일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **PLEN-1**

발표분야: 기조강연

발표종류: 특별강연, 발표일시: 목 16:30, 좌장: 박승민

실험실 연구에서 사업으로: 화학/바이오센서 연구팀의 사례

남학현

광운대학교 화학과

바이오 및 화학센서들에 대한 연구는 실생활에서의 응용이 목표인 경우가 많으며, 종종 연구자들은 연구 결과물로 상업화를 시도하는 경향이 있다. 화학 및 바이오센서 기반의 소형 장비들, 예를 들어 미세유로를 사용한 칩과 소형화한 전기화학 또는 광학 측정 장비들은 기존의 분석기술들의 분석성능을 약간 희생하는 대신 편리하고 경제적이며 대량생산이가능하여 누구나 복잡하고 어려운 분석을 간단히 시행할 수 있는 방법을 제공해준다는 측면에서 와해성기술(disruptivetechnology)의 범주에 속하며 상업성이 크다.

차근식 남학현 교수 팀은 1992 년도부터 광운대학교 화학센서연구 그룹을 이끌면서 소형화한 이온센서, 면역센서, 특히스크린프린팅 기술에 기반을 둔 일회용센서의 개발을 주도하였고, 이 분야에서 주목을 받을만한 다수의 논문과 특허를 출간하였으며, 국내 및 국제 기업들과 다양한 산학과제를 수행하는 경험을 축적하였다. 1990 년대 말부터 2000 년 초반까지 불었던 창업회사들에 대한 열기 속에서 차근식 남학현 교수 팀은 열성적인 5 명의 대학원생들과 함께 그 동안의 연구결과를 상업화할 수 있는 길을 찾기 위하여 아이센스 회사를 창업하였다. 그러나 화학만을 전공한 연구자들로서 기업의 연구 및 개발, 제품개발의 과정, 대량생산, 회사의 경영 방식 등에 대한 지식이 전무하였기에 회사를 운영하는 과정에서 발생하는 많은 도전적 문제들에 직면하였고 그러한 난제들을 창의적으로 해결해야 했다. 다행히도 첫 제품으로 목표했던 혈당센서를 3 년만에 성공적으로 개발 출시하였고, 주변의 많은 도움으로 지속적 성장을 하여 회사는 2013 년 코스닥에 등록을 할 수 있었다.

이 세미나에서는 화학 연구자로서 경험한 창업의 과정 및 학술적 연구에서 상업화의 과정, 기업의 경영에 관한 경험들을 소개하고자 한다. 본 강연의 내용이 산학연구와 상업화를 크게 강조하고 있는 현 정부 및 각급 대학, 국공립 연구기관들에서 종사하는 연구자들에게 약간의 도움이라도 되기를 희망한다.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **AWARD-1**

발표분야: 기념강연

발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 강헌

Some Simple Ideas in Perturbation Theories

이상엽

서울대학교 화학부

In this talk, I will present two general methods in the perturbation theories that would be useful in statistical mechanics and quantum mechanics.

The first one is a new method of solution for the Fredholm integral equations of the second kind. The method would be useful when the direct iterative approach to the integral equation leads to a divergent perturbation series solution. In such case one usually employ the Padé approximation, but we have found that our method gives much more accurate results than Padé approximation method for the same computational cost. A main advantage of the new method comes from the fact that the solution has the same structure as the exact solution. By using the method, we have derived a very accurate expression for the steady-state rate constant of diffusion-influenced bimolecular reactions involving long-range reactivity. We consider the general case in which the reactants interact via an arbitrary central potential and hydrodynamic interaction. The rate expression becomes exact in the two opposite limits of small and large reactivity, and also performs very well in the intermediate regime.

The second one is a variant of the Brillouin-Wigner perturbation theory, which can be easily extended to the quasi-degenerate case. A main advantage of the new theory is that the computing time required for obtaining the successive higher-order results can be made to be minimal after the fourth-order calculation. We illustrate the accuracy of the new perturbation theory for some simple model systems like the perturbed harmonic oscillator, the perturbed particle in a box, and the electronic problems of very small molecular systems.

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장소: 광주 김대중컨벤션센터
발표코드: **POLY1-7**
발표분야: Current Trends in Self-healing Polymeric Materials
발표종류: 분과기념강연, 발표일시: 목 11:30, 좌장: 박태호

Photothermally triggered cytosolic drug delivery via endosome disruption using a funtionalized graphene oxide

김원종

포항공과대학교(POSTECH) 화학과

In the present work, functionalized reduced graphene oxide (PEG-BPEI-rGO) has been developed as a nanotemplate for photothermally triggered cytosolic drug delivery by inducing endosomal disruption and subsequent drug release. PEG-BPEI-rGO has ability to load more amount of Doxorubicin (DOX) than unreduced PEG-BPEI-GO via π-π and hydrophobic interactions, showing high water stability. Loaded DOX could be efficiently released by glutathione (GSH) and photothermal effect of irradiated near IR (NIR) in test tubes as well as in cells. Finally, it was concluded that more cancer cell death efficacy was observed in PEG-BPEI-rGO/DOX complex-treated cells with NIR irradiation rather than that in no irradiation.Paclitaxel (PTX) is one of the most effective chemotherapeutic drugs used in breast, ovarian, lung, head and neck cancers. However PTX has very low solubility in water and physiological conditions. To enhance its solubility, PTX would be formed inclusion complex with β-cyclodextrin (β-CD). β-CD is a cup-shaped molecules that consists of 7 glucopyranoside units and has hydrophobic cavity and hydrophilic exterior. It has long-term biocompatibility, low toxicity and do not elicits any immune response. It has also well-known host-guest interactions with many small molecules and portions of large compounds, such as benzoate moiety of PTX. Herein, we designed self-assembled nanoparticles for PTX delivery toward tumor cell. Self-assembled nanoparticles were constructed through host-guest chemistry between PTX and CD. CD and PTX are covalently conjugated with poly maleic anhydrides that provide higher solubility of nanoparticles. This inclusion complex showed enhanced antitumor effect than PTX. In this study, we also developed novel nitric oxide (NO) delivery system using catecholamine and diazeniumdiolates. Although the surface NO delivery garners paramount importance in various biomedical applications, the prospect of local NO delivery strategies in implementing in widespread practical application is significantly impaired by the associated low NO-loading capacity, leaching out arising from the weak coating ability, heavy thickness (µm-mm). Herein, a novel surface nitric-oxide (NO) delivery system was developed. Simple two-step reactions comprising catecholamine and diazeniumdiolates enable virtually any material surfaces to release NO with appreciable storage. The modified surfaces showed the antibacterial activity without cytotoxicity. Hence our novel strategy presents the potential for various NO-mediated biomedical applications.

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장소: 광주 김대중컨벤션센터
발표코드: **POLY1-1**
발표분야: Current Trends in Self-healing Polymeric Materials
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이현정

초분자 네트워크형 자가 치유 고분자의 최근 연구 개발 동향

정재우

숭실대학교 유기신소재파이버공학과

자가 치유(self-healing) 고분자는 외부 환경에 의해 손상을 입은 고분자가 스스로 결함을 감지하여 자신의 구조를 복구함은 물론 원래의 기능을 회복할 수 있는 지능형 재료로 최초 자연계 생체 시스템이 스스로 복구되고 치유되는 것을 모방한 대표적 생체 모사 시스템 중 하나이다. 재료의 손상은 재료 자체의 물성과 기능의 손실을 야기하고 전체 제품의 내구성과 성능 지속성에 막대한 영향을 미치므로 손상을 억제함은 물론 재료가 지닌 구조와 기능에 대해 근원적 복구가 가능한 자가 치유 재료가 만들어 진다면 기존 소재 개발 및 응용에 패러다임을 획기적으로 바꿀 수 있어 이에 대한 관심이 급증하고 있다. 최근, 수소결합, π-π 상호작용, van der Waals 힘, 정전기적 인력, 금속 배위결합과 같은 비공유결합을 근간으로 올리고머 및 고분자에 초분자 형태의 네트워크 구조를 형성시켜 재료의 초기 파단 시 분자인식 및 재배치와 같은 자기집합적 특성의 발현으로 재료를 치유하고자 하는 연구가 활발히 진행되고 있다. 이들은 별다른 자극 없이도 손상된 부분이 수 차례나 복원될 수 있다는 점에서 기존 자가 치유 고분자의 한계를 극복할 수 있는 신개념 자가 치유 시스템으로 큰 주목을 받고 있다. 이에 본 심포지움에서는 초분자 네크워크 구조가 도입된, 특히 수소결합, π-π 상호작용, 정전기력, 금속 배위결합을 중심으로 초분자 네트워크형 자가 치유 고분자의 최근 연구 개발 동향에 대해 소개하고자 한다.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **POLY1-2**
발표분야: Current Trends in Self-healing Polymeric Materials
발표종류: 심포지엄, 발표일시: 목 09:22, 좌장: 이현정

Microencapsulation of 2,6-dimethylphenol for Self-Healing Asphalt

홍영근

수원대학교 신소재공학과

Microcapsules loaded with healing agent were successfully prepared in which 2,6-dimethylphenol(DMP) or SBS/DMP as healing agent form core, and urea/formaldehyde resin forms shell of the microcpasule. Microcapsule-contained asphalts showed better mechanical properties than non-contained ones. As time passed the impact strengths of microcapsule-contained asphalts was getting higher than that of its original. As the rest time of 3 and 7 days passed for microcapsule(SBS/DMP)-contained and microcapsule(DMP)-contained asphalt, respectively, their original strength was restored. This tells that microcapsule(DMP or SBS/DMP)-contained asphalts have the excellent self-healing ability. SEM and X-ray photos show that DMP on asphalt fracture surface, which burst out of the microcapsules when cracks occurred on surface of the asphalt, were polymerized to polyphenyleneoxide(PPO) and this PPO filled the crack and healed the damage.

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장소: 광주 김대중컨벤션센터

발표코드: **POLY1-3**

발표분야: Current Trends in Self-healing Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 09:44, 좌장: 이현정

Self-Healing Polymer Composite and their Applications

정용채

한국과학기술연구원(KIST) 탄소융합소재연구센터

초기 손상들은 눈에 보이지 않을 정도의 미세균열로부터 시작하게 되는데, 소재의 반복적인 사용은 소재 물성의 저하와 매트릭스 손상으로 인한 하중의 재분배를 일으켜 인장강도, 피로수명 등과 같은 지배 물성에 영향을 준다. 이후 수명이 다한 소재들을 새롭게 대체하는 과정에서 발생하는 재생산비, 그 때 발생하는 에너지 소비와 유지 및 관리비 등이 크게 소요된다. 이와 같은 문제점 등을 해결하기 위하여 많은 연구자들은 자연에서 흔히 볼 수 있는 스스로 치유되는 능력에 초점을 두어 연구하고 소재에 그 개념을 부여하기 시작하였다. 자가치유 또는 자가복구 시스템이란 “인위적인 조작 없이 열, 전기, 광등과 같은 특수한 환경에 따라 스스로 이러한 결함들을 감지하여 복구할 수 있는 특성을 가지도록 설계한 시스템”을 지칭한다. 본 발표에서는 이러한 미래지향적 자가치유 고분자 복합소재에 대한 이해와 최근 기술개발 동향에 대해 살펴보고자 한다.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **POLY1-4**
발표분야: Current Trends in Self-healing Polymeric Materials
발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 정용채

Graphene based self-healing composites

안석훈

한국과학기술연구원(KIST) 전북분원 복합소재기술연구소

For decades, scientists have paid great attention for the developments of self-healing materials to improve the safety and life time of materials. Various self-healing systems such as embedding micro-capsules or microvascular networks, and reversible polymers have been intensively studied. However, the study of self-healing composites based on nanocarbon materials such as graphene and graphene oxide is now focused because unique properties of graphene and graphene oxide have been recently recognized. In this presentation, the trend for self-healing composites based on graphene will be presented. In addition, the research topics covered in 4th International Conference on Self-Healing Materials (ICSHM2013) will be shared.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **POLY1-5**

발표분야: Current Trends in Self-healing Polymeric Materials

발표종류: 심포지엄, 발표일시: 목 10:42, 좌장: 정용채

Self-healing Polymer Coatings in Corrosive Environments

조수현

POSCO 기술연구원 강재2연구그룹

Self-healing polymer coatings, at a very simplistic level, mimic the self-healing nature of skin in living systems. Polymer coatings are commonly applied to metal substrates to prevent corrosion in aggressive environments such as high humidity and under salt water. Once the polymer coating has been breached, for example due to cracking or scratches, it loses its effectiveness, and corrosion can rapidly propagate across the substrate. The self-healing system we will describe prevents corrosion by healing the damage through a healing reaction triggered by the actual damage event. The anti-corrosion properties of the self-healing polymer on metal substrates are investigated by corrosion resistance and electrochemical tests as well as microscopic observation. To confirm the stability of healing agent in coating solution, thermomechanical properties of healing agent containing microcapsules are demonstrated by the first use of a silicone microcaptilever. Even after scratch damage completely through the substrate, the coating is able to heal, while control samples which do not include all the necessary healing components reveal rapid corrosion propagation. This self-healing coating solution can be easily applied to most substrate materials, and is compatible with most common polymer matrices. Due to the environmental stability of PDMS poly-condensation, this coating may be used in severe environments such as high humidity, marine, and aerospace applications. Furthermore, the self-healing coatings are highly effective for forming an anti-corrosion barrier.

