐거움 측면에서 차이가 없었던 결과는 과학 탐구의 본성에 대한 명시적-반성적 탐구 학습 프로그램이 학생들에게 인지적 부담을 줄 가능성이 있음을 의미한다. 실제로 학생들은 소집단 토론 활동이나 과학 탐구의 본성에 대한 이해, 자신의 생각을 글로 쓰고 발표하는 활동 등을 수업에서의 어려움으로 인식하는 것으로 나타났다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

발성사고법을 이용한 학생들의 과학 글쓰기 과정 탐색

유지연 <u>강석진</u>[1] 노태희[*]

서울대학교 화학교육과 [1]전주교육대학교 과학교육과

최근에는 효과적인 과학 글쓰기 전략 개발을 위해 완성된 글뿐 아니라 글쓰기에서 나타나는 학생들의 인지 과정에 대한 종합적인 이해가 강조되고 있다. 이 연구에서는 학생들의 과학 주제에 대한 문제 해결 글쓰기 과정의 특징을 분석하였다. 의사소통 기술과 성취수준을 고려하여 선정된 중학교 2 학년 학생 7 명을 대상으로 발성사고법을 활용한 글쓰기 활동을 한 후 면담을 실시하였다. 연구 결과, 학생들의 문제해결 글쓰기 과정은 아이디어나 내용의 생성, 글의 개요 조직, 구체적인 목표의 설정, 생성한 내용의 변환, 글에 대한 평가 및 수정의 6 가지 과정 요소로 분류되었다. 또한 학생에 따라 각 과정 요소가 나타나는 빈도나 순서의 측면에서 차이가 있었다. 글쓰기 과정에서 과정 요소들이 나타나는 유형을 체계적 전략, 암묵적 계획 전략, 시행착오 전략, 임의적 전략의 4 가지로 분류하였다. 전략의 유형에 따른 가장 두드러진 차이는 개요 조직이었다. 시행착오 전략이나 임의적 계획 전략에서는 개요 조직 과정이 없음으로 인해 시행착오가 나타나거나 글의 완성도가 낮은 경향이 있었다. 암묵적 계획 전략 유형에서는 개요 조직이 암묵적으로 이루어져 글의 흐름이 명확하지 못하는 문제가 있었다. 평가 측면에서도 전략 유형에 따른 차이가 나타났다. 임의적 전략의 경우에는 체계적인 평가가 전혀 이루어지지 못하였고, 암묵적 계획 전략이나 시행착오 전략에서는 조직 평가가 나타나지 않았다. 이에 대한 교육적 함의를 논의하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

화학평형 이동시 반응속도 변화에 대한 그래프를 이용한 교수방법의 효과

최병순[*] 염은숙[1]

한국교원대학교 화학교육과 [1]청주여자상업고등학교 방과후 부서

이 연구에서는 고등학교에서 심화선택 과목으로 화학Ⅱ를 선택한 3 학년 학생 132 명을 대상으로 화학평형 이동시 반응속도 변화에 대한 수업에서, 그래프를 이용한 수업이 화학평형 이동 시 반응속도 변화를 이해하는데 도움이 되는지를 연구하였다. 연구 결과, 화학평형 이동시 반응속도 변화에 대한 학생들의 이해는 그래프를 이용해 학습할 때 높았으며, 그 효과는 학업성취 수준이 높을수록 좋았다. 그러나 그래프 해석을 언어로 표현하는 데는 학업성취 수준에 관계없이 모든 학생들이 어려움을 느끼는 것으로 나타났다. 문항에 대한 심층 분석 결과, 평형 이동시 역반응 속도의 변화에 대해 일부 학생들은 ‘정반응과 반대 반응이므로 속도도 반대로 나타난다.’ 와 같이 기계적으로 진술하였으나, 그래프를 이용한 학습이 이와 같은 기계적 해석을 감소시킨 것을 알 수 있었다. 그러나 그래프를 이용한 수업도 학업성취 수준이 낮은 학생들에게는 효과가 없는 것으로 나타나, 이들을 위한 맞춤형 교수전략이 요구된다 하겠다.

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TIMSS 2011 결과 분석(I): 초등학교 화학영역문항에 대한 과학 학력 추이 분석

공영태

진주교육대학교 과학교육과

국제적인 과학 학력 비교 조사로 널리 알려진 TIMSS(Trends in International Mathematics and Science Study)는 4 년 주기로 이루어지고 있으며 4 학년(초등학교 4 학년)과 8 학년(중학교 2 학년) 학생들의 수학 및 과학성취도를 조사하고 있다. TIMSS 조사의 원래 목적은 매스컴에서 발표되는 국가별 순위를 매기는 것이 아니라 국제적인 수준에서 비교하고 그 변화를 파악하여 참여국들의 교수학습의 실제와 교육 정책을 상호 비교할 수 있는 정보를 제공하려는데 그 목적을 두고 있다.지난 연말에 발표된 TIMSS 2011 조사결과에 따르면 우리나라 초 4 학생의 수학 성취도는 2 위, 과학 성취도는 1 위, 중 2 학생의 수학 성취도는 1 위, 과학 성취도는 3 위로 매우 높은 성취를 보였다. 이번 연구에서는 초등학교 화학영역문항에 대한 우리나라 아동들의 과학학력추이분석을 행하고자 하였다. 지난 TIMSS 2003 및 TIMSS 2007 조사 결과에 기초하여 우리나라 아동의 추이분석을 행함으로써 이로부터 얻어지는 결과는 국제수준에서 합의된 교육과정 내용에 기초하여 과목별 성취도를 파악하고, 나아가 각종 배경변인과 학생들의 학업 성취도와의 연계분석을 근거로 성취 결정 요인을 분석하여 교육 개혁의 방향을 설정하고 교육과정 정책을 수립하기 위한 기초 자료로 활용될 수 있을 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

TIMSS 2011 결과 분석(II): 중학교 화학영역문항에 대한 과학 학력 추이 분석

공영태

진주교육대학교 과학교육과

국제적인 과학 학력 비교 조사로 널리 알려진 TIMSS(Trends in International Mathematics and Science Study)는 4 년 주기로 이루어지고 있으며 4 학년(초등학교 4 학년)과 8 학년(중학교 2 학년) 학생들의 수학 및 과학성취도를 조사하고 있다. TIMSS 조사의 원래 목적은 매스컴에서 발표되는 국가별 순위를 매기는 것이 아니라 국제적인 수준에서 비교하고 그 변화를 파악하여 참여국들의 교수학습의 실제와 교육 정책을 상호 비교할 수 있는 정보를 제공하려는데 그 목적을 두고 있다.지난 연말에 발표된 TIMSS 2011 조사결과에 따르면 우리나라 초 4 학생의 수학 성취도는 2 위, 과학 성취도는 1 위, 중 2 학생의 수학 성취도는 1 위, 과학 성취도는 3 위로 매우 높은 성취를 보였다. 이번 연구에서는 중학교 화학영역문항에 대한 우리나라 아동들의 과학학력의 추이분석을 행하고자 하였다. 지난 TIMSS 2003 및 TIMSS 2007 조사 결과에 기초하여 우리나라 아동의 추이분석을 행함으로써 이로부터 얻어지는 결과는 국제수준에서 합의된 교육과정 내용에 기초하여 과목별 성취도를 파악하고, 나아가 각종 배경변인과 학생들의 학업 성취도와의 연계분석을 근거로 성취 결정 요인을 분석하여 교육 개혁의 방향을 설정하고 교육과정 정책을 수립하기 위한 기초 자료로 활용될 수 있을 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

중학생 대상 과학 도서 독후활동 프로그램 개발

김경은 한재영[1]

남성중학교 과학 [1]충북대학교 사범대학 화학교육과

독서 교육은 소양(literacy)을 기르고 자기주도적으로 학습을 하도록 하는 데 중요한 역할을 한다. 독서 교육을 위해서는 도서를 안내하고 독서 시간을 확보해주는 것 뿐 아니라, 재미있고 다양한 독후활동을 통해 동기를 부여하고 독서의 효과를 높이는 것이 필요하다. 이러한 독서 교육은 국어 교과 이외의 다른 여러 교과의 학습과 연계되어 이루어질 필요가 있다. 독서 교육이나 독후활동에 대한 연구는 초등학교 학생을 대상으로 주로 이루어지고 있으며 중학생을 대상으로 과학과 같은 특정 교과에 대하여 수행한 연구는 매우 적다. 이 연구에서는 중학교 과학 학습에서 과학 도서를 활용하는 방안을 마련하기 위해 독후활동 프로그램을 개발하였다. 중학교 1 학년에서 배우는 과학 내용과 관련되고 중학생의 수준에 적합한 도서를 탐색하고, 독서를 한 후 하는 다양한 형태의 정리활동을 조사하였다. 독후활동으로 4 컷 만화 그리기, 시 작성하기, 편지쓰기, 기사문 작성하기 등을 선정하고, 적절한 과학 도서와 연결지어, 실제 과학 수업에서 활용할 수 있는 과학 도서 독후활동 프로그램을 개발하였다. 개발한 프로그램과 그 일부를 수업에 활용한 결과를 예시함으로써 중학교 대상 과학 독후활동의 적용 가능성을 제안하고자 한다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

과학고 학생들의 개인차에 따른 과제연구의 수행과 그 결과에 대한 인식 : 사고양식과 학습양식을 중심으로

신동선 김봉곤[1,*]

경남과학고등학교 과학교육부 [1]경상대학교 화학교육과

과제연구는 연구를 통한 영재교육 프로그램으로 대부분의 과학고 정규 교육과정에 개설되어 있다. 과제연구의 목표는 학생들이 자기주도적으로 연구문제(과제)를 해결하는 과정에서 과학적 연구방법을 경험하고 과학적 태도를 함양하며, 이를 통해서 문제해결력을 기르는데 있다. 과제연구는 특수목적고인 과학고의 설립취지와도 부합되는 교과로서 매우 중요하지만, 학생들의 교과목에 대한 흥미와 관심, 자발적인 참여 등에서 상당한 차이를 보이고 있다. 따라서 과제연구의 효과적인 운영방안을 모색하기 위해서, 과학고 학생들의 개인차(individual difference)에 따른 과제연구의 인식과 학습효과에 대해서 질적 연구를 수행하였다. 연구는 경남소재 G 과학고 화학영재학급 소속 학생 전원을 대상으로 하였으며, 학생들의 개인차는 Sternberg 사고양식과 Kolb 학습양식 검사지를 사용하여 개인의 특성을 분석하였다. 과제연구에 대한 인식은 과제 연구의 필요성, 연구 주제 선정, 문제 해결과정, 지도교사나 외부 전문가의 역할에 대한 인식, 과제 연구의 성과에 관한 내용으로 인터뷰 프로토콜을 개발하여 심층 면담에 활용하였다. 본 연구의 수행결과, 모든 학생들이 과학고 교과로써 과제연구의 필요성에 대해서 긍정적으로 인식하고 있었다. 그리고 과제연구는 팀 활동으로 이루어지는 교과이므로 다른 사고양식을 가진 학생들의 조합일수록 수행과 그 효과에 대한 긍정적인 인식이 높게 나타났다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