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장소: 광주 김대중컨벤션센터
발표코드: **POLY1-6**
발표분야: Current Trends in Self-healing Polymeric Materials
발표종류: 심포지엄, 발표일시: 목 11:04, 좌장: 정용채

Microcapsule-type Self-healing Protective Coatings

정찬문* 송영규

연세대학교 화학과

A protective coating is used to protect surface of a material from various deterioration factors. When cracks form and propagate in the coating, water, chloride ion, and carbon dioxide would penetrate through the cracks. This results in deterioration of the materials, leading to reduction in their serviceability. In this work we have developed self-healing protective coating systems for concrete or metal in which microcracks or scratches can be repaired by sunlight or atmospheric moisture. Healing agent-loaded microcapsules are embedded in a coating matrix to obtain a self-healing protective coating. Upon damage-induced cracking, the microcapsules are ruptured by the propagating crack fronts, resulting in release of the healing agent into the crack plane by capillary action and then self healing is achieved through polymerization of the healing agent.

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장소: 광주 김대중컨벤션센터
발표코드: **POLY2-1**
발표분야: Polymer Self-Assembly and Nanopatterning
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 정연식

Long-Range Orderd Selfassembly of Novel Block Copolymers for Nanolithography and Metallic Nanostructure Fabricaiton

한양규

한양대학교 화학과

Self-assembled nanoscale patterns from block copolymers are highly promising for future nanofabrication due to their extremely high resolution and cost-effectiveness. However, simultaneous achievement of long-range ordering and good pattern transfer capability still remains challenging. Here, we report that a novel acrylamide-based hard-soft hybrid block copolymer can unprecedentedly and simultaneously achieve extended long-range ordering and outstanding pattern transfer capability due to high etch-selectivity, high etch-resistance, and the capability to incorporate inorganic components. The unique molecular structure of the diblock copolymer also creates unusual bulk morphologies having a four-fold symmetry, which cannot be explained by traditional self-assembly theories. Moreover, the capability of selective incorporation of metal salt ions enables fabrication of diverse functional nanostructures such as aligned nanowires and nanomeshes with extraordinary structural regularity. This novel hybrid block copolymer with unique characteristics and outstanding versatility may pave a new pathway to create, tailor, and transform nanoscale patterns with high fidelity.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **POLY2-2**

발표분야: Polymer Self-Assembly and Nanopatterning

발표종류: 심포지엄, 발표일시: 목 13:52, 좌장: 정연식

그래핀 유연 기판을 이용한 10나노미터급 플렉서블 나노패터닝

김상욱

한국과학기술원(KAIST) 신소재공학과

블록공중합체 나노패터닝이나 광리소그라피등 나노패턴공정들은 균일한 두께의 유기박막의 형성이 필요하고 열처리나 노광공정이 요구되어 3 차원적인 기판이나 플렉서블한 기판에는 적용이 어려운 것으로 알려져있다. 본 발표에서는 용액공정으로 형성한 그래핀 기판을 기계적으로 유연한 기판으로 이용하여 다양한 3 차원적인 구조와 플레서블구조의 표면을 나노패턴화하는 연구들을 소개할 것이다. 더불어 ALD 공정을 통해 블록공중합체 나노패턴의 패턴밀도를 2 배향상시켜 PS-b-PMMA 고분자를 이용하여 5 나노미터급의 나노패턴을 형성하는 기법도 소개할 것이다.

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발표코드: **POLY2-3**
발표분야: Polymer Self-Assembly and Nanopatterning
발표종류: 심포지엄, 발표일시: 목 14:14, 좌장: 정연식

Block copolymer nanopatterning with shear alignment

김소연

울산과학기술대학교(UNIST) 에너지 및 화학공학부

Microphase separation of block copolymers in thin films can generate periodic structures and its application has been widely investigated due to its easy processability and low price. In this talk, recent progress in nanopatterning with shear-aligned block copolymers is discussed. For example, cylinder-forming block copolymers can be used as etch masks for the fabrication of nanowire grids, with both fine resolution and scalability. However, achieving a high aspect ratio in these nanostructures, where reactive ion etching is employed for pattern transfer, requires strong etch contrast between two blocks of the copolymer. We achieve this strong contrast by using metal-containing block copolymers: materials which either contain metal as synthesized: iron-containing polystyrene-b-poly(ferrocenylisopropylmethylsilane) (PS-PFS) forming PFS cylinders was employed, and a spin-coated film was aligned by shearing with a polydimethylsiloxane pad. The highly aligned stripe patterns can be used as UV polarizers with high efficiency of (>90%). Furthermore, nanosqure arrays with shear-alignment is introduced. Square or rectangular patterns do not naturally form by spontaneous self-assembly of a simple diblock copolymer, and are a challenge to create. A simple method to create nanoqsquare/rectangular arrays is demonstarted by building up a double-layer film of a cylinder-forming diblock, where each layer is sequentially deposited, shear-aligned independently, and cross-linked. Oxygen reactive ion etching is used to reveal the grid structures, and these grids can in turn form nano-wells in the silicon substrate when the cylinder-forming block is very etch-resistant under the conditions used for silicon etching.

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발표분야: Polymer Self-Assembly and Nanopatterning
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김소연

Directed Assembly of High-Molecular-Weight Block Copolymers and Perpendicular Orientation of Lamellar Microdomains

류두열

연세대학교 화공생명공학과

Nanoscopic assembly of block copolymer (BCP) thin films is currently of interest as a bottom-up approach for generating templates with well-defined periodic arrays of spherical, cylindrical, lamellar morphologies in typically 10 to 50 nm-scale. Despite a variety of morphological arrays of BCP, the spontaneous microphase separation in the thin films results in a random orientation of microdomain arrays with defects or parallel orientation due to preferential interaction of one block with the substrate, which limits the potential applications. The perpendicular orientation of microdomains was achievable by controlling the interfacial and surface interactions as an external field, particularly in polystyrene-b-poly(methyl methacrylate) (PS-b-PMMA) system, where the difference in surface energies of the two blocks was little. Furthermore, the substrates were readily tuned with the balanced (or neutral) interfacial interactions toward each block. On the other hand, the translational ordering of long-chained block copolymer is hindered by its very low chain mobility due to highly entangled conformation. In this study, we used a high-molecular-weight PS-b-PMMA to order and direct the orientation of lamellar microdomains in BCP films on a variety of substrates using a solvent vapor annealing process with tetrahydrofuran (THF) that is a neutral solvent for the two blocks of PS-b-PMMA, followed by quickly evaporating the solvent to preserve the film structure. We also demonstrate the wall guidance effect on perpendicularly oriented lamellae in topographic line and disk photoresist patterns as well as the interlamellar d-spacing compliant to the patterns.

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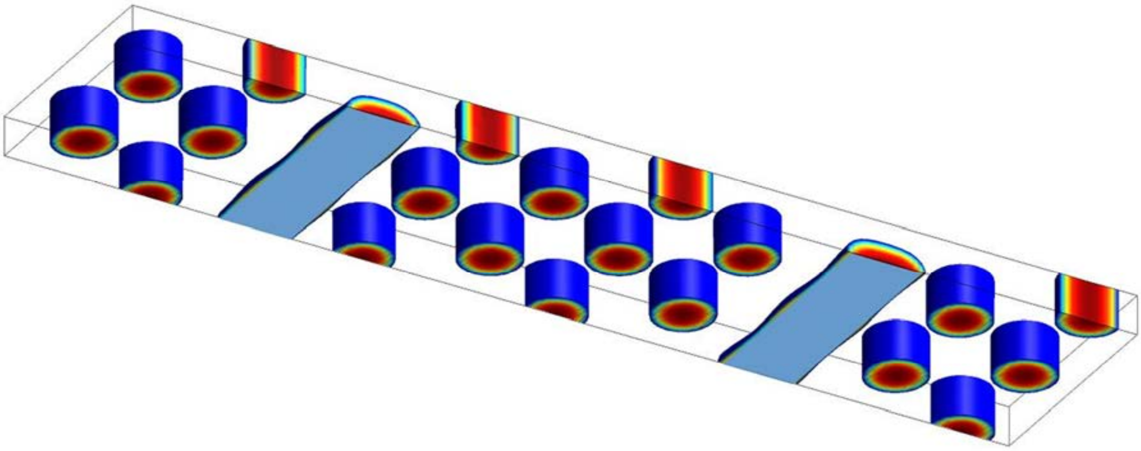
발표코드: **POLY2-5**
발표분야: Polymer Self-Assembly and Nanopatterning
발표종류: 심포지엄, 발표일시: 목 15:12, 좌장: 김소연

Theoretical Study on Nanopatterning Through Block Copolymer Nanostructures

김재엽

울산과학기술대학교(UNIST) 자연과학부

The recent trends in block copolymer nanoscience can be summarized by the following keywords: large area, low defects, short period, alignment direction control and top down/bottom up assembly. It has been well known that microphase separation of block copolymers create various shapes of nanostructures in 10 ~ 100nm of lengthscale, but the resulting morphology usually contains various types of topological defects which sneak in due to entropic fluctuation and incomplete annealing; thus it is highly desirable to develop a strategy reducing the defect probability.One idea to overcome this problem is to introduce physically patterned substrate which breaks the planar symmetry. Block copolymer films deposited on such substrates form periodic structures with little defects following the template pattern. With the help of Self-Consistent Field Theory (SCFT), I have theoretically studies a few systems with such physical patterns and comparison with experiments shows that well-aligned nanostructures with non-traditional domain shapes can be created if parameters are properly tuned.Another attractive idea is to introduce chemically patterned substrate. By controlling the chemical pattern shape, period and interaction strength, a wide parameter space can be explored. With the combination of physical pattern, even hierarchical 3-dimensional ordering of nanopatterns may become possible in the near future.