2007개정 및 2009개정 교육과정에 의한 과학 교과서의 MBL 관련 내용 분석

김학범 차정호*

대구대학교 과학교육학부

실험과 동시에 실시간으로 실험값 측정 및 기록이 가능한 MBL(microcomputer-based laboratory)이 국내에 도입된 지 오랜 시간이 지났다. 그동안 MBL 과 관련된 연수나 자료 개발에 많은 시도가 있었으며, 2 차례의 교육과정 개편을 겪으면서 교과서에 MBL 을 이용한 실험이 반영되기도 하였다. 이 연구에서는 2007 개정 과학교과서와 2009 개정 과학교과서를 중심으로 교과서에 수록된 MBL(microcomputer-based laboratory) 관련 내용을 분석하였다. 두 교육과정기에 개발된 과학 및 화학 교과서를 대상으로 MBL 이 언급되거나 사용된 실험을 추출하여 대상 학년, 내용 영역, 단원, 사용된 센서, 출판사 등의 측면에서 분류하고 그 특징을 분석하였다. 이에 대한 교육학적 함의도 함께 논의될 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

9학년 과학 교과서 화학 영역 삽화 분석

박인선 곽옥금 김봉곤 박종근*

경상대학교 화학교육과

2007 개정 과학과 교육과정에 따른 중학교 3 학년 과학교과서 8 종을 대상으로, 화학 단원에 포함된 삽화의 종류, 소재 및 역할을 비교·분석하였으며, 삽화 역할의 유형을 세분화하였다. 삽화의 종류는 사진, 그림, 도해, 만화, 도표 및 기타로, 삽화의 소재는 과학적 상황, 자연적 상황 및 생활적 상황으로, 삽화의 역할은 동기유발, 실험안내, 자료제공, 실험결과 제시 및 기타로 분류하였다. 연구 결과 삽화의 종류에서는 "사진"이, 삽화의 역할은 "자료제공"이 각 세부항목 중에서 빈도수가 가장 높게 제시되었고, 삽화의 소재는 "과학적 상황"이 가장 높게 제시되었다. 삽화 역할 유형의 동기유발에서는 "사진"이, 실험 안내에서는 "실험 과정에서 도구만 담은 장면"이, 실험 결과 제시에서는 "실험 수행 후 표만 제시"가, 자료 제공에서는 "사진" 항의 빈도수가 가장 높았다. 본 연구에 사용된 분류틀은 우종옥 등이 제시한 분석틀을 기초로 하여, 본 연구 목적에 합당하게 재수정하여 사용하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

초등 과학 교과서 읽기자료의 활용 실태와 인식 연구

강석진

전주교육대학교 과학교육과

과학 읽기자료를 이용한 교육은 학생들의 성취도 뿐 아니라 과학에 대한 흥미, 과학에 대한 태도, 과학자에 대한 이미지 등을 함양하는데 효과적인 것으로 보고되었다. 이에 따라 2007 개정 과학교육과정에 따른 초등학교 과학 교과서에도 읽기자료가 대폭 도입되었으나, 읽기자료의 구체적인 활용 실태와 읽기자료에 대한 교사와 학생들의 인식에 대한 조사는 부족한 실정이다. 이 연구에서는 2007 개정 과학교육과정에 따른 초등학교 과학 교과서의 읽기자료에 대한 교사와 학생의 인식 및 읽기자료의 활용 실태를 조사하였다. 이를 위해 읽기자료에 대한 인식과 활용 실태 조사를 위한 설문지를 개발하여, 초등학교 교사 181 명과 학생 643 명을 대상으로 설문을 실시하였다. 읽기 자료에 대한 인식 조사 결과, 많은 교사들이 읽기자료의 필요성에 대하여 공감하고 있었다. 또한 읽기자료의 단원 관련성이나 정확성에 대한 만족도는 상대적으로 높았으나, 읽기자료의 난이도와 제시 방식에 대한 만족도는 상대적으로 낮았다. 학생들은 읽기자료에 대한 만족도가 모든 측면에서 긍정적인 경향이 있었고, 교사에 비하여 읽기자료에 대한 만족도가 상대적으로 높았다. 읽기자료의 활용 실태에 대한 조사 결과, 대부분의 교사들이 읽기자료를 적극적으로 활용하고 있었고, 활용 시간은 평균 5 분 정도인 것으로 나타났다. 학생들은 읽기자료를 자세히 읽는 비율이 70% 이상일 정도로 적극적으로 활용하고 있었지만, 학년이 높아질수록 그 비율이 낮아지는 경향이 있었다. 이 연구의 결과를 바탕으로, 교사와 학생들이 활용하기에 적합하고, 보다 흥미롭고 다양한 내용의 읽기자료를 개발하는데 필요한 몇 가지 지침을 제안하였다.

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중학교 3학년 학생들의 과학 동아리 활동에 적용한 STEAM 탐구 수업 전략의 효과

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지식정보기반 사회에서는 새로운 지식을 생성하고 활용하기 위해 하나의 학문 분야에 갇힌 사고에서 벗어나 여러 학문 분야를 통합하여 사고할 수 있는 융합적 사고가 요구된다. 이러한 요구에 따라 본 연구에서는 학생들의 과학기술에 대한 흥미와 이해를 높이고 융합적 사고를 바탕으로 한 문제해결 능력을 신장시키고자 STEAM 수업을 개발하고 학생들에게 적용하였다. 순환학습을 바탕으로 공학설계의 과정을 도입하고 수공 활동을 강조하여 STEAM 수업을 개발하고, 서울 소재 중학교 3 학년 30 명 학생으로 구성된 과학 탐구반 동아리 활동에 1 년 동안 18 차시에 걸쳐 시행하였다. 학생들의 과학에 대한 흥미 향상 정도를 알아보기 위하여 TORSA 흥미 검사지를 이용하였으며, 중학생용 창의적 문제 해결력 검사지를 이용하여 창의적 문제 해결력의 향상을 살펴보았다. 연구 결과 동아리 활동을 한 학생들에게서 창의적 사고의 부분에서는 유창성과 독창성 영역에서 통계적으로 유의미한 향상이 나타났고 비판적 사고의 부분에서는 자료해석과 결론 도출 부분에서 실험반 학생들이 통계적으로 유의미한 향상을 보임을 알 수 있었다. 또한 학생들이 과학에 대해 느끼는 흥미도 향상되었음을 볼 수 있었다.

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인지분류를 통한 개별맞춤형 스마트교육 e교과서 개발-중학교 1학년 입자모형을 중심으로

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21 세기 사회는 고도화된 기술의 발달과 디지털 패러다임의 변화로 빠르고 다양하게 변화하고 있다. 현재 학생들이 살아갈 세상에서 정말로 필요한 기술과 기능은 현재 우리가 사용하고 가르치고 있는 기술과 기능이 다를 수도 있다. 전통적인 학교 체제에서의 학습을 떠올려보면 교실이라는 특정한 물리적 공간에서 정해진 수업 시간에 따라 획일화된 서책형 교과서로 3R(읽기, 쓰기, 셈하기)중심의 강의식 수업을 받는 모습을 떠올릴 수 있다. 이와 같이 시간, 공간, 도구, 강의 내용, 강의 방법 등에 제한이 있는 전통적인 학교 체제에서 탈피하여 새로운 교육으로 발 디딜 수 있도록 도와주는 것이 바로 스마트교육인 것이다. 이를 위한 21 세기의 핵심 역량은 3R 이 아닌 4C(의사소통능력, 협업능력, 창의성, 비판적 사고)로 요약할 수 있다. 알 수 없는 미래를 살아갈 우리의 학생들에게 21 세기 핵심역량인 의사소통능력, 협업능력, 창의성, 비판적 사고능력을 키워주는 것이 21 세기 교육의 핵심이라고 할 수 있다. 스마트(SMART) 교육의 (Self-directed)는 학생 스스로 학습을 계획하고 수행하는 자기 주도적 학습을 의미한다. M(Motivated)은 다양한 학습활동 및 학습내용들을 활용하여 학습자들의 흥미를 유발하는 학습을 의미하다. A(Adaptive)는 과거의 전통적인 획일적 수업에서 벗어나 학생 개별의 수준과 적성을 고려한 수업을 의미하고, R(Resource Enriched)은 디지털 콘텐츠 및 온라인 학습과정을 활용하여 학습자들에게 풍부한 교육 콘텐츠를 제공하는 수업을 의미한다. 마지막으로, T(Technology Embedded)는 교실 공간에서 벗어나 언제 어디서나 학습을 지원하는 기술기반의 학습을 의미한다. 과학 교육에서 스마트교육을 잘 펼칠 수 있는 내용은 '학습자 스스로가 지식과 개념을 학습'하는 것이다. 여기에서 지식과 개념을 학습한다는 것은 수많은 자료 속에서 학습과 관련된

자료를 찾아내고 이를 지식 습득에 활용하는 것이다. 또한 과학지식의 습득은 실생활과 관련된 자료로 이해할 때 가장 학습이 잘 이루어진다. 그리하여 현재 우리 주위에서 과학지식과 관련된 현상을 찾고 이것이 과학지식과 어떠한 연관이 있는지 관련 정보를 탐색하면서 지식을 찾아낸다. 스마트교육은 개별학습자의 능력에 맞는 수업을 중시하기 때문에, 다양한 학습형태를 추구한다. 그리하여 개인 특성에 맞는 차별화된 교육을 제공하는 것이 중요하다. 따라서 본 연구에서는 중학생의 인지확인 및 인지갈등을 통하여 인지분류를 한 후, 그에 맞는 수업을 제공하는 개별맞춤형 e-교과서를 개발하였다.

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두뇌의 편집과정 분석을 통한 본 과학자의 창의적 사고과정 이해와 과학교육에의 적용에 대한 고찰

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이 연구의 목적은 두뇌의 편집과정 분석을 통해 과학자의 창의적 사고과정을 이해하고 이를 과학교육에 적용하여 학생들의 창의성을 신장시키는데 있다. 이를 위해 두뇌의 편집과정에 대한 문헌과 자료를 분석하고 근대 과학의 성립기인 19 세기 과학이 보다 복잡하고, 정교화된 시대의 과학자로 Avogdro 의 사고과정을 분석하였다. 우선 문헌 연구를 통해 두뇌에서 일어나는 기억의 편집과정을 분석하였다. 기억은 대뇌피질의 측두엽에 저장된다. 그 이후 측두엽에서는 기억의 편집과정이 계속해서 일어나면서 창의적인 사고도 생성한다. 어려운 상황이나 당장 답을 할 수 없는 문제를 만났을 때 측두엽에서는 이를 해결하기 위해 기억을 재생하게 되는데 이 과정에서 단순한 회상이 아니라 기억이 편집과정을 거치게 된다. 따라서 기존에 없던 새로운 생각을 하게 되며 이 생각이 창의적 해결이 될 수 있는 것이다. 이 과정을 잘 이해한다면 이를 학생들의 창의성 교육에 새로운 모델을 제시할 수 있으리라 기대되었다. 두뇌의 편집과정에 대한 보다 완벽한 이해와 창의성 교육의 모델제시를 위해 Avogdro 관련 문헌을 수집하여 분석하였다. Avogdro 는 실험 현상인 기체반응의 법칙을 설명할 수 있는 입자론이 무엇인가를 문제 상황으로 인식하고 해결하려고 노력한다. 이 과정에서 그는 그가 이해하고 있던 돌턴의 원자설로 문제를 해결하려고 시도했지만 예측가능성의 부재로 문제해결에 실패하고 만다. 막다른 골목에 도달한 상태에서 그는 부분압력의 법칙과 Boyle 의 법칙, Gay-Lussac 의 논문을 접하게 된다. Avogdro 는 ‘물질이 반응할 때 간단한 정수비로 결합한다’고 주장한 Proust 의 일정성분비의 법칙이 입자설의 증거가 됨을 알 고 있었다. 그리고 Boyle 의 논문에 있는 기체는 같은 압력에서 같은 부피를 나타낸다는 사실을 자신의 사전지식인 돌턴의 부분압력의 법칙과 연결하여 생각하게 된다.

또한 Gay-Lussac 이 ‘기체는 다른 기체들과 반응할 때, 결합하는 기체들 사이에 간단한 정수비가 성립된다’고 주장한 기체 반응의 법칙과 관련하여 ‘입자와 부피의 관계’에 주목하고 결국 입자의 개수가 그 기체의 압력을 결정하고, 모든 기체가 같은 압력에서 같은 부피를 나타낸다면 동일조건에서 같은 부피에 들어있는 입자의 개수는 같을 것이라는 결론에 도달하게 된다. 이렇게 실험현상인 기체반응의 법칙을 해결하기 위한 Avogdro 의 사고의 과정은 그가 알고 있던 사전지식의 편집과정을 거치면서 두 개 혹은 그 이상의 기억들이 편집되면서 창의적 사고로 문제를 해결하게 된다. Avogdro 의 경우에서 볼 수 있듯이 두뇌에서 기억의 편집과정은 창의적 사고를 이끌어 내고 나아가 문제해결에 도달하게 된다. 이는 사전지식을 충분히 고민할 수 있는 시간적인 여유와 기존 지식들에 대한 폭넓은 이해가 필수적으로 필요함을 이야기하기도 한다. 현재 우리나라 과학교육은 지식을 암기식으로 학습하고 시간 내에 문제를 빨리 해결하는 것을 학생들에게 강요하고 있다. 창의적인 사고를 할 수 있는 기억의 편집과정을 위한 조건이 결여되어 있는 것이다. 과학 지식이 암기식이 아닌 폭넓은 이해로 학생들에게 기억되는, 자신의 기억을 편집할 수 있는 기다림이 있는 학교 교육 요구된다.

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자연모사 태양전지를 적용한 중등과학 창의융합실험 설계 및 모듈 개발

김현주 이재관*

조선대학교 화학교육과

지구온난화 및 화석연료의 한계를 필두로 한 환경, 에너지 문제는 글로벌 핵심 이슈로서 고효율 에너지기술 및 신재생에너지와 같은 친환경 기후변화대응기술 개발이 미래 지구생태계 및 생활환경의 최선 및 필수 대안으로 대두되고 있다. 그러나 급변하는 과학기술개발에 대한 환경변화에도 불구하고, 초?중등 및 대학 교육현장에서는 이러한 패러다임의 현실적인 변화에 대한 중요성을 인식하지 못하는 안타까운 현실에 직면하고 있으며, 학생들에게 환경, 에너지의 중요성을 강조하고 효과적으로 교육에 적용하여 학생들로 하여금 올바른 미래에너지에 대한 가치관과 호기심, 그리고 희망을 심어주어야 하는 교육적 의무의 실행이 요구된다. 현재의 과학교육과정에서 변화에 대한 필요성을 공감하고 점진적인 변화를 위한 노력들이 절실히 요구 되지만, 우리나라의 교육현실의 특수성은 현실적인 변화에 대한 소극적인 태도를 많이 보여주고 있다. 이러한 현실을 인지하고, 학생들에게 과학기술에 대한 관심도를 높여주고, 미래에너지의 중요성과 활용성을 몸소 체험하고 흥미를 느껴 친근한 느낌을 부여할 수 있도록, 아주 작은 변화에 대한 교육적인 접근 노력들이 필요하다. 최근 미래 에너지 기술로 많은 관심을 받고 있는 자연계의 광합성원리를 응용한 자연모사 태양전지 기술은 초·중등 및 대학 교과과정 내용과 가장 연계성이 높아 다양한 융합교육콘텐츠 개발에 적합하다. 이를 적용하여 중등과학 교과과정과 연계한 융합적 사고와 문제 해결력을 배양할 수 있는 창의융합실험을 설계하고 탐구모듈의 개발에 관한 연구내용을 소개하고자 한다.

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열화상 카메라를 이용한 화학 반응의 가시화 방안

박기철 강성주*

한국교원대학교 화학과

열화상 카메라는 화학 변화과정에서 수반되는 열 출입을 수치와 그래프로 제공할 뿐만 아니라 화학에 대한 더 많은 정보를 제공해 준다. 따라서 본 연구를 통해 적외선 열화상 카메라를 과학 교육 현장에 적용하는 방안을 마련하고자 한다.열화상 카메라로 엔탈피의 변화가 작은 탄산 칼슘의 앙금 생성 반응을 촬영한 결과, 온도 변화가 색깔 변화로 나타나므로 흡열 반응임을 쉽게 확인할 수 있었다. 중화 적정의 경우에도 용액이 혼합되는 부분에서의 반응 여부가 화면의 색깔 변화로 나타나므로 묽은 농도의 반응에서도 지시약을 사용하지 않고 중화점을 찾을 수 있으며, 온도계의 접촉에 의한 열손실이 발생하지 않아 아주 적은 양의 용액을 사용한 반응의 온도 변화도 측정할 수 있다. 전기 분해 관찰을 통해 전극 반응의 엔탈피 변화 크기와 생성 물질의 종류와 상태에 따라 전극 주변 용액 온도 변화의 크기와 양상이 다르게 나타난다는 것을 발견하였고, 전해질의 이동과도 관련이 있음을 짐작할 수 있었다.열화상 카메라는 일반 온도계로 측정하기 어려운 상태 변화와 엔탈피 변화가 작은 화학 반응도 관찰할 수 있게 해 주었으며, 무엇보다 결과 뿐만 아니라 변화 과정을 역동적으로 보여주어 쉽고 재미있는 화학에 대한 요구가 증가하고 있는 현실에서 변화의 과정을 역동적으로 볼 수 있는 열화상 카메라의 활용은 학생들의 화학에 대한 흥미와 관심을 크게 제고할 수 있는 방안이 될 수 있을 것으로 기대한다.

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멘토링 대화분석에서 나타난 멘티의 교수실행측면에 대한 멘토의 지원

이동원 이미경[1] 남정희[1]

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교사의 수준은 학생의 성취도에 영향을 주는 가장 중요한 변인 중 하나이다. 하지만 많은 경우에 초임 교사들은 수업에 대한 전문성을 충분히 갖추고 있지 않으며, 이러한 수업 전문성의 부족은 초임교사들이 교직생활에 적응하는데 어려움으로 작용한다. 그러나 같은 수업 전문성의 측면이라 하더라도 세부적인 부분에서 교사들이 어려움을 느끼는 부분들은 상이하며 이들을 고려하지 않은 일괄적인 형태의 도움은 교사들이 수업 전문성을 발달시키는데 효과적이지 않을 수 있다. 따라서 이번 연구에서는 멘티가 교수실행측면에서 실제로 어떠한 어려움을 가지고 있으며, 멘토링에서 멘토가 멘티에게 교수실행측면에서 어떠한 지원을 하는지 알아봄으로써 교수실행측면에서 효과적인 멘토링을 위한 멘토의 역할을 알아보고자 하였다. 이를 위해 4 쌍의 멘토, 멘티가 1 년간의 멘토링 프로그램에서 수행한 멘토링 대화, 멘티 저널, 멘티 간담회 등의 내용을 수집하였다. 그리고 이들의 담화에서 나타나는 PCK 요소를 추출한 뒤 이들 중 공통적으로 나타나는 부분을 범주화하여 멘티가 교수실행측면에서 실제로 필요하다고 생각했던 부분과 멘토링에서 멘토가 제공한 지원을 비교분석하였다.

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일반화학실험에서의 글쓰기형 마인드맵 적용 효과

박정은 강순희[1,*]

이화여자대학교 과학교육학과 [1]이화여자대학교 과학교육과

본 연구는 글쓰기와 마인드맵을 이용한 창의적 문제 해결력 신장 수업 전략을 개발하고 그 효과를 검증하고자 하였다. 창의적 문제 해결 과정에서는 창의적 사고력과 비판적 사고력이 핵심적이 사고이다. 창의적 사고력을 발산적 사고로 정의하였으며, 비판적 사고력은 여러 가지 사고들 중 더욱 합리적인 하나의 사고로 수렴하는 사고로 정의하였다. 따라서 창의적 문제해결력을 신장하기 위한 기존의 수업 모형인 발산하기 모형, 수렴하기 모형, 발산 수렴 함께 하기 모형을 바탕으로 글쓰기와 마인드맵을 이용한 창의적 문제 해결력 신장 수업 전략을 개발하였다. 개발한 수업 전략을 사범대학 예비 과학교사들을 대상으로 한 학기동안 적용하여 창의적 사고력, 비판적 사고력, 과학에 대한 태도 변화에 효과가 있는지 알아보았다. 그 결과, 창의적 사고력의 하위 범주 중 유창성, 융통성, 독창성에서 통계적으로 유의미한 신장이 나타났으며 비판적 사고력과 과학에 대한 태도에서는 유의미한 차이를 나타내지 않았다.