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장소: 광주 김대중컨벤션센터
발표코드: **POLY2-6**
발표분야: Polymer Self-Assembly and Nanopatterning
발표종류: 심포지엄, 발표일시: 목 15:36, 좌장: 김소연

Ultrahigh-resolution Nano-Transfer Printing Applicable to Applicable to a Broad Range of Surfaces

정연식

한국과학기술원(KAIST) 신소재공학과

Nanotransfer printing (nTP) technology offers outstanding simplicity and throughput in the fabrication of transistors, metamaterials, epidermal sensors, and other emerging devices. Nevertheless, the development of a large-area sub-50 nm nTP process has been hindered by fundamental reliability issues in the replication of high-resolution templates and in the release of generated nanostructures. This talk will present a solvent-assisted nanotransfer printing (S-nTP) technique based on high-fidelity replication of ultrahigh-resolution (8 ? 20 nm scale) patterns using a dual-functional bilayer polymer thin film. The master substrates were prepared by patterning the surface of a silicon wafer through photolithography and/or block copolymer (BCP) lithography followed by plasma etching. In particular, we employed BCP nanolithography for the fabrication of 8 ? 20 nm scale templates. For uniform and fast release of nanostructures on diverse receiver surfaces, interface-specific adhesion control was realized by employing a polydimethylsiloxane (PDMS) gel pad as a solvent-emitting transfer medium, providing unusual printing capability even on biological surfaces such as human skin and fruit peels.

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발표코드: **IND-1**

발표분야: Current Trends of Engineering Plastics

발표종류: 심포지엄, 발표일시: 목 09:35, 좌장: 이익모

Aliphatic Polyketone, its Charactristics and Applications

이원

효성 연구소

Aliphatic Polyketone, its Charactristics and Applications Weon Lee, Sang Sun WooR&D Business Labs, Hyosung Corporation, Anyang city, KoreaPhone: +82-10-5423-4180, Fax : +66-2218-7627, *E-mail: weonleet@hyosung,comAbstractAliphatic Polyketone(APK) is made up the perfect alternating copolymerization of CO and Olefins that has the property of polar and nonpolar respectively. Pd-phosphines is well known as its catalyst. APK has the high degree of crystallinity and fast crystallization rate because of its simple structure. In addition, compact crystal structure and high crystallinity of APK allow various outstanding characteristics such as excellent gas barrier, tribological and resilience properties, and resistance to fuels and chemicals including acid and base. APK is expected to lead the markets in the applications of automotive, electronics and industrial parts based on its differentiated characteristics. Hyosung is building the commercial plant with a capacity of 50,000 annual tons by March 2015, using proprietary catalyst technology. Keywords: .Hyosung, Aliphatic polyketone, High crystallinity, Gas barrier, Chemical resistance

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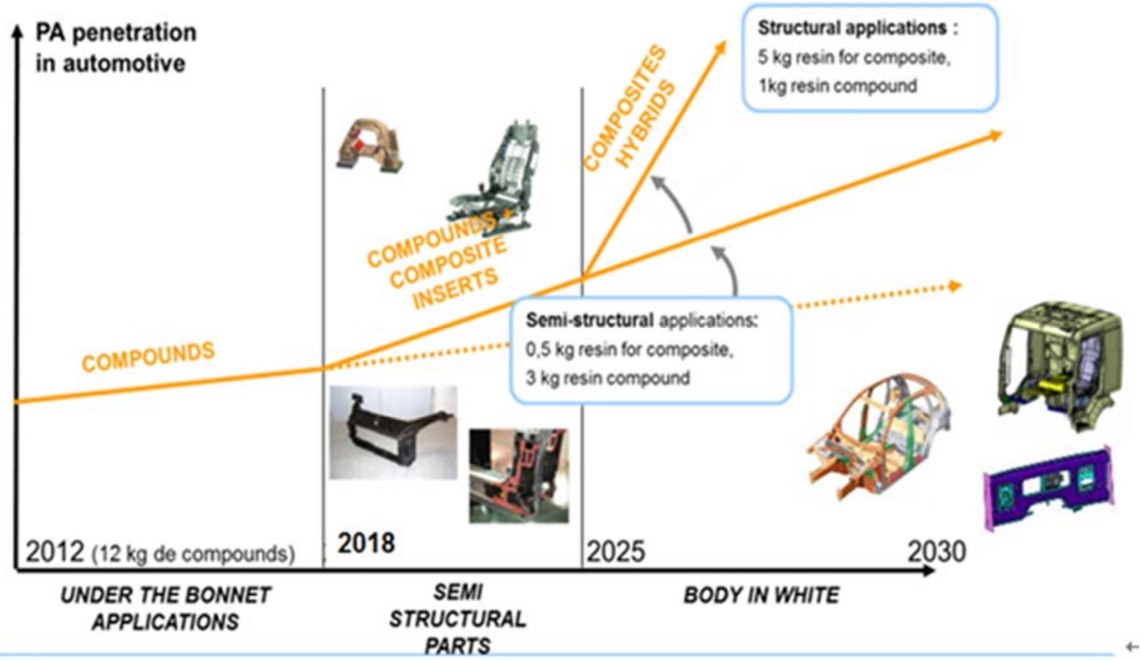
발표코드: **IND-2**
발표분야: Current Trends of Engineering Plastics
발표종류: 심포지엄, 발표일시: 목 10:05, 좌장: 이익모

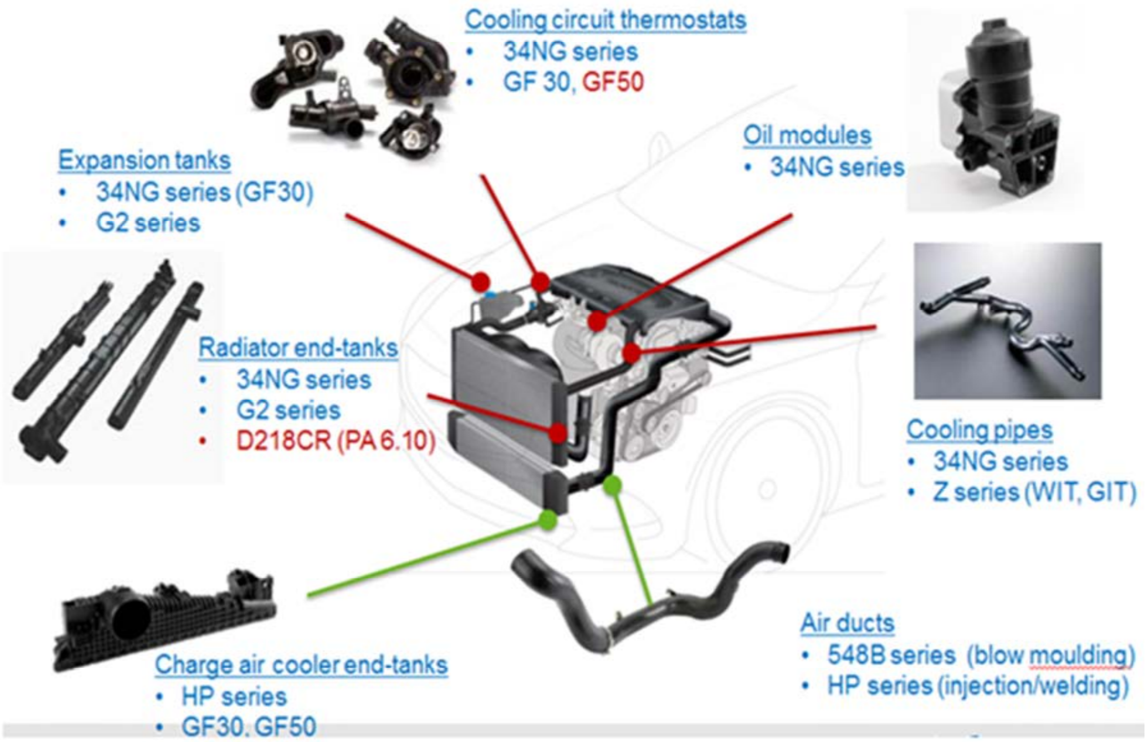
Material development trend of polyamide for automotive applications

이광상

한국솔베이 수지응용연구소

Under recent fuel efficiency and environmental regulations there are new demanding challenges for automotive applications, esp. metal replacement(such as engine mount, oil filter module, air intake manifold), thermal management(such as thermostat housing and charge air cooler), fluid barrier(such as cooling tanks and pipes) and fire protection(such as new FMVSS302 engine cover).In addition, new powertrain as xEV or fuelcell, safer mobility, bio and eco trends would be continued.


PA penetration in automotive
Structural applications :
5 kg resin for composite,
1kg resin compound
COMPOSITES HYBRIDS
COMPOUNDS + COMPOSITE INSERTS
COMPOUNDS
Semi-structural applications:
0,5 kg resin for composite,
3 kg resin compound
2012 (12 kg de compounds)
2018
2025
2030
UNDER THE BONNET APPLICATIONS
SEMI STRUCTURAL PARTS
BODY IN WHITE


Cooling circuit thermostats
• 34NG series
• GF 30, GF50
Oil modules
• 34NG series
Expansion tanks
• 34NG series (GF30)
• G2 series
Radiator end-tanks
• 34NG series
• G2 series
• D218CR (PA 6.10)
Cooling pipes
• 34NG series
• Z series (WIT, GIT)
Air ducts
• 548B series (blow moulding)
• HP series (injection/welding)
Charge air cooler end-tanks
• HP series
• GF30, GF50

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발표코드: **IND-3**
발표분야: Current Trends of Engineering Plastics
발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 이익모

Lightweight solution with engineering plastic for automotive part

제형호

한국바스프 Perfomance material

It is very clear that engineering plastic is one of effective and potential material to make a lightweight car. In case of glass fiber reinforced plastic, it was divided with short glass reinforced plastic, long glass fiber and endless glass fiber reinforced depends on length and we can approach with different design and processing according to length of glass fiber. One of importance things to engineering plastic development is mechanical simulation technology. Will be introduced that engineering plastic application in accordance with fiber length and advanced CAE(Computer Aided Engineering) solution for plastic development in automotive part.

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발표코드: **IND-4**

발표분야: Current Trends of Engineering Plastics

발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 이익모

New Material Development Trend in SABIC

방태훈

SABIC KOREA MAEKETING

SABIC, a major petrochemical company based in Saudi Arabia has been actively expanding their business area from petrochemicals to other value added downstream products including engineering plastics. They merged GE Plastics, a global leading company in engineering plastics industry in 2007 .You will get more information on SABIC as one of the most rapidly growing global chemical company and you may be able to get new understanding on engineering plastics resin development trend in various industry segments together with some practical examples.

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발표분야: Current Trends of Engineering Plastics
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친환경 PPS 제조 기술 개발(Development of New Polyphenylene Sulfide Manufacturing Process)

차일훈

SK케미칼(주) 화학연구소

poly(phenylene sulfide) (PPS)는 난연, 내열성 및 내화학성이 뛰어난 고성능 polymer의 하나로, 자동차 경량화 소재, 전자 부품 소재 및 내화학성이 요구되는 섬유와 관련되어 그 수요 및 용도가 급격히 확산되고 있다. SK 케미칼에서 개발한 친환경 PPS 제조기술 개발은 conventional 제조방법인 용매를 사용하는 solution polymerization 이 아닌 melt polymerization 으로 개시(Initiation)-전파(Propagation)-종결(Termination)의 mechanism 으로 진행된다. 원부 원료인 p-DIB (Paradiiodinebenzene or 1,4diiodinebenzene)과 황 (Sulfur)이 반응하여 사슬이 길어지는데, 온도가 상승 시, 황의 결합 고리가 깨지며 생성된 황 라디칼이 p-DIB의 요오드와 반응하여 고분자가 합성된다. P-DIB와 황이 반응하며 발생되는 요오드는 monomer 공정으로 이송되어 p-DIB 를 만드는데 다시 사용된다. Conventional process 로 생산된 PPS 와는 달리 chlorine 이 없고, solvent 를 사용하지 않으며, 부산물로 Nacl 이 발생하지 않아 대량의 세척용 물이 필요 없고, 생산된 제품도 powder 가 아니어서 기존 제품대비 친환경적인 제조 공법이다. 또한 고온에서 진공하에 polymerization 이 진행되므로 conventional 제조공법에 많이 존재하는 outgas 함량이 작다.