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다문화·탈북 가정 학생의 과학 학업성취 특성 분석

김현경

한국교육과정평가원 교육평가본부

본 연구에서 다문화·탈북 가정 학생을 국제결혼 가정 자녀(국내출생 자녀, 중도입국 자녀), 외국인가정 자녀, 탈북 가정 자녀로 유형화하고, 이러한 다문화 유형별로 과학과 문항유형별, 내용영역별 학업성취 특성을 계량적, 질적 방법으로 분석하여, 다문화·탈북 가정 학생이 어려움을 겪고 있는 학업 상황을 탐색하였다. 연구 결과, 과학의 국가수준 학업성취도 평가에서 다문화 집단에게 불리하게 작용하는 차별 기능을 가지는 것이 무엇인지를 문항별 및 문항군 별로 분석한 결과, 과학 문항은 다른 교과의 문항에 비해서 그림, 기호, 그래프 등의 도식 사용이 많고, 일상의 용어와 더불어 새롭고 생소한 과학 용어들이 많기 때문에 다문화 집단에게 불리한 방향으로의 영향을 주는 측면이 드러났다. 분석을 통해 드러난 점들을 정리하면 첫째, 일상의 언어는 외국인 가정 학생들에게, 과학의 언어는 탈북 학생들에게 불리하게 작용하고 있다. 둘째, 과학적 도식은 다문화 집단, 특히 타국에서의 과학 교육의 경험을 가진 집단에게 불리한 요인이 된다. 셋째, 중도 입국 국제 결혼 집단과 탈북 학생들이 특히 과학 문항에 대해 높은 불리함을 보였다. 넷째, 역사나 지리 등의 문화적인 요소들을 반영하고 있는 문항들은 탈북 제외 다문화 집단에게 불리하게 작용했다. 마지막으로, 중학교에서 학년이 올라갈수록, 지식 보다는 탐구 문항에서 다문화 학생들은 어려움을 보였다. 이를 위해, 다문화 학생에 대한 지원을 준비할 때 특히 과학과의 경우에는 다른 다문화 집단과는 구별하여, 다른 나라의 과학 교육 경험을 가진 중도입국 학생들을 위한 교육적인 지원이 필요하며, 교육 공백을 가진 탈북 학생들을 위한 보충 교육 자료 및 교재들의 개발에도 지원이 이루어져야 할 것이다.

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고등학교 화학 교과서에 기술된 열역적 개념에 대한 분석

장낙한

공주대학교 화학교육과

고등학교 화학 교과서에 기술된 압력, 확산 등의 열역학적 개념에 대하여 분석하였다. 모든 화학 교과서에서 이 개념들을 설명할 때 분자 운동론을 도입하면서 개별적인 분자 운동에 초점을 맞추고 있었다. 즉, 분자량의 차이에 의한 충돌 빈도나 평균 속력의 차이로 이 개념들을 설명하고 있다. 특히 확산식과 같은 수리적인 표현은 학생들에게 열역학적 개념이 미시적인 개념으로 오해하도록 기술되어 있었다. 이로 인해 이 개념들이 거의 아보가드로수에 해당하는 입자수에 의한 벌크(bulk) 상태에 대한 현상임에도 불구하고, 학생들과 교사들은 원자 상태에 해당하는 미시적인(microscopic) 개념으로 잘못 이해하고 있었다. 따라서 올바른 열역학적 개념을 가지게 하기 위해 예비교사들에게 물리화학 수업에서 통계열역학적 개념에 대한 수업이 반드시 필요하리하고 생각된다. 또한 화학 교과서에서 이 개념들을 기술할 때 확산식과 같은 수리적인 표현뿐만 아니라 모형과 같은 시각적 자료를 활용하여 거시적인(macroscopic) 개념이 정착되도록 하는 것이 더 유용하리라고 생각된다.

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중등 과학영재 인성교육 프로그램의 적용 효과

유미현

아주대학교 교육대학원

본 연구의 목적은 Betts 의 자발적 학습자 모형을 바탕으로 과학영재 인성교육 프로그램을 개발하여 과학영재 수업에 적용하는 것이다. 개발 적용된 과학영재 인성교육 프로그램은 존경하는 과학자 탐구, 과학자 인터뷰, 영재들의 수다, 과학자 연구 윤리, 과학영재를 위한 정서적 멘토링 등이다. 이를 위해 경기도 소재 대학부설 과학영재교육원 중등화학심화반 학생을 실험집단으로, 중등물리심화반 학생들을 비교집단으로 각각 배치하였다. 실험집단에 1 년에 걸쳐 인성교육 프로그램을 실시하고 학생들의 과흥분성, 정서지능, 사회적 성숙에 미치는 효과를 조사한 후 연구 결과 및 이에 따른 시사점을 논의하였다.

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Acylated Polyethyleneimines as Temperature-Sensitive Draw Solutes for Producing Highly Pure Usable Water in Forward Osmosis

목영봉 이연*

서울대학교 화학부

Temperature-sensitive materials (TSMs) have enormous potentials for obtaining clean water in desalination and purification. Well dissolved TSMs in low temperature, show good drawing ability when they are facing feed solution containing salts or other contaminants with semipermeable membrane interface. As processing temperature goes up, TSMs becomes aggregated above a certain temperature; LCST (lower critical solution temperature) phase-transition temperature. By their abruptly decreased osmotic pressure it is possible to obtain very low salt water as product using osmosis.Although TSMs with low molecular weights show high osmotic pressure, adequately high MW TSMs have several benefits. Because it shows much low osmotic pressure at high temperature, it will be possible to produce more low salt productive water. Also, the hydrodynamic volume of high MW TSMs are larger than low MW ones, it will show higher membrane rejection than that of low MW ones. Among many TSMs, acylated polyethyleneimines are easy to synthesize and controll MW and LCST transition.Therefore, synthesis, LCST characterization, osmotic drawing and rejection efficiency of temperature-sensitive acylated polyethyleneimine derivatives will be introduced in this research.

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Enhanced photocatalytic hydrogen prodution on Ag/TiO_2 in the presence of Thiocyanate

최여선 최원용[1,*]

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Due to energy and environmental issues, hydrogen from photocatalytic water splitting has been actively investigated since not only solar light and water are abundant but also hydrogen as an energy carrier can be widely utilized. However, to achieve high photocatalytic efficiency, it is hard to avoid the use of Pt as a cocatalyst that is expensive and rare. Therefore, the replacement of Pt by relatively low cost materials has been paid attention to more and more in photocatalysis. Silver nanoparticles can be considered as an alternative co-catalyst due to its relatively low cost and good ability for electron storage. on the other hand, it still exhibits lower efficiency than Pt for photocatalytic water splitting. Herein, the addition of thiocyanate (SCN^-) brings about significant enhancement for hydrogen production under UV irradiation, which is attributed to the complexation with silver nanoparticles on TiO_2. The complexation of SCN^- with silver nanoparticles was confirmed by various techniques including Raman spectroscopy, energy-dispersive spectroscopy (EDS), and X-ray photoelectron spectroscopy (XPS). As a result, the hydrogen evolution rate(41 μmol/h) of SCN^--Ag/TiO_2 was observed three times higher than that of Ag/TiO_2 (12 μmol/h). This study suggests the strategy how to improve hydrogen production efficiency via the complexation of silver with thiocyanate and will open the opportunity for a variety of combination between metal nanoparticles and molecular ions.

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Preparation of Organic-based Radical Battery using Polyviologen Anode andPoly(TEMPO radical) Cathode

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In this experiment, poly(tripyridinio mesithylene) (PTPM) as an anode-active material and poly(2,2,6,6-tetramethylpiperidine-4-yl acrylamide)-poly(acrylicacid) (PTAm-PAA) as a cathode-active material was researched. PTPM has a cross-linked structure which leads to a long life time. It shows two electron reversible redox behavior which helps the radical battery to have high theoretical capacity. PTAm-PAA is rapidly and reversibly oxidized. Moreover, its high molecular weight helps in the formation of film and in having a long cycle life. The capacity of PTPM half-cell was 115 mAh/g, and it maintained 95 % capacity after 200 cycles. The capacity of PTAm-PAA half-cell was 106 mAh/g, and it maintained 98 % capacity after 200 cycles. Full-cell was fabricated with PTPM anode, PTAm-PAA cathode and aqueous NaCl electrolyte. The cell voltage of the full-cell was 1.1 and 1.5 V coinciding with difference of PTPM and PTAm-PAA voltages. The capacity of full-cell was 114 mAh/g and it maintained 95 % capacity after 200 cycles. According to the C rate, the rate performance of the full-cell was changed but the discharging capacity of the full-cell was 114 mAh/g at 15 C. (76 % coulombic efficiency)

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Polyether Ionomers Containing Various Cross-Linkable Moieties for Fuel Cell Applications

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We synthesized novel PEMs with sulfonated poly(arylene ether)s(SPAE) copolymers as electrolyte membranes with various cross-linking moieties to develop stable PEMs. Among those novel SPAE copolymers, cross-linkable sulfonated copolymers, ESFx-BPys and SHQx-TFVys, had especially good properties. These cross-linked SPAE copolymers exhibited high glass-transition temperatures over 200 ^{o}C and thermal degradation temperatures around 300 ^{o}C. Also, the tensile strength was improved from 62.3 to 85.9 MPa, which is over three times than that of Nafion(27.7 MPa). The cross-linked SAPE copolymers had excellent proton conductivity(0.098 - 0.151 S/cm) compared to that of Nafion 117(0.091 S/cm). In addition, The H_2/O_2 single cell performance tests of the cross-linked membranes and Nafion 212 were performed. The CSHQ90-TFV10 exhibited the higher maximum power density(1.053 W/cm^2) than that of Nafion 212 (0.844 W/cm^2).

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Preservation of NZVI reactivity by natural electron transfer mediator for reductive degradation of chlorinated organic

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In this study, we demonstrated that natural electron transfer mediator (riboflavin) keep the nanoscale zerovalent iron (NZVI) reactivity alive during the reductive dechlorination of chlorinated organic (i.e., carbon tetrachloride (CT)). Addition of riboflavin (1 ?M) to NZVI suspension showed the increase of CT degradation during third cycle reactions, while a significant reduction of NZVI reactivity for CT degradation was observed in the absence of riboflavin. Mechanism study revealed that riboflavin can effectively absorb on NZVI surface at the first step, then reduced by NZVI and excavate the passive NZVI surface during the CT degradation. The results obtained from this study can be properly applied to the development of novel remediation technologies using riboflavin to preserve NZVI reactivity and extend its longevity at the remedial sites contaminated by chlorinated organics.

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One-Pot Synthesis of Peacock-Shaped TiO2 Light Scattering Layer with TiO2 Nanorods Film for Dye-Sensitized Solar Cells

<u>강순형</u>

전남대학교 화학교육과

Nowadays, the exploration of new photoelectrode architectures to improve the light-harvesting and charge-collection properties of sensitized solar cells and related devices has been regarded as a challenging work. Here, we demonstrate one-pot synthesis of peacock-shaped TiO2 light scattering layer with TiO2 nanorods film for dye-sensitized solar cells by hydrothermal method controlling the acid ratio of HCl and CH3COOH. In the case of 1:2 ratio of HCl:CH3COOH, the one-dimensional (1-D) TiO2 nanorods (NRs) film was synthesized with a length of 2 μm, whereas 1-D TiO2 NRs film with peakcock shaped TiO2 nanobundles as a light scattering layer (LSL) was acquired in the 2:1 ratio of HCl:CH3COOH. This LSL showed the remarkably dual functions in an aspect of high light harvesting attributable to the large surface area due to micrometer-sized TiO2 nanobundles consisting of small-sized TiO2 NRs with approximately 30~40 nm sized diameter and light scattering effect in the long wavelength of 550-700 nm. Accordingly, this dual functions of LSL result in the sharp increased conversion efficiency (3.93 %) about above two times compared to that (1.49 %) of TiO2 NRs film synthesized in 1:2 rato of HCl:CH3COOH.

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Developement and characteriztion of anodic TiO2 nanotubes and nanoparticles based bilayered photoanode for dye-sensitized solar cells

강순형

전남대학교 화학교육과

Dye-sensitized solar cells (DSSCs) have been widely attracted due to low manufacturing cost, environmental friendliness, and high efficiency. However, there are still several drawbacks to attain the conversion efficiency above 15 % for the commercialization. In particular, in the photoanode comprised of TiO2 nanoparticles, the trap-limited diffusion process leads to the high charge recombination with a reduction of electron collection efficiency, even though it shows large surface area ensuring a high dye loading for light harvesting. One-dimensional TiO2 nanotube (TONT) by electrochemical two-step anodization in 0.25 wt% NH4F of ethylene glycol was suggested to overcome this problem. Herein, the overcoating of TiO2 nanoparticle was introduced to support the surface area because nanotubular structure has low surface area resulted from large inner diameter (approx. 100 nm) of nanotube. This bilayered TiO2 nanotube/nanoparticle film was characterized by XRD, FE-SEM, and J-V analysis.

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Catalytic nitrate reduction by bimetallic Pd-Cu catalysts supported on Hematite(α-Fe2O3)

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In this study, catalytic nitrate reduction was investigated by bimetallic Pd-Cu catalysts supported on hematite(α-Fe2O3). A variety of hematite catalysts was synthesized using different types of iron bearing soil minerals (IBSMs) (i.e., maghemite (γ-Fe2O3), lepidocrocite (γ-FeOOH), goethite (α-FeOOH), hematite (α-Fe2O3)). Different catalysts prepared from different IBSMs were chracterized by BET, X-ray diffraction, temperature programmed reduction, and transmission electron microscopy. Nitrate was significantly reduced (97%) by Hematite/Pd/Cu-hematite in 90 min, while the lowest removal efficiency (24%) was obtained by Hematite/Pd/Cu-lepidocrocite. The highest N2 selectivity (71%) was obtained by Hematite/Pd/Cu-hematite, while Hematite/Pd/Cu-lepidocrocite showed the lowest selectivity (40%) in this study.

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Catalytic nitrate reduction by bimetallic TiO2/Pd/Cu with formic acid

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Formic acid was used as a reducing agent for catalytic nitrate reduction by TiO2/Pd/Cu catalyst. The formic acid has been known to be easily decomposed into hydrogen and carbon dioxide on a noble metals. Therefore, we used the formic acid as the reducing agent during catalytic nitrate reduction in this study. The removal of nitrate and its selectivity to nitrogen gas was significantly influenced by the concentration of formic acid (3.2-19.2mM). 45% of nitrate was removed in 1h at 19.2 mM of formic acid, while 10% of nitrate removal efficiency was obtained at 3.2 mM of formic acid. In contrast to the nitrate removal, the highest selectivity to nitrogen gas (71%) was obtained at 3.2 mM of formic acid, while 19.2mM of formic acid showed the lowest selectivity (27%). The catalytic performance of TiO2/Pd/Cu with formic acid was compared to that with hydrogen gas.

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How Computational Chemistry Helps Mechanistic Understanding of Environmental Nanominerals Reactivity

권기덕

강원대학교 지질학과

Hexagonal birnessite (δ-MnO2) and mackinawite (FeS) are layer-type Mn oxide and Fe sulfide minerals ubiquitous in soils and natural waters. They are major players to determine the contaminant dynamics in subsurface environments mainly through the high capacity in sorption and redox reactions. These minerals are typically found as nanoparticles which are difficult to study the structure and surface chemistry by experimental techniques alone. This presentation introduces recent computational chemistry studies to provide new insights that are not experimentally available about underlying principles in some metal scavenging mechanisms of birnessite and redox mechanisms of mackinawite.

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Sol-gel Synthesis of Ultrathin TiO_2 Nanodisk at the Interface between Organic Solvent and Ice

김건우 최원용*

포항공과대학교 환경공학부

The synthesis of two-dimensional TiO_2 through simple method is fundamental challenge in material science and photochemistry. Recently, there have been much efforts on development of two-dimensional TiO_2 because of its great potential for application in solar energy conversion or electronic devices. However, studies on the synthesis of two-dimensional TiO_2 and the effects of the two-dimensional structure on physicochemical properties of the semiconductor have not been conducted well. In this study, we synthesized ultrathin two-dimensional TiO_2 through a novel and simple sol-gel method and found that the two-dimensional TiO_2 exhibits optical and surface characteristics that are considerably different from those of TiO_2 nanoparticles. The synthesis of two-dimensional TiO_2 was achieved by the sol-gel reaction occurring at the interface between organic solvent and ice. Reaction of titanium precursor dissolved in hexane solvent with pieces of ice results in the formation of ultrathin TiO_2 nanodisk with thickness of 0.5~1 nm and diameter of 5~20 nm. Direct observation of the two-dimensional structure in the field-emission scanning electron microscopy (FE-SEM) images confirmed the formation of ultrathin two-dimensional TiO_2. Optical and surface characteristics of the two-dimensional TiO_2 were analyzed by UV-visible absorption spectroscopy, zeta potential and BET surface area measurements.

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Recovery of Lead and Electric Power Generation Using a Double Microbial Fuel Cell Arrangement

최찬수

대전대학교 응용화학과

In order to recover lead from lead ion-containing wastewater, a double microbial fuel cell (MFC) arrangement was used that supplies a power lacking 0.071 V which is the needed amount to operate a single MFC. In this double MFC arrangement, a slight little voltage could be supplied using the first MFC (Cell 1) consisting of an anode containing acetate and a cathode containing Cr(VI) ions, which reaches a voltage as high as 1.55 V in the standard state that can supply enough power to recover lead from the wastewater in the cathode chamber of the second MFC (Cell 2). The anode chambers of Cell 1 and Cell 2 were supplied with acetate media in a continuous mode with a peristaltic pump. The cathode chamber of Cell 1 was filled with $HCrO_4^-$ catholyte to generate enough electric power. The voltages across Cell 2, which plays a role as a load resistor of Cell 1, were measured using the Lab View system. Remaining concentrations and recovery efficiencies of lead ions in the cathode chamber of Cell 2 were examined with time. After 60 hours, the remaining concentrations of lead ions were 4.82± 0.38 ppm, 10.71±0.49 ppm, and 27.33±0.35 ppm for 50 ppm, 100 ppm, and 200 ppm initial lead ion concentrations, respectively. The recovery efficiency of lead ions was 90.37±0.76%, 89.29±0.49%, and 86.33±0.18% for 50 ppm, 100 ppm, and 200 ppm initial cadmium concentrations, respectively.Lead recovery needs only a very small amount of voltage to accelerate reaction speed and Cell 1 can supply a voltage as high as 1.55 V. One may think that using such high voltage only for recovery of heavy metals is not an efficient utilization. While recovering the metals, it is recommended to drain electrical energy from the cell arrangement. A load resistor could be connected in parallel between Cell 1 and Cell 2 to achieve efficient utilization. In conclusion, this experiment verifies that lead recovery using the present arrangement of MFCs was very successful.

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Photoelectrochemical Water Oxidation of $BiVO_4$ electrodes coupled with Cobalt-Phosphate Complexes

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To enhance the efficiency of water oxidation of $BiVO_4$ photoanode, $BiVO_4$ is modified with Cobalt Phosphate Catalyst (CoPi) by using electrodeposition and photodeposition. Amounts of CoPi that deposited on the surface of electrode are increased by following deposition method of CoPi on substrate for a certain time. Photoelectrochemical activities of $BiVO_4$/CoPi were performed by changing deposition times in each deposition methods. Among them, $BiVO_4$/CoPi ED 30m which is followed by stepwise ED (5m + 5m + 20m) has the most highest photocurrent, 0.77 mA cm^{-2}, which is more twice than that of bare $BiVO_4$, 0.33 mA cm^{-2}. Optimized CoPi ED resulted in a CoPi overlayer of approximately 850 nm thick, which showed an electrochromic-like behavior that was likely due to limited access of phosphate into $BiVO_4$ across the CoPi layer. Optimized CoPi PD, however, had very thin and rather uniform CoPi dispersion and did not show electrochromic-like behavior. Despite the lesser amount of CoPi, the PEC performance of $BiVO_4$/CoPi (PD) was comparable to that of $BiVO_4$/CoPi (ED). The primary role of CoPi has been suggested as a hole-conducting electrocatalyst making the photogenerated electrons more mobile and, consequently, increasing conductivity and boosting the PEC water oxidation performance of $BiVO_4$. To understand more information about $BiVO_4$/CoPi electrode, surface analysis such as SEM, XPS etc was performed.