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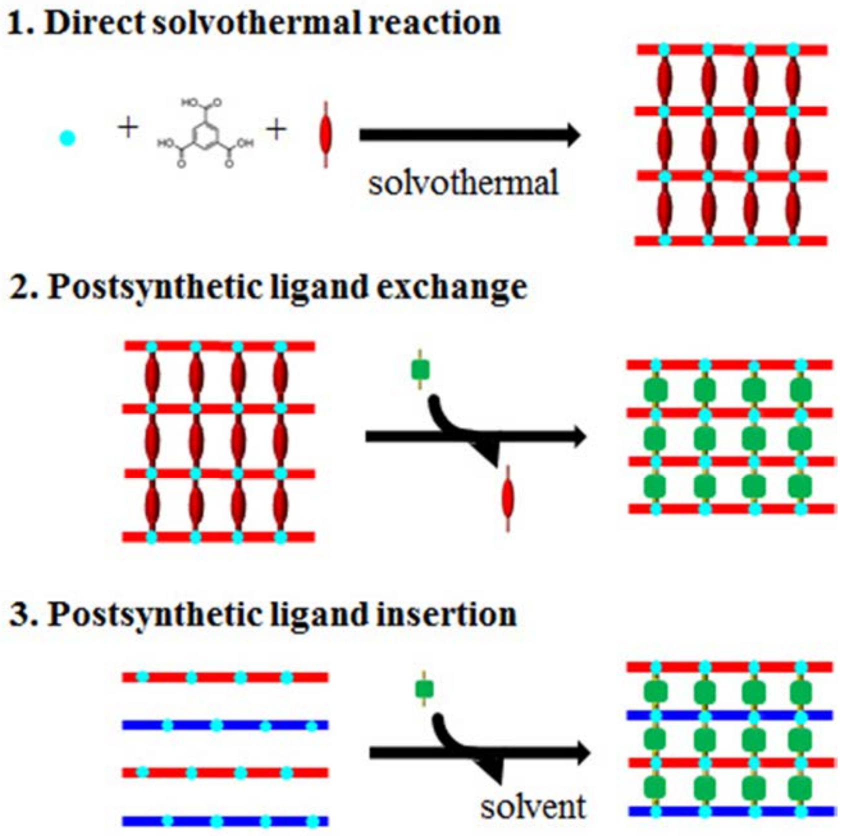
발표코드: **INOR1-1**
발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 홍창섭

Postsynthetic Modifications of Metal-Organic Frameworks: Framework Ligand Exchanges and Insertions

나명수

울산과학기술대학교(UNIST) 화학과

Isoreticular and polymorphic 3-D MOFs were prepared via the combination of direct solvothermal reactions using Ni(II) ion and 1,3,5-benzenetricarboxylic acid as building components and dabco, 4,4'-bipyridine or pyrazine as a pillar between the sheets, postsynthetic ligand exchanges of the MOFs prepared via the direct solvothermal reactions and postsynthetic ligand insertions into a 2-D MOF. The appropriate pore dimensions, surface areas and adsorption enthalpies of the MOFs combined well to produce the largest working CO2 capture capacities via the pressure swing adsorption process, even though their BET surface areas and adsorption enthalpies are not so large.


1. Direct solvothermal reaction
HO
O
HO
O
OH
O
solvothermal
2. Postsynthetic ligand exchange
3. Postsynthetic ligand insertion
solvent

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **INOR1-2**

발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks

발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 홍창섭

Electrochemical Sensing of Carbon Dioxide with a Metal-Organic Framework Material

정낙천

대구경북과학기술원(DGIST) 신물질과학과

The detection of carbon dioxide, a highly oxidized and largely inert gas, has proven difficult within mixtures of multiple gases owing to the presence of competing gas such as oxygen, carbon monoxide and water vapor ? all of which are far more chemically active. It stands to reason, therefore, that the clear benefits of having robust and inexpensive devices to provide a quantitative analysis of CO2 concentrations in admixture with other gases provides more than enough impetus for the continued development of such devices. Much of the present sensing technology depends largely upon spectroscopic methods which become unreliable when the mixture of gases contains spectroscopically similar resonances. Alternative methods, such as semiconducting field effect transistors, and semiconductive oxide sensors operate constantly at temperatures in excess of 200 °C (upwards of 800 °C) making them both power hungry and potential ignition sources in areas with flammable or explosive gases. Here, we present the possibility for MOFs to act as platforms for sensing analytes at relatively low temperatures.

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발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 홍창섭

Role of high-valent metal ions in the structures and properties of porous metal-organic frameworks

전형필

한양대학교(ERICA) 응용화학과

The great success of metal-organic frameworks (MOFs) as a new class of crystalline porous materials owes much to the coordination chemistry of divalent metal ions, such as Zn(II) and Cu(II). With minor exceptions, most of the best-known MOFs are based on coordination bonds between M(II) ions and anionic ligands with O- or N-donors. Recently, there has been a growing interest in synthesizing new MOFs using high-valent transition metal ions, such as Ti(IV) or Zr(IV). This is partly because such MOFs often display excellent hydrothermal and chemical stability required for practical applications. In a synthetic point of view, however, it is not always straightforward to incorporate the tetravalent metal ions into the frameworks of MOFs, and thus the building blocks and known topologies are not as diverse as those based on divalent metal ions. This presentation intends to review current trends in developing new MOFs with high-valent metal ions. Also presented will be a M(II)-M(IV) heterometallic approach in the synthesis of new MOFs and gas sorption behavior of Ti(IV)-carboxylate clusters which are potential building blocks for new MOFs.

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발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 10:25, 좌장: 정낙천

Networking of Macrocycles via Exocyclic Coordination

이심성

경상대학교 화학과

Macrocyclic ligands show high selectivity for specific metal ions and small molecules, and these features make such molecules attractive candidates for chemical sensing applications. Crown ethers have typical macrocyclic structures with polyether linkages where the oxygen donors are often separated by an ethylene unit (-O-CH_2-CH_2-O-).Because the oxygen lone pairs in crown ether type macrocycles are directed inward, the preorganized macrocyclic cavity tends to form complexes where metals coordinate inside the cavity (endo-coordination). However, sulfur-containing macrocycles (thia-macrocycle) often demonstrate metal coordination outside of the cavity (exo-coordination). This coordination behavior results from the different torsion arrangements adopted by the X-CH_2-CH_2-X atom sequence (X = O, gauche; X = S, anti) in thia-macrocycles.Exo-coordination is synthetically attractive because it would provide a means of networking macrocyclic building blocks in diverse arrangements. In fact, exo-coordination could allow the construction of more elaborate network assemblies than are using conventional endocyclic coordination which gives metal-in-cavity products. Exo-coordination can also serve as a tool for crystal engineering through the use of diverse controlling factors. Although challenges remain in the development of exo-coordination-based synthetic approaches and, in particular, for the architectural control of supramolecular coordination platforms, we have established several strategies for the rational synthesis of new metallosupramolecules. In this presentation, we describe our recent studies of the assembly of metallosupramolecules and coordination polymers based on sulfur-containing macrocycles that employ simple and versatile exo-coordination procedures. Initially, we focus on the unusual topological products such as sandwich (1:2, metal-to-ligand), club sandwich (2:3), and cyclic oligomeric complexes as discrete network systems. The primary structures we achieve in these networked macrocycles are one to three dimensional coordination polymers (or MOFs) based on homo- and heteronuclear metal systems. Using crystal engineering methods, we have also investigated variation in the donors, interdonor distances, ligand isomer structures, and the effect of counter anions on the chemical and physical properties of the products.Understanding the relationship between structure and function in these exo-coordination products is an important step in the design of these new supramolecules for practical applications. We investigated the photophysical properties of the exocyclic complexes and a chromogenic macrocycle, which exhibited cation-selective and anion-controlled color change depending on an exo- or endo- ligand binding mode. Overall, we suggest that the exocyclic coordination behavior provides a versatile strategy for the preparation of new molecular networks and materials.References1.Park, S.; Lee, S. Y.; Park, K.-M.; Lee. S. S. *Acc. Chem. Res.* 2012, *45*, 391.2.Kim, S.; Lindoy, L. F.; Lee, S. S. *Coord. Chem. Rev.* In press (DOI: 1016/j.ccr.2014.08.011).3.Lindoy, L. F.; Park, K.-M.; Lee, S. S. *Chem. Soc. Rev.* 2013, *42*, 1713.4.Lee, E.; Lee, S. Y.; Lindoy, L. F.; Lee, S. S. *Coord. Chem. Rev.* 2013, *257*, 3125.5.(a) Lee, J. Y.; Lee, S. Y.; Sim, W.; Park, K.-M.; Kim, J.; Lee, S. S. *J. Am. Chem. Soc.* 2008, *130*, 6902. (b) Lee, J. Y.; Kim, H. J.; Jung, J. H.; Sim, W.; Lee, S. S. *J. Am. Chem. Soc.* 2008, *130*, 13838.6.(a) Lee, S. J.; Jung, J. H.; Seo, J.; Yoon, I.; Park, K.-M.; Lindoy, L. F.; Lee, S. S. *Org. Lett.* 2006, *8*, 1641. (b) Lee, H.; S. S. Lee. *Org. Lett.* 2009, *11*, 1393. (c) Lee, S. J.; Lee, J.-E.; Seo, J.; Lee, S. S.; Jung, J. H. *Adv. Func. Mater.* 2007, *17*, 3441.

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발표코드: **INOR1-5**
발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 정낙천

Functional Metal-Organic Frameworks: Their Preparations and Applications

허성

한국외국어대학교 화학과

Crystalline nanoporous metal-organic frameworks (MOFs) are zeolite-like functional inorganic-organic hybrid materials. Theoretically, infinite number of MOFs could be prepared by simply combining various metal ions with diverse polytopic organic bridging ligands. Once MOFs exhibit permanent porosity, their channels can be utilized for a wide range of new applications. These may contain hydrogen/methane storage, selective carbon dioxide sorption, substrate-dependent heterogeneous catalysis, encapsulation of functional guests, targeted drug delivery, and proton conduction. The combination of the bridging ligands with suitable metal ions is a key parameter for the preparation of functional nanoporous MOFs. In this sense, we demonstrate several new MOF systems with their crystal structures and applications. The successful preparation of zeolitic MOF with interesting topology was possible by choosing a suitable metal ion with commercially available ditopic ligand. Catenation isomers of MOF having the same connectivity between metal ion and ligand were observed by changing the reaction solvent. Catalytically active MOF with openly accessible Lewis basic sites was prepared by using less symmetric ditopic bridging ligand. Very large dye molecule could be encapsulated into the large channels of MOF. Molecular wires could be assembled inside the preorganized MOF channels. All these examples suggest that many more new applications by functional MOFs would be possible.

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발표코드: **INOR1-6**
발표분야: Current Trends in Inorgnaic Chemistry: Metal-Organic Frameworks
발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 정낙천

Transformation of Metal-Organic Frameworks into Functional Nanomaterials

문회리

울산과학기술대학교(UNIST) 화학과

Coordination chemistry, which is the classical branch of inorganic chemistry, is concerned with the interactions of organic ligands with metal centers. Rational design of organic and metal building blocks has successfully enabled the genesis of variety of coordination polymers or metal-organic frameworks (MOFs) that are of fundamental scientific importance as well as provide a myriad of practical applications. Our research is primarily focused on the design of new MOFs and their use as 'precursors' of new nanostructured materials. Since MOFs are composed of organic and inorganic part, well-tailored MOFs can be transformed to metallic/metal oxide nanomaterials or carbon-based materials under appropriate reaction conditions. To understand and develop this "transformation chemistry", in-depth understanding of coordination chemistry is of crucial importance. In this talk, we present the design of functional MOFs and their applications such as sensing, catalysis, and carbon capturing. In addition, novel synthetic strategies that exploit a MOF-driven, self-templated route towards nanoporous metal oxides and porous graphene materials via thermolysis will be also discussed.

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발표코드: **INOR2-1**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이은성

Design and synthesis of novel chiral 6-NHC toward transition metal catalysis and continuous flow reaction

박진균

부산대학교 화학과

We recently reported the design, synthesis, and novel reactivity of a family of 6-membered annulated chiral N-heterocyclic carbene (6-NHC) copper(I) complexes.[1-6] Chiral 6-NHC ligand structure was inspired by OLED materials. The steric properties and electronic properties of chiral 6-NHC ligand were evaluated by the X-ray and IR analysis of 6-NHC-Rh complexes.[1,4] This family of copper(I) complexes exhibited high enantioselectivities for β-borylation reactions and stereoconvergent allylic substitutions.[2-4] It also gave high diastereoselectivities in catalyst controlled double allylic substitutions for the synthesis of 1,2-polyols[4] and high regioselectivities in hydroborations of propargylic substrates.[5,6] Finally, we demonstrated practical applications of flow reaction for the continuous synthesis using NHC-copper complexes in β-borylation reactions.[7] Further details will be provided in the presentation.

References

1. Jin Kyoon Park, Hershel H. Lackey, Matthew D. Rexford, Kirill Kovnir, Michael Shatruk, D. Tyler McQuade*. Org. Lett. 2010, 12, 5008-5011.
2. Jin Kyoon Park, Hershel H. Lackey, Brian A. Ondrusek, D. Tyler McQuade*. J. Am. Chem. Soc. 2011, 133, 2410-2413.
3. Jin Kyoon Park, D. Tyler McQuade*. Angew. Chem. Int. Ed. 2012, 51, 2717-2721.
4. Jin Kyoon Park, D. Tyler McQuade*. Synthesis 2012, 44, 1485-1490.
5. Jin Kyoon Park, Brian A. Ondrusek, D. Tyler McQuade*. Org. Lett. 2012, 14, 4790-4793.
6. Brain A Ondrusek, Jin Kyoon Park, D. Tyler McQuade*. Synlett. 2014, 239-242
7. Suzanne M. Opalka, Jin Kyoon Park, Ashley R. Longstreet, D. Tyler McQuade*. Org. Lett. 2013, 15, 996-999.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **INOR2-2**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 이은성

Cyclometalated Iridium Complexes with Substituted *o*-Carboranes: Impact of *o*-Carborane Substitution on the Photophysical Properties

이민형

울산대학교 화학과

Cyclometalated Ir(III) complexes with substituted *o*-carboranes may constitute a new class of color-tunable phosphorescent emitters in organic light-emitting diodes (OLEDs). However, detailed understanding of the role of *o*-carborane in controlling the emissive properties of iridium(III)-cyclometalates has not been clarified. To this end, we have prepared a series of *o*-carborane substituted $(C\^{}N)_2$Ir(acac) complexes with various 2-R-*o*-carborane functionality in the ligand and investigated the effect of the position of carborane substitution and 2-R group on the photophysical properties of cyclometalated Ir(III) complexes. X-ray crystal structures were determined to see the variation in the carborane cage structure. UV/vis absorption and phosphorescence measurements under various conditions exhibited that the photophysical properties in terms of quantum efficiency and phosphorescence wavelength are dependent on the substitution position of carborane, 2-R substituent, and polarity of medium. Finally, it was shown that the complexes can be used as a highly efficient phosphorescent emitting material in PhOLEDs. Details of synthesis, characterization, and photophysical and electroluminescent properties of complexes will be discussed with theoretical calculations.

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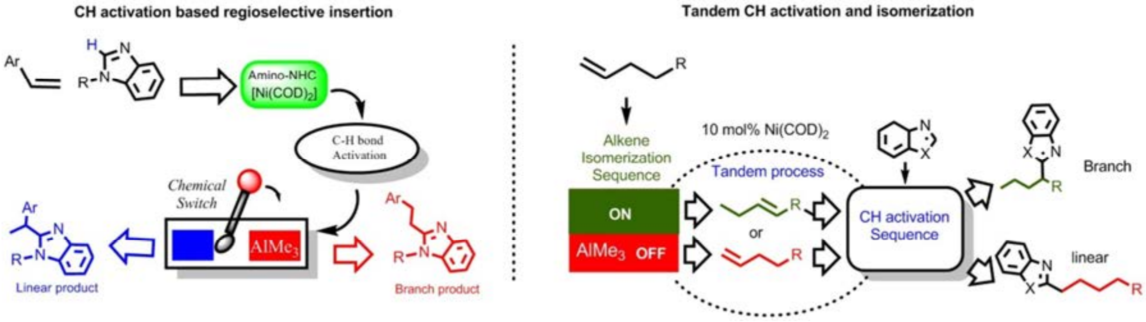
발표코드: **INOR2-3**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 이은성

Adding Ligand-and-Main Group Element Dimensions to The C-H Bond Activation

Tiow-Gan Ong

Institute of Chemistry, Academia Sinica, Taiwan

The past decade has seen the increasing reports of C-H bond activation and functionalization of compound via C-H bond activation, which would obviate the additional steps and limitations associated with the perfunctionalization substrates in the catalytic coupling process. We envisage that addition of $AlMe_3$ would act cooperatively in tandem fashion with nickel to invoke a new selectivity in pyridine and heteroarenes with the help of ligand NHC. In addition, we describe the development of a reactivity strategy for Ni-catalyzed heteroaromatic C-H bond functionalization based on using chemical switch like $AlMe_3$ that selectively generates linear or branched adducts.



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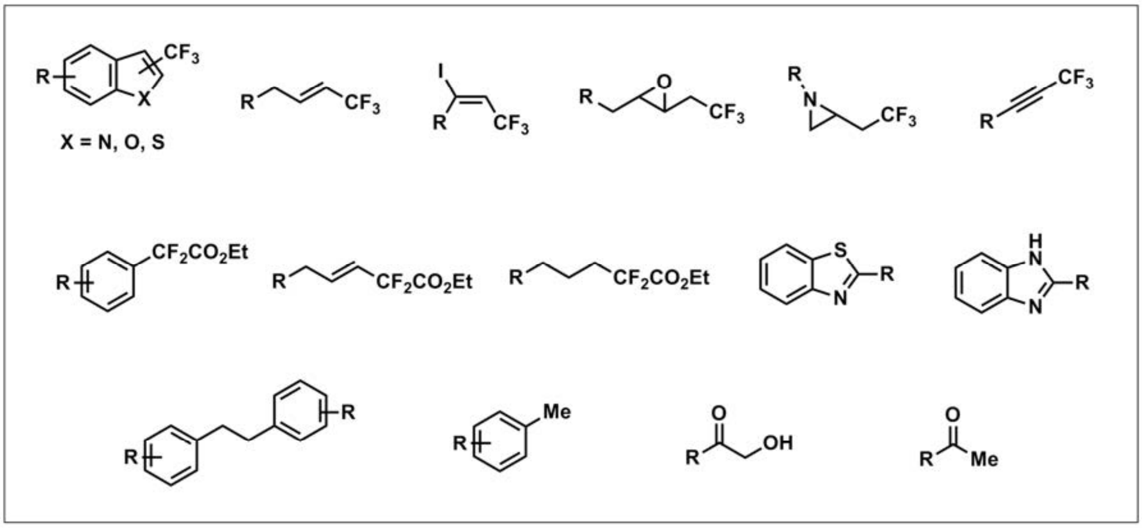
발표코드: **INOR2-4**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 이민형

Radical Transformations with Ru-, Ir-, and Pt-based photoredox catalysts

조은진

한양대학교 응용화학과

Recently, visible light photoredox catalysis has attracted substantial attention due to its environmental compatibility and versatility in promoting a large number of synthetically important reactions. We have developed several radical transformations using Ru-, Ir-, or Pt-based photoreox catalysts under visible light irradiation. The methods allowed access to a variety of fluoroalkyl group-containing molecules, such as -CF2R, -CF3, -C3F7, and -C4F9 groups, and benzofused heterocycles including benzothiazoles and benzimidazoles.In addition, various homocoupled-, hydroxylated- and dehalogenated compounds have been efficiently generated employing Hantzsch ester as a photoreductant.



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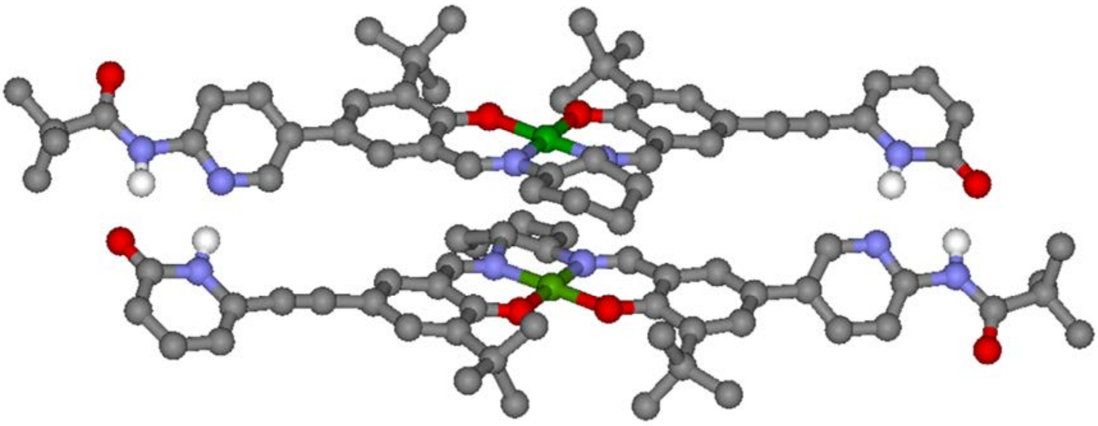
발표코드: **INOR2-5**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 이민형

Exploring New Ligand Designs for Asymmetric Catalysis

홍석원

광주과학기술원(GIST) 신소재공학부

Chiral cooperative catalysis enabling simultaneous activation of both an electrophile and a nucleophile has emerged as a powerful strategy in catalytic asymmetric synthesis. In our laboratory, a series of novel hydrogen-bond functionalized salen-transition metal catalysts have been developed to facilitate bimetallic or bifunctional activation of both reaction partners. For example, a self-assembling dinuclear Co(II)-salen catalyst featuring the pyridone/aminopyridine H-bonding pair results in significant rate acceleration as well as excellent enantioselectivity in nitro-aldol reaction. Bis-urea functionalized salen-Co(III) complexes exhibited significant rate acceleration in hydrolytic kinetic resolution of epoxides even at low catalyst loading (0.05 mol%). The bis-urea salen-Co(III) complexes are also excellent catalysts for anti-selective asymmetric Henry reaction where broad substrate scope, good yield, excellent enantio- and diastereoselectivity were observed. During this presentation, synthesis of ligands/catalysts, applications in asymmetric transformations, and plausible mechanisms will be discussed in detail.



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발표코드: **INOR2-6**
발표분야: Organometallics: New Trends in Catalysis
발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 이민형

Insights into Dioxygen Activation/Alkene Oxidation Mediated by Iridium

Jan-Uwe Rohde

울산과학기술대학교(UNIST) Chemistry

Molecular oxygen is a much desired oxidant for the functionalization of organic compounds, as it is readily available and inexpensive. Thus, synthetic and catalytic methods that use O_2 offer in principle significant economic and environmental advantages. The development of selective methods, however, remains a challenging task. In this context, organometallic O_2 reactivity is an area of growing interest, because it offers insights into possible oxygenation mechanisms and provides a basis for the design and development of new catalytic methods. In this talk, I will present a project from my research group that is aimed at the activation of O_2 and other small molecules by low-valent Ir alkene complexes. We investigate the mechanisms of such reactions and the properties of intermediates with the goal of developing synthetic cycles of small-molecule activation and atom transfer. This work has led to the identification of (alkene)peroxo intermediates, where both the oxidant and the substrate are bound to the metal center. Such species are intriguing, because they have been proposed as key intermediates in stoichiometric and catalytic alkene oxygenation.