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Reactivity and Electrochemical behavior of Fe/FeS Nanoparticles in Simulated and Real Groundwater

김은주 장윤석*

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The reactivity and electrochemical behavior of freshly-synthesized FeS-coated iron nanoparticles (Fe/FeS) were examined under various solution conditions in order to evaluate the potential advantages of Fe/FeS in field treatment. Ionic strength, hardness (Ca^{2+}/Mg^{2+}), and humic acid (HA) imposed significantly different effects on the reactivity of Fe/FeS. While the addition of Ca^{2+} and Mg^{2+} greatly increased the TCE reduction rate, HA caused less than a 50% rate decrease. Interestingly, when HA and Ca^{2+}/Mg^{2+} coexist, the negative impact of HA could be overcome, possibly due to the conformational change of HA upon adsorption into nFe/FeS. The present study provides compelling evidence that the field performance of Fe/FeS will not be significantly diminished by environmental conditions.

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Corrosion Electrochemistry and Surface Reactivity of Bimetallic Iron Nanoparticles

김은주 장윤석*

포항공과대학교 환경공학부

The deposition of a secondary metal to the iron surface significantly enhances the reactivity of remediation systems. Herein, we investigated and related the electrochemical corrosion properties of iron-based bimetals (Fe/Pd, Fe/Co, Fe/Cu, and Fe/Ni) and their reactivity toward trichloroethylene (TCE). Electrochemical characterizations reveal that Fe/Pd was most susceptible to corrosion, while Fe/Cu was most resistant. All metal depositions increased rates of TCE reduction, but the magnitude of rate enhancement greatly differed with Fe/Pd > Fe/Ni > Fe/Co >> Fe/Cu. From linear regression analyses, we found strong relationships between experimental rate constants and corrosion current (icorr) and exchange current density (i0) values, suggesting that both galvanic corrosion and atomic hydrogen were responsible for the enhanced reactivity of bimetallic particles.

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Production of hydrochar from biomass contained food waste and sewage sludge and its characteristics

박효선 배선영*

서울여자대학교 화학과

Due to London Dumping Convention, disposal of wastes which could create hazards to human health or living resources in the ocean is gradually prohibited. It demands to convert biomass into the value added products. Hydrochar can be converted by hydrothermal carbonization (HTC) from biomass which consists of food waste and sewage sludge disposal. In this study, hydrochar was formed from food waste or mixtures of sewage sludge and food waste (SFWC) at 230 ℃ for 8 hr. The food waste which contained the moisture content about 83.7% was composed of the cooked rice, the cabbage, the rind of a watermelon, and the mackerel. Mixed biomass contained respectively 2%, 5%, and 10% sewage sludge in food waste. The moisture content of sewage sludge was about 78.7%. The highest yield of hydrochar was obtained from 10% SFWC. The higher ratio of sewage sludge in food waste showed the higher yield of hydrochar. Hydrochar had more carbon content than biomass as feedstock confirmed by elemental analysis. Functional groups in food waste and its hydrochar were identified by FT-IR. SEM images confirmed that hydrochar has more fine porosity than biomass. The optimum condition of hydrochar production was determined by the results of iodine number (986 mg/g) and BET measurement.
Keywords : Hydrochar, Food waste, Sewage sludge, Iodine number, BET

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Sand Fixation with Polymer Solutions

심지연 황유라 배선영*

서울여자대학교 화학과

Dust storm such as Asian dust blown from arid regions adversely affects human health and harm environmental aspects. It reduces the quantity of solar radiation, increases patients with lung respiratory and premature deaths, and damages flight, and so on. Among various means of dust emission reduction, three kinds of polymers such as polyacrylamide (PAM), polyacrylic acid (PAA), and poly (acrylamide-co-acrylic acid) (PAM-co-PAA) at a concentration of 0.5%, and 1.0% were evaluated and sodium lauryl sulfate(polymer solution : sodium lauryl sulfate = 11 : 1) and 1,6-Hexadimethylene diisocyanate (polymer solution : sodium lauryl sulfate : 1,6-Hexadimethylene diisocyanate = 11 : 1 : 0.1) were added in the polymer solution. These composites were sprayed on sand surface and dried at 21.8℃ (±2.8℃) and relative humidity 23.4% (±5.0%). As a result, desiccation curves were constructed for 30 days. Our results indicated that polymer composites sprayed onto sand surface enhanced aggregative strength of sand particles and caused desiccation of liquid proceed slowly. Among the polymer solutions evaluated in this study, the most effective polymer with various mixing ratio was determined. Further, the depth of polymer penetration and compressive strength will be investigated. Keywords: Dust, Polymer, PAM, PAA, Sand

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Characterization of Hydrochar of Food Waste via Hydrothermal carbonization

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서울여자대학교 화학과

Hydrothermal carbonization(HTC) that converts biomass into biofuel is one of thermal conversion methods and used to produce hydrochar. HTC is able to react materials contained water in relatively low temperature. It is useful in terms of energy requirement unlike pyrolysis. Hydrochar created by HTC possess large surface areas, microporous structure, active functional groups and high pH. It can be used as absorbents for these characteristic. This study is based on the characteristics of the hydrochar through the physical and chemical composition analysis, we investigate adsorption ability for heavy metal. The biomass used in the study was obtained at W dormitory restaurant in Nowon-gu and composed of 41.5 % cereal, 27.8 % fruits, 18.5 % vegetables, 4.5 % meat , fish and 10.7 % of others (bark, paper, etc.). The moisture content of biomass was 81.43% (wt/wt). In order to determine the optimum conditions, hydrochar was generated at 220 ℃ and 230 ℃, for 1 hour, 2 hours, 4 hours, 6 hours and 8 hours, respectively. To select the optimum conditions, iodine number and methylene blue number have been measured. As a result, surface area of the hydrochar showed the highest at 230 ℃ for 4 hr. From the results obtained from computation of surface area, 230 ℃ for 4 hr was the optimum condition for biochar production. Physicochemical characterization of the biochar generated at the optimal conduction was investigated including elemental analysis(C, H, N, O), FT-IR, SEM, compositional analysis and carbon's acidic oxygen surface functional groups. Keywords : Biomass, HTC(Hydrothermal carbonization), Hydrochar, Adsorption, Surface area

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The screening of new microalgae for biofuel production at AMD area

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Economic and environmental friendly, bioenergy (biofuels) production from microalgae has become one of the most promising and sustainable alternatives. Many studies have been reported that physiochemical conditions to increase the lipid content are influenced by the growth condition of microalgae in medium. In toxic environmental condition (lower pH, exist variety heavy metal ions), the growth rate of microalgae might be reduced. Recently, many previous studies focused on high biomass production as well as high lipid productivity. For incubating specific microalgae with high contents of fatty acids, neutral lipids, and polar lipids in the natural environment, the isolation and characterization of microalgae in toxic environmental condition have been exploited1). Therefore, the goal of this study is to select the best algal strain to achieve the following objectives: i) high biomass production and specific growth rate ii) maximize lipid productivity and high quality biodiesel. Four green microalglae were isolated from 30 algal cultures (Nephroselmis sp. KGE1, Uronema sp. KGE3, Micractinium sp. KGE4, and Scenedesmus sp. KGE7) and selected based on their searching the NCBI BLAST and new strains uploaded GenBANK. The similarity of the new species is very low based on comparing with BLAST (89 %, 94 %, 89 %, and 97 %). Palmitic acid (C16:0), Linolelaidic acid (C18:2n6t), and γ-Linolenic acid (C18:3n6) were found as a major fatty acid. Total fatty acid(TFA) in Nephroselmis sp. KGE1, Uronema sp. KGE3, Micractinium sp. KGE4, and Scenedesmus sp. KGE7 represents 76.8%, 74.5%, 61.6%, and 80.9%, respectively.

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Human Risk Assessment of Heavy Metal from the Rinsing Wastewater of PCB Industry

장다영* **김종부[1]** **서항복[2]** **박종오[3]** **최영하[4]**

해동테크놀로지 기업부설연구소 [1](주)해동테크놀로지 기업부설연구소 [2](주)해동테크놀로지 대표이사 [3](주)해동테크놀로지 상무 [4](주)해동테크놀로지 이사

국내의 PCB(Printed Circuit Board)산업시장은 2000 년대 초부터 상승세를 보이며 세계 PCB 산업시장에서 약 13%의 점유율을 가지고 있다. 또한 매년 성장률이 약 10%를 기록하면서 PCB 생산량도 급증하고 있는 추세이다. 이에 따라 PCB 제조공정에서 발생하는 폐수에 관심이 집중되고 있다. 특히 PCB 제조 공정 중 에칭(Etching)과 박리(Stripping)공정 이후에 세정공정에서 발생하는 저농도 구리는 에칭과 박리공정에 비하여 농도가 낮기 때문에 수거효율이 낮아 폐수처리장으로 유입된다. 수질 및 수생태계 보전에 관한 법률에 따르면 구리는 특정수질유해물질로 분류되며 독성이 강하여 그 처리 없이 수체 내 환경으로 방출될 경우, 매우 낮은 농도의 구리 함유 폐수라 하더라도 흡착, 화합물의 형성 그리고 화학적 결합 등을 통해 환경에 축적되어 수질의 탁도, 냄새, 색 등을 변화시키는 등 생태계에 악영향을 주며 생물농축 등의 경로를 거쳐 인채 내에서는 간기능 장애, 위장장애, 피부장애 등의 인체에 치명적인 영향을 미치는 질병을 유발시킬 수 있기 때문에 구리에 관한 규제의 필요성이 제기되고 있다.본 연구에서는 PCB 제조에서 에칭과 박리공정 이후에 세정공정에서 발생하는 폐수를 분석함으로써 그에 따른 유해성을 평가하기 위하여 PCB 제조업체의 에칭 및 박리공정 세정폐수를 분석하였다. 구리농도는 에칭 및 박리 세정 폐수에서 각각 약 440ppm 과 약 100ppm 으로 측정되었다.이는 환경정책기본법에서 규정하는 사람의 건강보호를 위한 해역환경기준인 0.02ppm 과 비교하였을 때 매우 높은 수치로 나타내고 있다. 국내에서 아직 저농도의 구리를 회수하는 기술이 많이 연구되고 있지 않은 가운데 중금속이 폐수처리장으로 유입되기 이전에 회수할 수 있는 방법을 강구해야 할 것이다. 본 연구는 지식경제부와 한국산업단지공단의 생태산업단지구축사업의 일환으로 수행되었으며, 이에 감사를 표한다.

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Persulfate/Zerovalent Iron mediated oxidation of chlorinated organic compounds

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Persulfate (PS: S2O82?) is a strong oxidant (E? = 2.1 V) that can generate free sulfate radicals(SO4??, E?= 2.6 V) under certain conditions. Various agents (heat, ultraviolet light, high pH, hydrogen peroxide, and transition metals) are used to activate persulfate and generate the sulfate radical (SO4?.?). Persulfate activation by zerovalent iron (Fe(0)) has recently attracted increasing interest as zerovalent iron is environmentally benign and relatively economical. We applied the Fe(0)+PS system for the removal of chlorinated organic contaminants(COC) and the oxidative decomposition process was investigated. The various combination of COC/Fe(0)/PS was studied in order to find the optimum ratio, and Fe(0)-activated dissociation of PS was monitored to obtain information about the duration of PS under the given amount of Fe(0). For continuous removal of contaminants the repeated spikes of Fe(0)+PS was necessary due to the sulfate radical scavenging by Fe(0) and Fe2+ which was generated through oxidation of Fe(0).

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SO2 absorption by nitrile-functionalized amines

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경희대학교 화학과

Several functionalized amines bearing a nitrile group, including N-butyl-N-propionitrile amine (BAPN), N,N-diethyl-N-propionitrile amine (DEAPN), N,N-dibutyl-N-propionitrile amine (DBAPN) were synthesized and their SO2 absorption capacities were evaluated. For comparison, the SO2 absorption capacities of N-tert-butylethanol amine (TBAE) and N-methyl-N,N-diethanol amine (MDEA) were also tested. Absorption-desorption cycle experiments clearly demonstrate that the amines bearing a nitrile group are more efficient than those containing a hydroxyethyl functional group or groups in terms of absorption rate and regeneration although the amines containing a hydroxyethyl functional group or groups showed higher SO2 absorption capacities than those containing a nitrile group. Computational calculations with MDEA and DBAPN revealed that the hydroxyethyl-functionalized MDEA absorb SO2 through both chemical and physical interactions, whereas the DBAPN bearing a nitrile group absorb SO2 through a physical interaction.

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Novel ionic liquids bearing ether-functionalized anion and their properties

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Novel room temperature ionic liquids (RTILs), [DMIm][MPEG200P] and [DMIm][MPEG350P], bearing ether-functionalized anion were prepared by monomethylated polyethylene glycol (MPEG-200 and MPEG-350) and their physical and electrochemical properties were studied. The ILs exhibited high thermal stabilities over 200 oC and have wide electrochemical window over 5 V. [DMIm][MPEG200P] and [DMIm][MPEG350P] showed relatively low ionic conductivities of 9.3 and 5.71 mS cm-1 at 100 oC, respectively. Interestingly, however, after added 1 mole eq. of LiTf2N into each IL, the ionic conductivities of [DMIm][MPEG200P] and [DMIm][MPEG350P] were increased up to 12.0 and 11.7 mS cm-1 at 100 oC, respectively, although both ILs became soft gel.

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Factors affecting struvite crystallization

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Struvite ($MgNH_4PO_46H_2O$) is a white inorganic crystalline material and has gained interest as a route to phosphorus recovery. Precipitation of struvite is affected by several factors, such as pH, concentrations of Mg^{2+}, PO_4^{3-} and NH_4^+ and presence of other interfering ions, such as calcium (Ca^{2+}). It is highly pH-dependent, as activities of both NH_4^+ and PO_4^{3-} are affected by solution pH. It has been well documented that pH for struvite precipitation is 8.0-10.7. This optimum pH range is related to PO_4^{3-} solubility and the presence of N as NH_4^+ in solution. High NH_4^+ concentration enhances struvite precipitation and has the extra advantage of pH buffering in solution. Previous studies of struvite mainly focused on improving effluent quality from anaerobic processes that produced PO_4^{3-} and ammonia. Inthis study, effects of the molar ratio $[Mg^{2+}]:[NH_4^+]:[PO_4^{3-}]$ and pH were investigated. The structure, morphology, composition and thermal properties of the prepared precipitates were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectrometry (EDS), and thermogravimetric analysis (TGA).

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Overestimation of total Fe(II) concentrations during acid extraction of Fe(II)/Fe(III) (hydr)oxides in the presence of sulfide

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This study compared the total Fe(II) concentrations measured by X-ray spectroscopy and acid extraction in the presence of Fe(II)/Fe(III) (hydr)oxides and sulfide. The proportion of Fe(II) in the solid phase, as determined by X-ray spectroscopy in the goethite system, was consistent with that determined from the chemical extractions. Fe(II) determined by X-ray spectroscopy in the ferrihydrite and lepidocrocite systems followed the trend with time observed in the chemical acid extraction data, but the amount determined by X-ray spectroscopy in the long-incubation samples was significantly lower. It is possible that the decrease in pH during the acid extraction procedure promoted redox reactivity between the more soluble parent Fe(III) (hydr)oxides and the sulfide species (or other reductants) resulting from dissimilatory sulfate reducing activity. Therefore, total Fe(II) concentrations determined by acid extraction of Fe(II)/Fe(III) (hydr)oxides in the presence of sulfide may overestimate the amount of Fe(II) present in the system at pH 7. Because the acid extractions in the current work were performed in a consistent manner for all points, the temporal profile observed for the Fe(II) dynamics will likely not be affected; however, the amounts of Fe(II) in the lepidocrocite and ferrihydrite system may need to be scaled by a factor to estimate Fe(II) content at pH 7. More detailed studies will be conducted to constrain this factor, but based on a comparison between the acid extractions and the x-ray spectroscopy data its value is of the order 0.6-0.7 for our experimental conditions.

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Direct observation of aluminium ions produced via pulsed laser ablation in liquid: a 'turn-on' fluorescence study

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경상대학교 화학과

An Al metal plate was ablated by a pulsed Nd-YAG laser to produce nano-structured Al and gamma-Al_2O_3 in deionized water without any surfactants or catalysts. In this study, direct evidence for the production of Al^{3+} ions from the plasma plume is presented for the first time by characterizing the absorption and emission spectra of their $[Al(salophen)]^+$ complex. Very interestingly, a remarkable increase in the fluorescence intensity was observed when the Al_{3+} ions, produced via the pulsed laser ablation, complexed with the salophen ligand. This fluorescence 'turn-on' behaviour of $[Al(salophen)]^+$ was investigated by DFT/TD-DFT calculations. Based on these results, mechanisms for the production of aluminium and alumina nanoparticles in the pulsed laser ablation in liquid (PLAL) process are proposed.

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Alternative Extracellular Electron Shuttles for the Transformation of Explosive Compounds

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We investigated the potential of aloe as the eco-friendly extracellular electron shuttle (EES) for stimulating iron and contaminant reduction. EES, the compounds containing quinone functional groups are known to transfer electrons from the cell to the Fe(III) (hydr)oxides or contaminants. Therefore, EES can promote the reduction of Fe(III) or the degradation of contaminants such as hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). We compared the rate and extent of Fe(III) reduction in the presence of Geobacter metallireducens and several quinone containing compounds including anthraquinone-2,6-disulfonate(AQDS), humic acid, and aloe extracts. All EES tested in this study stimulated Fe(III) reduction. Although the rate and extent of Fe(III) was fastest in the presence of AQDS, Fe(III) reduction was also 2-3 times faster with aloe. This suggests the extracts from aloe can be a viable source of electron shuttles and can be used to degrade or reduce contaminants (e.g., RDX, Cr, U). We will further determine if low-cost, easily obtained aloe can promote the reduction of RDX and heavy metals.

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CO2 adsorption by carbon-coated silica aerogels

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

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Low Concentration Explosives and Their Degradation Products Analysis by Nanoscale Zero-Valent Iron(nZVI) Using LC-ESI-MS/MS

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포항공과대학교 환경공학부

Explosives, especially RDX(1,3,5-trinitro-1,3,5-triazine) and TNT(2,4,6-Trinitrotoluene), have been widely used for a long time at many military installations. Their extensive use has led to widespread contamination in soil and water. RDX and TNT are known to be toxic to various aquatic and terrestrial organisms, thus necessitating their removal from polluted environments. Recently, nanoscale zero-valent iron(nZVI) have been developed for several environmental remediation technologies. Especially, nZVI has demonstrated effective degradation of explosives. In this study, RDX degraded by reduction with nZVI has been investigated by several degradation products including nitroso-RDX metabolites (e.g., MNX, DNX, and TNX). In addition, major intermediate products obtained from TNT degradation, including 2,6-DNT, 2,4-DNT, 2A-4,6-DNT and 4A-2,6-DNT, were identified using LC-ESI-MS/MS. Acquisition was performed in the multiple reaction monitoring mode (MRM) depending on the compound. In conclusion, LC-ESI-MS/MS study for explosives analysis showed the presence of several key products carrying important information on the initial reactions involved in the degradation of explosives.

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Catalytic Reductive Dechlorination of m-Dichlorobenzene (m-DCB) by Nickel-Palladium Nanoparticles via Pulsed Laser Ablation in Liquid.

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Nickel and nickel oxide nanoparticles exhibit useful optical or electrical functions as well as catalytic actions. Among various particle fabrication methods, pulsed laser ablation in liquid (PLAL) is currently attracting great interest due to its simplicity and versatility. In this study, a pulsed Nd:YAG laser (1064 nm, 10 Hz, 7 ns) is used to produce the nickel and nickel oxide nanoparticles in deionized water and methanol. The morphological and optical properties of nickel and nickel oxide nanoparticles size and optical properties of the nanoparticles were characterized by field emission scanning electronic microscope (FE-SEM), X-ray diffraction (XRD) and ultraviolet-visible spectroscopy (UV-vis). Synthesized palladium/nickel (Pd/Fe) bimetallic nanoparticles were applied to dechlorinate dichlorobenzene (DCB) under various conditions. Rapid dechlorination of dichlorobenzene (DCB) suggests that nickel nanoparticles can be used for remediation of polychlorinated aromatic compounds in the environment.

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Reductive Dechlorination of Groundwater Waste using Bimetallic Nanoparticles Produced by Pulsed Laser Ablation in Liquid (PLAL).

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Disposal of chlorinated organic wastes in such a way as to minimize the environmental hazards has become an urgent issue nowadays. Synthesis and use of reactive metal particles have shown significant environmental implications for the remediation of groundwater and sediment contaminated with chlorinated compounds. However, groundwater waste such as tichloroethylene(TCE), tetrachloroethylene(PCE) cannot be easily and effectively decomposed with currently available biological and chemical treatment methods. The good of this work is an effective dechlorination of chlorinated compounds using Fe nanoparticles produced via a pulsed laser ablation in liquid (PLAL). The present work presents a relatively simple method to fabricate Fe nanoparticles for the dechlorination of chlorinated compounds. Fe nanoparticles were produced by laser ablating onto an Fe plate immersed in deionized water with a reducing agent, ascorbic acid. Rapid dechlorination of chlorinated compounds suggests that Pd/Fe bimetallic nanoparticles can be used for remediation of polychlorinated compounds in the polluted environment.