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발표코드: **PHYS1-1**

발표분야: Computational Chemistry in Materials and Biology

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이상욱

Atomistic observation of the lithiation and delithiation behaviors of silicon nanowires using reactive molecular dynamics simulations

한상수

한국과학기술연구원(KIST) 계산과학연구단

For the practical use of silicon nanowires (Si NWs) as anodes for Li-ion batteries, understanding their lithiation and delithiation mechanisms at the atomic level is of critical importance. We discuss the mechanisms for the lithiation and delithiation of Si NWs determined using a large-scale molecular dynamics (MD) simulation with a reactive force field (ReaxFF). The ReaxFF is developed using results from first-principles calculations for various crystals and molecules. During the lithiation process, Li atoms penetrate into the lattices of the crystalline Si (*c*-Si) NWs preferentially along the or direction, and then the *c*-Si changes into amorphous LixSi (*a*-LixSi) phases due to the simultaneous breaking of Si-Si bonds as a result of the tensile stresses between Si atoms. Before the complete amorphization of the Si NWs, we observe the formation of silicene-like structures in the NWs that are eventually broken into low-coordinated components, such as dumbbells and isolated atoms. Additionally, during delithiation of LixSi NWs, we observe the formation of a small amount of *c*-Si nuclei in the *a*-LixSi matrix below a composition of $Li_{1.4}Si$ ~ $Li_{1.5}Si$, and we demonstrate that the two-phase structure can be thermodynamically more favorable than the single-phase *a*-LixSi.

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발표코드: **PHYS1-2**
발표분야: Computational Chemistry in Materials and Biology
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First-principles molecular modeling for electronic/photovoltaic applications

장윤희* **Yves Lansac**[1]

광주과학기술원(GIST) 신소재공학 [1]*University of Tours*

With a series of (time-dependent) density functional theory calculations, force field development, and molecular dynamics simulations, we try to understand the working principles of various organic and inorganic materials used in non-volatile memories, field-effect transistors and organic solar cells, and try to design a high-performance low-cost material or architecture for electronic and photovoltaic applications. Several examples include: (1) push-pull-type low-band-gap polymers used in bulk heterojunction organic solar cells and their structure, electronic structure, optical properties, charge transfer rates, power conversion efficiencies and stabilities; (2) shuttlecock-shaped fullerene derivatives known to exhibit a rectification behavior when self-assembled between gold electrodes and their field-dependent self-assembly and orientation-dependent charge transport; and (3) graphene-based channel materials whose on/off ratio is improved by a thin-film deposition of ferroelectric polymer such as polyvinylidene fluoride.

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발표분야: Computational Chemistry in Materials and Biology
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 이상욱

Structure and Dynamics of the Self-Assembled Monolayer at the Nanoscale

장준경

부산대학교 나노소재공학과

Using molecular dynamics simulations, we show that the minimum diameter of ordered self-assembled monolayer (SAM) structures of alkanethiols on Au(111) is 1.9 nm at room temperature. The tilt direction of the alkyl chain precesses around the center of the nanoscale SAM. We also investigate the nanometer-wide SAM lines. The packing structure in the SAM line was compared with that in a bulk SAM. A stable SAM line must be at least 1.7 nm wide, and two lines can merge if they are less than 3.0 nm apart. This probably sets the ultimate resolution of SAM patterns. We studied the evolution of a droplet of 1-octadecanethiol into a circular island of SAM. The packing of sulfur atoms preceded the alignment and packing of alkyl chains. The SAM islands resembled the bulk SAM, but it contained defects where the molecules were standing upside down on the surface. We found two mechanisms pertaining to the growth of a SAM island in the direct-write lithography. In the first mechanism, the molecules penetrated into the SAM islands by pushing away the molecules below. In the other mechanism, the molecules diffused, reached the periphery of the SAM islands, and slid down to the surface. The chemisorption of sulfur atoms made the present droplet spread more slowly than a droplet interacting nonspecifically with a surface. A droplet laterally moving across the surface was also simulated to emulate the growth of a SAM line. The alkyl chains of the SAM line were directed preferentially toward the line direction.

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발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 허지영

Prediction of Protein Structure and Interaction by GALAXY Protein Modeling Programs

석차옥

서울대학교 화학부

Recently developed GALAXY protein modeling programs are introduced and advantages and disadvantages of these programs are discussed. The GALAXY package consists of the template-based modeling program GalaxyTBM, the loop/terminus modeling program GalaxyLoop, the model refinement program GalaxyRefine, the homo-oligomer prediction program GalaxyGemini, the ligand binding site prediction program GalaxySite, the protein-ligand docking program GalaxyDock, and the protein-protein docking program GalaxyPPDock. These programs have been tested with some success in community-wide competitions Critical Assessmentof Techniques for Protein Structure Prediction (CASP) and Critical Assessment of PRediction of Interactions (CAPRI). For the development of these programs, modeling problems have been posed as global optimization problems of designed energy functions. The free energy functions of GALAXY have been carefully designed by combining physical chemistry principles and structure and sequence information. Efficient conformational search methods such as conformational space annealing and triaxial loop closure have been employed. Freely accessible web servers of the modeling programs are available at http://galaxy.seoklab.org,and some programs can be downloaded from http://galaxy.seoklab.org/softwares.

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발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 허지영

Improved network community structure improves function prediction

이주영* Steven Gross[1] Juyong Lee[2]

고등과학원 계산과학부 [1]UC Irvine, USA [2]NIH, USA

We are overwhelmed by experimental data, and need better ways to understand large interaction datasets. While clustering related nodes in such networks?known as community detection?appears a promising approach, detecting such communities is computationally difficult. Further, how to best use such community information has not been determined. Here, within the context of protein function prediction, we address both issues. First, we apply a novel method that generates improved modularity solutions than the current state of the art. Second, we develop a better method to use this community information to predict proteins' functions. We discuss when and why this community information is important. Our results should be useful for two distinct scientific communities: first, those using various cost functions to detect community structure, where our new optimization approach will improve solutions, and second, those working to extract novel functional information about individual nodes from large interaction datasets.

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Novel model and stochastic kinetics for quantitative understanding of vibrant reaction networks in living cells

성재영* 김지현 임유림 박성준 양길석 송상근

중앙대학교 화학과

For quantitative understanding of probabilistic behaviors of living cells, it is essential to construct a correct mathematical model of intracellular networks interacting with complex cell environment, which has remained a formidable task. Here, we present a novel model and stochastic kinetics for a vibrant intracellular network interacting with cell environment, employing a complete description of cell state dynamics and its coupling to the system network. By applying the present kinetics to a vibrant gene expression network model, we obtain simple analytic results for the gene expression variability and the environment-induced correlations between the expression levels of dual reporter genes. The theoretical results compose a unified framework for quantitative understanding of various gene expression statistics observed across a number of different systems. Our analyses reveal the relative contribution of the constituent processes of gene expression to the overall gene expression statistics, which is found to be dramatically different depending on the promoter strength, the gene expression machinery, and the cell type.

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발표분야: Recent Trends in Physical Chemistry
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 방윤수

Nanotectonics

한상우

한국과학기술원(KAIST) 화학과

The morphology of noble metal nanocrystals and their spatial organization explicitly determine their plasmonic, electronic, and catalytic characteristics. Accordingly, several strategies have been developed for preparing metal nanocrystals with well-defined geometries and for constructing two- and three-dimensional assemblies of nanocrystal building blocks with ordered structures. However, the lack of simple and versatile methods for preparing multi-scale structures with designed properties and spatial regularity has slowed the adaption of these unique structures to practical applications. Herein, facile wet-chemical synthetic processes for the fabrication of noble metal nanocrystals and their designer assembly and patterning toward functional materials as well as their applications in catalysis, sensors, and plasmonics are reported.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **PHYS2-4**
발표분야: Recent Trends in Physical Chemistry
발표종류: 분과기념강연, 발표일시: 목 15:00, 좌장: 조성

Time-resolved fluorescence for the dynamics and structure in electronic excited state

주태하

포항공과대학교(POSTECH) 화학과

Chemical reactions in electronic excited states usually occur promptly within a few hundred femtoseconds. Time-resolved spontaneous fluorescence (TF) is a powerful tool for the study of the dynamics, although pump/probe transient absorption is employed much more frequently. Over the years, we have developed highly time-resolved fluorescence method that enables launching coherent vibrational wave packets and observation of the nuclear motions in the excited state through the modulation of the TF signal by the wave packet motion. Thus, TF recorded with a time-resolution shorter than the periods of vibrations provides the "vibrational spectrum" of the emitting species as well as the dynamics. The intensity of a band in a vibrational spectrum by TF (VSTF) is weighted by the vibrational reorganization energy along the relevant nuclear coordinate. This "selection rule" facilitates the identification of the molecule and the emitting state and elucidation of the electron-nuclear coupling between the states involved. We have applied this method to the excitation and relaxation of a Franck-Condon state, internal conversion from S_n to S_1, intramolecular charge transfer, energy transfer in porphyrins, and intramolecular proton transfer reactions.

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발표코드: **PHYS2-2**
발표분야: Recent Trends in Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 방윤수

Raman Metrology for Surface Scientific Investigation of 2-Dimensional Systems

류순민

포항공과대학교(POSTECH) 화학과

Atom-thick crystals have served as unique systems to explore new physics and chemistry in two dimension. Raman spectroscopy has proven to be a versatile analytical tool for two-dimensional systems because of the varying spectral features for different thickness, stacking, defect density, charge density (n), mechanical strain (ε), temperature, etc. Such multimodal sensitivity, however, turns into difficulty when multiple unknown variables are to be determined simultaneously. Despite the strain-sensitivity of the Raman G and 2D modes, for example, optical characterization of native strain in graphene on silica substrates has been hampered by excess charges interfering with both modes. In this talk, I will show that the effects of strain and charges in graphene can be optically separated from each other by correlation analysis of the two modes, enabling simple quantification of both.[1] Employing the proposed analysis, I will address our recent findings on important surface scientific issues of graphene such as structural deformation caused by substrates and thermal perturbation,[1] interfacial charge transfer,[2] and molecular intercalation[3] through graphene-substrate interface.References[1]J. E. Lee, G. Ahn, J. Shim, Y. S. Lee, and S. Ryu,* “Optical Separation of Mechanical Strain from Charge Doping in Graphene”, Nature Commun. 3, 1024 (2012)[2]S. Ryu, Li Liu, S. Berciaud, Y.-J. Yu, H. Liu, P. Kim, G. W. Flynn, and L. E. Brus, “Atmospheric Oxygen Binding and Hole Doping in Deformed Graphene on a SiO2 Substrate”, Nano Lett. 10, 4944 (2010)[3]D. Lee, G. Ahn and S. Ryu,* “Two-Dimensional Water Diffusion at a Graphene-Silica Janus Interface”, J. Am. Chem. Soc. 136, 6634 (2014)

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **PHYS2-3**
발표분야: Recent Trends in Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 방윤수

Chemical Exchange 2DIR Spectroscopy for Ultrafast Dynamics

이경구

군산대학교 화학과

Femtosecond two-dimensional infrared (2DIR) spectroscopic method has been used in studying a variety of chemical exchange processes occurring on picosecond timescales under thermal equilibrium conditions. In 2DIR spectroscopy, a specific target mode is vibrationally-labeled with an initial excitation frequency $\omega\tau$. After a finite waiting time (T_w), the emission frequency ω_t of the initially vibrationally-labeled mode can be experimentally measured. The 2DIR spectrum is then displayed in a two-dimensional frequency space, i.e., ω_τ and ω_t. The spectral correlation between the initial excitation and final emission frequencies is measured as a function of T_w. Therefore, the time evolution of the 2DIR spectra as a function of T_w provides dynamical information about the molecular systems under study. Chemical exchange 2D IR spectroscopy can be used for studying the microscopic aspects of ultrafast dynamics, such as solute?solvent complexation, hydrogen-bond exchange, carbon?carbon bond rotational dynamics, ion pairing dynamics, fast conformational switching dynamics of proteins.In this talk, the experimental background will be presented briefly and the results of ultrafast dynamics occurring between components in electrolyte system will be discussed.

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발표코드: **PHYS2-5**
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발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 조성

Nobel Fluorescence-free Single-Molecule Detection Techniques and Bio-Applications

강성호

경희대학교 응용화학과

Novel optical single-molecule detection techniques have been developed based on fluorescence-free detections for quantitative analysis of bio-molecules. At this study, new detection techniques such as wavelength-dependent enhanced dark field illumination, total internal reflection scattering (TIRS), and Nomarski differential interference contrast (DIC) techniques will be introduced, which can be also applied to super-resolution (SR) microscopy. Those are expected tools to provide crucial information and essential approaches for understanding various characterizations, dynamics of single-biomolecules and nanoparticles as well as the molecular interactions at the single-molecule level.

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발표코드: **PHYS2-6**
발표분야: Recent Trends in Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 조성

Charge Separation and Recombination Dynamics in Organic Photovoltaics using Low-Bandgap Conjugated Terpolymers

김정호[*] 김태우[1] 전선홍[1] 김중한[2] 김범준[3] 이효철[1,*]

인하대학교 화학과 [1]한국과학기술원(KAIST) 화학과 [2]가톨릭대학교 화학과 [3]한국과학기술원 (KAIST) 생명화학공학과

In the development of bulk-heterojunction-type organic solar cells, low-bandgap polymers have recently attracted much interest with the aim of achieving better overlap with the solar spectrum and thus increasing the photoconversion efficiency. However, most common low-bandgap D-A copolymers do not exhibit broad absorption spectrum, but instead the absorption maximum is only red shifted, resulting in the decrease of the absorption in the visible region. As an alternative approach to circumvent this limitation, random terpolymers have been developed based on the copolymerization of one electron-rich unit and two different electron-deficient units (D-A-A) or two electron-rich units and one electron-deficient unit (D-D-A). The random terpolymers show broad absorption spectrum from visible to near-IR and the photoconversion efficiency of solar cells using those terpolymers dramatically changes depending on the composition of the repeat unit. While charge separation and recombination at the donor/acceptor interface are the most critical steps that govern the photoconversion efficiency, their dynamics and mechanism have never been explored for these novel low-bandgap terpolymers. In this work, we use femtosecond transient absorption (TA) spectroscopy to investigate the dynamics of charge separation and recombination in a bulk-heterojunction solar cell containing a random D-A-A terpolymer, PBDTT-DPP-TPD, and the one containing a D-A copolymer, PBDTT-TPD. From the TA measurement, we found that charge separation (CS) state is formed on sub-100 fs time scale for both D-A-A terpolymer and D-A copolymer solar cells. Subsequently, the CS state decays via a bimolecular process of charge loss between free electrons and holes in ~1 ps and geminate recombination in ~100 ps. Interestingly, we found that the fraction of the bimolecular charge loss and geminate recombination is apparently smaller at the D-A-A terpolymer heterojunction than at the D-A copolymer heterojunction, which is in agreement with higher

photoconversion efficiency of the D-A-A terpolymer solar cell. Thus, we revealed that the D-A-A terpolymer can maintain the CS state more efficiently than the D-A copolymer, leading to improved performance of solar cells.

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장소: 광주 김대중컨벤션센터
발표코드: **ANAL1-1**
발표분야: Analytical Chemistry for Environmental & Forensic Sciences
발표종류: 분과기조강연, 발표일시: 목 09:00, 좌장: 김태영

High Frequency, High Quality Measurement of Anthropogenic Ultra-trace Components in Atmosphere: What can we learn from these measurements?

김경렬

광주과학기술원(GIST) GIST대학

Man-made chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) have been widely used in many industrial applications such as degreasing solvents in semiconductor/electronics, foam-blowing agents, aerosol propellants and refrigerants. However, because of their involvement in stratospheric ozone depletion, the production and consumption of these compounds have been regulated by the Montreal Protocol on Substances that Deplete the Ozone Layer and its Amendments. High-frequency in situ measurements of a wide range of man-made halogenated compounds have been made at Gosan (Jeju Island, Korea) since November 2007 as part of AGAGE global network. These halogenated compounds are measured in 2 L ambient air samples every two hours using automated custom?built cryogenic pre-concentration system coupled with gas chromatograph and mass selective detector (GC-MSD) with relative measurement precisions typically less than 1%.Using an interspecies correlation method with annual and average of HCFC-22 emissions, which is calculated with an inverse method based on a Lagrangian particle dispersion model (FLEXPART), we could estimate the emission rates of anthropogenic halocarbons. Our results, a unique “top-down” approach, suggest that overall China is the dominant emitter of HCs in East Asia with global fractions reaching 20% of total global emissions for many individual species, while significant emissions are also found in South Korea, Japan and Taiwan for some specific compounds such as HFC-134a, SF6, CH3CCl3, and HFC-365mfc. Our results also confirm the signs of successful phase out of primary ozone-depleting species along with substantial emissions of replacement HCFCs. Further implication of these high frequency high quality data will be discussed at the meeting.

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발표코드: **ANAL1-2**
발표분야: Analytical Chemistry for Environmental & Forensic Sciences
발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 김태영

Identification of key physico-chemical properties of brominated flame retardants alternatives for the evaluation of environmental persistence

권정환

고려대학교 환경생태공학부

Flame retardants are widely used as additives to various plastic products having an effect of reducing or suppressing combustion by improving physico-chemical properties of plastic products. The use of flame retardants increased rapidly with increasing production of plastics. Recently, some brominated flame retardants, a few congeners of polybrominated diphenyl ethers (PBDEs), have been classified and banned according to the Stockholm Convention on persistent organic pollutants (POPs) because they are resistant to degradation and have long-range transport potential. After the regulation of the use of PBDEs, industry uses various alternative chemicals including other types of brominated flame retardants without rigorous evaluation of their physico-chemical properties that determine the potential of being POPs. Lack of information on their physico-chemical properties and global monitoring data makes it difficult to decide their environmental persistence. In this study, it is intended to evaluate the long-range transport potential and environmental persistence of selected alternatives using the OECD screening tool and to identify critical properties of alternatives determining their persistence. A few of alternative materials may be more environmentally persistent than BDE-47 that has been classified as POPs although the uncertainties associated with input parameters such as partition coefficients between phases. Recent sensitive techniques that can be used to determine partition coefficients was found to be useful in reducing the uncertainties in the model.

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발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 김성환

Simultaneous measurement of thermal ionization mass spectrometry for high accuracy and precision in isotopic analysis of uranium and its application to nuclear safeguards and nuclear forensics

박종호* 송규석

한국원자력연구원 원자력화학연구부

A thermal ionization mass spectrometer (TIMS) equipped with a multiple collector system was utilized for the study on the measurement accuracy and precision based on the detection methods and the amounts of uranium. Various amounts of samples were loaded in the mass spectrometer followed by being measured with three different detection configurations, which were multi-dynamic, dynamic, and simultaneous static detection methods. Only static detection method enabled us to ensure reliable accuracy and precision for the isotopic measurement of the uranium with 1 pg, which corresponds to the amount of uranium contained in a typical single-particle collected from a nuclear facility. Examples for isotopic analysis of uranium single-particles performed by TIMS with fission-track (FT) or scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM-EDS) techniques were shown as applications of this study to nuclear safeguards and nuclear forensics. The excellent agreement of the measurement with the certified value showed our single-particle analysis based on FT-TIMS and SEM-TIMS measurements suitable for the analysis of unknown uranium particles with high precision and accuracy.

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발표코드: **ANAL1-4**
발표분야: Analytical Chemistry for Environmental & Forensic Sciences
발표종류: 심포지엄, 발표일시: 목 10:55, 좌장: 김성환

Application of Analytical Chemistry to Environmental and Forensic Sciences: The Case Study of Isotope Data

류종식

한국기초과학지원연구원 환경과학연구부

The unclear, physical and biological chemistry of isotopes has profoundly influenced the environmental and forensic sciences, forming the basis for reconstructions of past climates, 'tracer' studies in the hydrosphere and lithosphere, and numerous other chemical tools. Recently, new technology using mass spectrometry, such as multi-collector inductively coupled plasma mass spectrometer (MC-ICP-MS), allows us to accurately and precisely measure relatively small isotope abundance variations. Analyzing isotopes thus offers powerful opportunities for directly tracing the elemental cycles, and the provenance of materials and people in environmental and forensic sciences. In this presentation, I will introduce analytical methods for particular isotopes and several case studies that show how isotopes can be used as a chemical proxy or chemical fingerprinting in environmental and forensic sciences.

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발표분야: Analytical Chemistry for Environmental & Forensic Sciences
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 김성환

Forensic applications of mass spectrometry for illicit drug testing

김진영

대검찰청 과학수사담당관실

Forensic toxicology deals with hundreds of drugs that are abused or illicit. These compounds should be rapidly and reliably detected and identified in biological samples on a routine analysis. Combined chromatography-mass spectrometric techniques have been most commonly used for this purpose. GC-MS has been considered as the ‘gold standard’ for forensic compound identification, while LC-MS has become an increasingly important technique due to its usefulness for the analysis of hydrophilic, thermolabile, and non-volatile compounds. The hemp plant Cannabis sativa is one of the most widely abused illicit substances in Korea. However the incorporation of THC-COOH into hair is very small, making quantification challenging due to the very high sensitivity required. The proposed cut-off concentration for the detection of THC-COOH in hair is 0.2 pg/mg from the Society of Hair Testing and 0.05 pg/mg under the federal regulations of the United States. To satisfy these analytical requirements, we have focused on GC-MS/MS methods for the determination of THCCOOH in hair. The developed method provided reliable data for use in forensic toxicology and results in a substantial increase in detection sensitivity by the combination of GC, NCI and MS/MS.

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장소: 광주 김대중컨벤션센터

발표코드: **ANAL2-6**

발표분야: Recent Developments in Chemical Analysis Methods

발표종류: 분과기념강연, 발표일시: 목 15:50, 좌장: 김준곤

The Role of Mass Spectrometry in the Omics Era

김영환

한국기초과학지원연구원 질량분석연구부, UST 생물분석과학과

Mass spectrometry is one of the key analytical technology on which the emerging -omics approaching are based, because it provide all the criteria to study -omics field such as high sensitivity, selectivity, throughput, robustness, flexibility, and linear dynamic range of quantification of complex biological samples. As you know, Korea Basic Science Institute (KBSI) is the government-supporting institute which performs R&D support and joint research to promote national science and technology development. I have worked for developing the MS-based analytical methods of biological molecules by using various kinds of mass spectrometers, since I entered KBSI 23 years ago. In this lecture, I would like to show the results for proteomics, glycomics, and lipidomics obtained through collaboration with the researchers in other universities and research institutes. I will also discuss the essential roles of mass spectrometry in -omics study.

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발표코드: **ANAL2-1**
발표분야: Recent Developments in Chemical Analysis Methods
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 차상원

Separation and Characterization of Stereoisomeric Polylactides using Electrospray Ionization Ion Mobility Mass Spectrometry

김준곤

포항공과대학교(POSTECH) 화학과

The separation and characterization of stereo-isomers of polylactide (PLA), synthesized by ring-opening polymerization of cyclic lactide dimer, are carried out using electrospray ionization ion mobility mass spectrometry (ESI-IM-MS) combined with molecular dynamics (MD) simulations. The IM-MS analysis shows intriguing difference between the collision cross section (Ω_D) value of poly-L-lactide (PLLA) and poly-LD-lactide (PLDLA) with respect to chain architecture (linear vs. ring) and stereo-regularity. It further seeks to investigate an experimentally observed intriguing difference between the mobility values of PLLA and PLDLA ions with respect to their chain architecture and stereoregularity using computational modeling. The hydrogen bond interaction is affected to the structure, morphology, and physical properties of PLA. The degree of crystallization of PLA is highly related to their weak hydrogen bond interaction. The potential application of IM-MS to separate and characterize stereo-isomeric polymers will be further discussed.