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REMPI and UV-UV Hole-burning Spectroscopic Investigation Persistent Organic Pollutants (POPs)

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경상대학교 화학과

Persistent oganic pollutants (POPs) are chemical substances that persist in the environment, bioaccumulate through the food and pose a risk of causing adverse effects to human health and the environment. In this study, resonance enhanced multi-photon ionization (REMPI) and UV/UV double resonance spectra of POPs in the gas phase are presented. And we calculated POPs using density functional theory (DFT) with a 6-311+G(d) basis set and obtained structural information. Furthermore, we further carried out calculations for POPs using time dependent-DFT (TD-DFT) to predict excited state molecular information.

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Preparation of nano-sized indium tin oxide(ITO) powder by co-precipitation

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In and Sn one known as important resources in many of industrial fields. Several counties in the world monopolize the supply of these resources to control their price and national securities. So that many countries consuming these material without supplying have difficulties in production of others. One way to avoid the supply difficulty is the recycling method of the materials for the discarded IT instruments or wastes of the sputtering target. Amount of spent with ITO target increases with display industry growth. Because ITO targets are usually sputtered onto glass plates by DC magnetron sputtering method. But in this process only less then 30% of ITO target is used to ITO glass. And the 70% of sludges remained on the chamber. We have tried to prepare nano-sized ITO powder from the waste of ITO target for resource recycling purpose. Nano-sized ITO powder was successfully prepared by using co-precipitation method. After heat treatment up to 500℃ for 6hr, it were homogeneous and single phase. and XPS, EDX, XRD, TGA and ICP were done for this sample. This work was supported the Energy & Resource Recycling of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Knowledge Economy (No.2010501010002B)

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Determination of optimal conditions for reductive transformation of tetrachloroethylene by bimetallic catalysts and hydrogen gas

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This study was conducted to determine optimal conditions for reductive dechlorination of tetrachloroethylene (PCE) by bimetallic catalysts. Bimetallic catalyst was applied to effectively degrade PCE, one of the recalcitrant toxic contaminants. We tested four second metals (Co, Ni, Cu, and Zn) and three noble metals (Pd, Pt, and Au) to synthesize bimetallic catalysts with meghemite as support material. Reductive dechlorination of PCE by bimetallic catalysts was observed in closed batch reactors containing certain contents of noble metal ion and zero-valent catalyst composed of second metal and maghemite in pH 7 MOPS buffer solution under 2% H2/98% N2 condition. Under the conditions of 3% second metal and 0.5% noble metal, PCE removal rates by different second metals were in the order of Ni, Co, Cu, and Zn. When Ni was used as second metal, PCE was removed by 40% in 6 hr. PCE removal rates based on different noble metals were in the order of Pd, Au, and Pt. In case of Pd, PCE was degraded by 40% in 6 hr. Remaining H2 gas concentrations with respect to noble metal were 0.3% (Pd), 1.0% (Pt), and 1.6% (Au) respectively after 6 hr reaction. When Ni contents as second metal composing catalyst were 1%, 3%, and 10%, PCE was removed by 36%, 40%, and 63% respectively. In case of different contents of Pd (0.5%, 1%, and 3%), PCE was removed by 40%, 50%, and 50% respectively. Ethane as a PCE degradation product in 3% Ni and 3% Pd condition was detected higher than that in any other catalyst composition, whereas the highest yield of ethylene as a PCE transformation product was produced in 10% Ni and 0.5% Pd catalyst composition.

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TiO_2-embedded carbon nanofibers을 이용한 광촉매적 수소생성

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무한한 에너지원인 태양광을 이용하는 광촉매적 물분해 수소 생산방법은 매우 전망이 밝은 분야이다. 광촉매 분말을 사용하는 경우 광촉매의 반응 후 TiO_2 분말을 다시 분리하여 제거하는 공정이 필요하다. 그러나 TiO_2/CNFs 는 분말의 분리, 제거공정을 생략 할 수 있는 경제성과 편이성이 돋보이는 (청정에너지를 위한) 광촉매의 새로운 형태이다. 분리해낸 TiO_2/CNFs 는 형태의 변형 없이 재사용이 가능하고, CNFs 는 비표면적이 크기 때문에 촉매 지지체로 응용했을 때 그 효율이 극대화 될 수 있다. TiO_2/CNFs 은 물에서의 안정성이 양호하고, 재생 가능하며, 지속적으로 사용 가능한 에너지원인 수소를 생산하기 위한 새로운 광촉매로 주목할 만하다.본 연구에서는 TiO_2 광촉매를 CNFs 지지체 위에 함양시키고 광촉매적 물분해로 수소를 생성한다. 고분자 Polyacrylonitirle(PAN)과 광촉매 TiO_2 을 섞은 용액을 전기방사하여 TiO_2/PANnanofibers 를 제작한다. TiO_2/PANnanofibers 는 온도를 점증적으로 올려 소성시키는 Carbonization 그리고 Oxidation 을 통해서 순차적으로 TiO_2/CNFs 로 완성된다. 자외선 조사 하에서 Pt deposition 을 하고 MeOH 를 electron donor 로 사용하여 수소의 생성효율 향상에 기여 할 수 있도록 한다. Pt deposition 이 된 TiO_2/CNFs 에 자외선을 조사 후 수소 생성량은 4.07 mmol/g 이다. 본 연구는 TiO_2/CNFs 를 광촉매적 물분해를 통한 수소생성 연구에 최초로 적용하였으며 지속적 연구개발을 통하여 효율 향상과 다양한 광촉매 반응 분야로의 응용을 기대할 수 있다.

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Quantification of aqueous U(VI) by laser-induced spectroscopy in the presence of Fe(II)

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Recent studies for understanding biogeochemical interaction mechanisms between U(VI) and natural reductants have demonstrated that iron bearing soil minerals such as greenrust, magnetite, and mackinawite can effectively reduce soluble U(VI) into insoluble U(VI) under reducing environments. Selective monitoring of U(VI) concentration in the aqueous phase and/or on the iron-bearing soil minerals is indispensable in assessing the reactivity of soil minerals. Since only U(VI) emits fluorescence signals under laser incident, laser spectroscopy has been widely used to study the qualitative and quantitative analysis of aqueous U(VI). However, due to the quenching effect of iron, laser spectroscopy has not been able to measure the reductive capacity of iron-bearing soil minerals for U(VI). In this study, we investigated the quantitative analysis of aqueous U(VI) by time resolved laser-induced fluorescence laser spectroscopy (TRLFS) in the presence of ferrous iron. As a results, the profile of U(VI) fluorescence intensity and lifetime was obtained as a function of ferrous iron concentration . The fluorescence intensity of U(VI) has been decreased as S-logistic curve with respect to the ferrous iron concentration. Based on the life-time measurement results, dynamic quenching without formation of U(VI)-ferrous iron complex was the major mechanism in this study.

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Synthesis and Characterization of LCST-Based Draw Solutes for Efficient Forward Osmosis

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Osmosis is a promising method for the efficient production of energy and water resources. Contrary to reverse osmosis (RO) which uses external pressure input, forward osmosis (FO) uses the difference of osmotic pressure between feed solutions and draw solutions with different concentrations and different osmotic activities.We designed several novel solutes with lower critical solution temperature (LCST) properties, which are dissolved in water at low temperatures, but are separated from water at high temperatures. The solutions based on these solutes show high osmotic pressure and abruptly reduced low osmotic pressure at temperatures lower and higher than the phase transition temperatures, respectively. We compared the LCST characteristics of various solutes and check the structure-LCST relationships for more efficient FO process using mild temperature change.

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Eco-friendly Forward Osmosis Using Novel Thermo-sensitive Materials as a Desalination Draw Solute.

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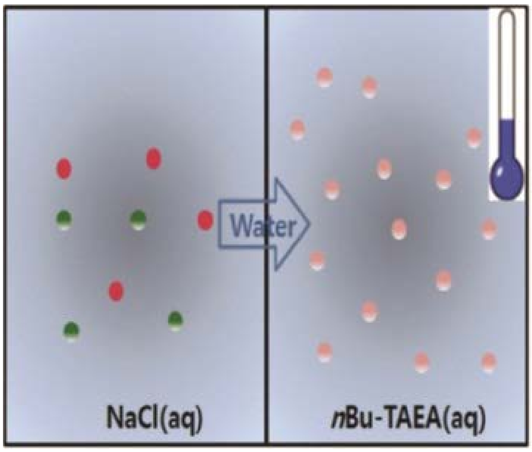
Various methods such as distillation and reverse osmosis (RO) for desalination have been researched to solve this clean water deficiency until now. However, those methods to obtain freshwater from seawater have to consume a lot of energy. Therefore, alternative method which could save consumption of energy for desalination is required. Meanwhile, Forward osmosis (FO) has been recognized as one of the most promising ways in regards of its eco-friendly and energy-efficient characteristics. The well-known FO draw solute, ammonium bicarbonate (NH4HCO3), has some limitations for eco-friendly, permanent FO process because it is required to high separation temperature (>60oC), complex solute removal process, and alkaline condition of the solution. To overcome these limitations of ammonium bicarbonate (NH4HCO3) solution for FO process, we selected thermo-sensitive materials as FO draw solute in this research. Thermo-sensitive materials are separated from solutions at certain temperature range. N-acylated tris(2-aminoethyl)amine which shows lower separation temperature, ~30oC, was used as FO draw solute in this work. The solution with the N-acylated tris(2-aminoethyl)amine draw solute in water is highly soluble enough to have osmotic pressure which can draw fresh water from seawater (0.60M NaCl equivalent) below a certain temperature (LCST).Above the LCST, the draw solute is separated from water and therefore the effective concentration of solution is lowered enough to release the drawn water into physiological saline (0.15M NaCl equivalent).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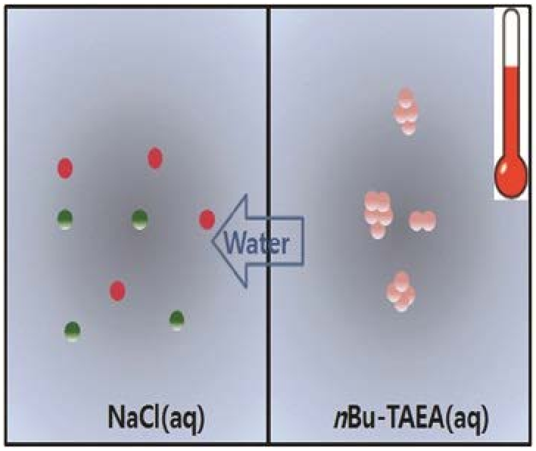
NaCl(aq)
*n*Bu-TAEA(aq)


Water
NaCl(aq)
*n*Bu-TAEA(aq)