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장소: 광주 김대중컨벤션센터

발표코드: **ANAL2-2**

발표분야: Recent Developments in Chemical Analysis Methods

발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 차상원

Better Bioanalysis using Gold Nanoparticles

이혜진

경북대학교 화학과

Bioanalysis via monitoring surface bioaffinity events such as DNA-DNA, RNA-DNA, protein-protein interactions have been extensively investigated for a wide range of biological applications. In this talk, we will highlight our latest efforts made on the development of ultrasensitive bioaffinity sensing platforms using biofunctionalized gold nanoparticles in conjunction with either surface plasmon resonace (SPR) or electrochemical techniques for the analysis of biologically and environmentally important molecules. For example, a novel surface sandwich bioaffinity assay in conjunction with antibody functionalized gold nanoparticles was developed for the quantitative analysis of protein biomarkers in serum samples [1]. Another example is a dual-nanoparticle sandwich configuration to achieve detection limits down to 0. 1 aM for biomarkers. The final example is the use of multilayers of gold nanoparticle-polyelectrolyte-enzyme on a disposable electrode platform for the highly sensitive analysis of catechol in tea smaples [2].

[1] H. R. Jang, A. W. Wark, S. H. Baek, B. H. Chung, H. J. Lee, Analytical Chemistry, 2014, 86, 814-819[2] M. N. Karim, J. E. Lee, H. J. Lee, Biosensors and Bioelectronics, 2014, 61, 147-151

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ANAL2-3**

발표분야: Recent Developments in Chemical Analysis Methods

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 차상원

Diverse Raman measurement schemes for reliable non-destructive analysis of samples: Axially perpendicular offset (APO) and axial illumination schemes

정회일

한양대학교 화학과

An axially perpendicular offset (APO) scheme able to directly acquire reproducible Raman spectra of samples contained in an oval container even under the variation of the container orientation has been demonstrated. It utilized the axially perpendicular geometry between the laser irradiation and photon detection, namely the irradiation through a sidewall of the container and gathering of Raman photon just beneath the container. The APO scheme provided the best accuracy when the axial offset distance was 10 cm. To rationalize the found optimal offset distance, a simulation based on Monte-Carlo method was used to study the characteristics of photon migration in the APO scheme. Next, we have demonstrated a simple and effective strategy, so called axial illumination schemes, to obtain representative Raman spectra of suspension samples with minimal influence by internal particle-settling. The proposed schemes irradiates laser radiation axially with the same or opposite direction of settling, so allowing laser photons to migrate through the settling-induced particle-density gradient formed in a suspension and widely interact with particles regardless of their settled locations. Therefore, transmitted Raman information gathered at opposite of the illumination could be better representative of overall suspension composition even with the occurrence of partial settling.

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발표코드: **ANAL2-4**

발표분야: Recent Developments in Chemical Analysis Methods

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김준곤

Lipidomics Platform to Find the Lipid Alteration in Biological Samples

김광표

경희대학교 응용화학과

Lipidomics is a systems-level analysis of lipid species, their abundance, biological activities, and subcellular localization. Many studies have reported the aberrant lipid metabolism in human disease. Thus, there are increasing interests in finding the lipid alteration between disease samples and controls. In lipidomics, it is critical to construct a well-designed platform to identify the differentially expressed lipids (DELs) in biological samples. First, we need an exhaustive lipid profiling method. Second, a robust statistical analysis of lipid profiles is required for the reliable data analysis. We described here an established lipidomics platform that consists of global lipid profiling based on LC/Qof MS and lipid quantification based on by LC/QqQ MS. High accuracy mass analysis was effective to profile various lipid, and multiple reaction monitoring was useful to sensitive and selective quantification. This platform was applied to the biological sample analysis, and its utility was demonstrated.

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발표코드: **ANAL2-5**
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2D correlation analysis in protein study

정영미

강원대학교 화학과

The advanced spectral analysis method was utilized to investigate structural changes of protein during transition from native to the intermediate state. 2D correlation spectroscopy is well established analytical technique to interpret the spectral data obtained under some type of perturbation (e.g., temperature, concentration, pH, etc.). Proteins are transformed from the native state into the intermediate states or into the denaturated state under low pH, high concentrations of denaturant, or heating. Despite some common features of intermediate state, a coherent picture of the intermediate state cannot be completed. In this presentation, pH-induced transition of proteins from the native to the intermediate state were analyzed by probing theirtertiary and secondary structure using 2D correlation spectroscopy. Full scenario of pH-induced transition mechanism of holo-form of bovine alpha-lactoablumin and ovalbumin will be discussed in more details.

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장소: 광주 김대중컨벤션센터

발표코드: **BIO1-1**

발표분야: Neurodegenerative Diseases in Life Chemistry

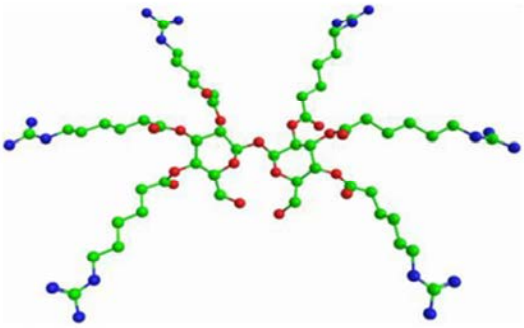
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 안대로

Preparation and Evaluation of BBB-permeable Trehalose Derivatives as Potential Therapeutic Agents for Huntington’s Disease

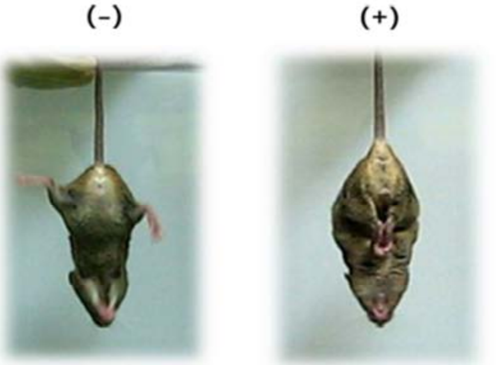
임정균

순천향대학교 나노화학공학과

Huntington’s disease (HD) is an autosomal dominant neurodegenerative disorder, and affects about 1 in 20,000 people in the US. The main cause of HD is assumed to be the mutation in the gene coding for huntingtin (Htt), and the mutated Htt contains an abnormally expanded polyglutamine stretch (polyQ>35), which tends to aggregate into insoluble amyloid-like fibrils. Many attempts were made to inhibit the polyglutamine-induced protein aggregation, and the non-reducing disaccharide trehalose was reported to alleviate the disease symptoms of HD transgenic mice. However, trehalose is known to be rapidly hydrolysed to glucose by trehalase enzyme present in the small intestine, and its uptake into tissues is regarded to be very low. In addition, there is no evidence that trehalose can cross the blood-brain barrier (BBB) and enter the mammalian brain. Here we show that BBB-permeable trehalose derivatives could be prepared by applying the delivery methods which are previously developed before, and the derivatives were found to efficiently prevent the aggregation of polyQ in the transfected HEK293 cells. Furthermore, the derivative (TD-G6), when given ad libitum to a transgenic mouse model of HD (Tg R6/2), was found to significantly prolong lifespan, improve motor functions and reduce the inclusion bodies in the mouse brain compared with the trehalose control. These data strongly suggest that the BBB-permeable trehalose derivative may be used as a potential therapeutic agent for HD, and that further refinement of the present delivery technology might have significant potential applications for the treatment of many other intractable degenerative neurological diseases.



Trehalose derivative



no sign

limb clasping symptom

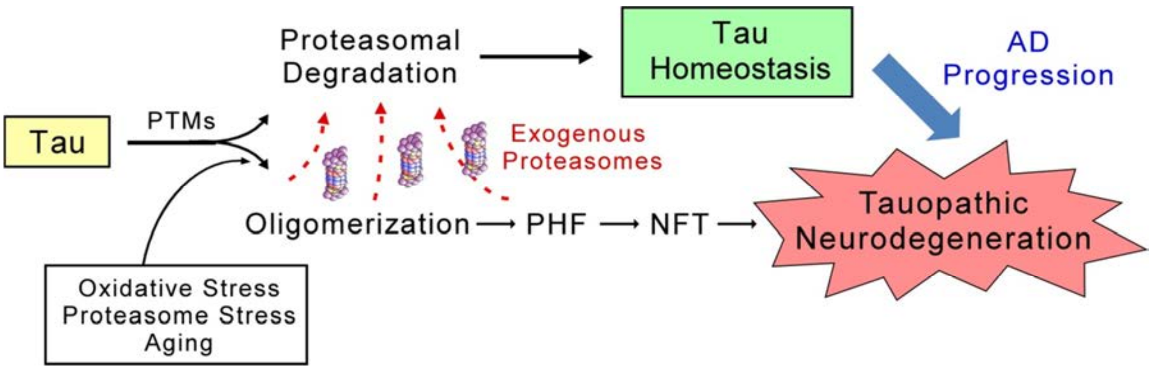
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **BIO1-2**
발표분야: Neurodegenerative Diseases in Life Chemistry
발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 안대로

Modulating Intracellular Protein Degradation and Its Implications in Neurodegenerative Diseases

이민재

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 (UPS) is responsible for the degradation of most intracellular proteins in eukaryotes. As our knowledge of biological processes in the systems has grown for the last 30 years, so have the ties between the systems 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. Moreover, we would like to emphasize that purified proteasomes can be directly transported into cells through mesoporous silica nanoparticle-mediated endocytosis. Proteasomes that were loaded onto nanoparticles through noncovalent interactions between poly-histidine tags and nickel ions fully retained their proteolytic activity. Cells treated with exogenous proteasomes were more efficient in degrading overexpressed human tau than endogenous proteasomal substrates, resulting in decreased levels of tau aggregates. Moreover, exogenous proteasome delivery significantly promoted cell survival against proteotoxic stress caused by tau and reactive oxygen species. These data demonstrate that increasing cellular proteasome activity through the direct delivery of purified proteasomes may be an effective strategy for reducing cellular levels of proteotoxic proteins.


Proteasomal Degradation
Tau Homeostasis
AD Progression
Tau
PTMs
Exogenous Proteasomes
Oligomerization
PHF
NFT
Tauopathic Neurodegeneration
Oxidative Stress
Proteasome Stress
Aging

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **BIO1-3**
발표분야: Neurodegenerative Diseases in Life Chemistry
발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 안대로

Alpha-Synuclein oligomers inhibit neuronal-SNARE mediated vesicle fusion: a new potential pathway of Parkinson’s disease

이남기

포항공과대학교(POSTECH) 시스템생명공학부/물리학

Parkinson’s disease and dementia with Lewy bodies are featured with the formation of Lewy bodies, composed mostly of α-Synuclein (α-Syn) in the brain. Although evidence indicates that the large oligomeric or protofibril forms of α-Syn are neurotoxic agents, the detailed mechanisms of the toxic functions of the oligomers remain unclear. Here we show that large α-Syn oligomers efficiently inhibit neuronal SNARE-mediated vesicle lipid mixing by using single-vesicle assay. Large α-Syn oligomers preferentially bind to the N-terminal domain of a vesicular SNARE protein synaptobrevin-2, which blocks SNARE-mediated lipid mixing by preventing SNARE complex formation. In sharp contrast, the α-Syn monomer has a negligible effect on lipid mixing even with a 30-fold excess compared with the case of large α-Syn oligomers. In addition, we show that large-sized αS oligomers, which are normally difficult to form, are readily generated by Aβ42-seeding and that these oligomers efficiently hamper neuronal SNARE-mediated vesicle fusion. Thus, the results suggest that large α-Syn oligomers function as inhibitors of dopamine release, which provides a clue, at the molecular level, to their neurotoxicity.

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발표코드: **BIO1-4**
발표분야: Neurodegenerative Diseases in Life Chemistry
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 안대로

NSF disassembles a single SNARE complex in one round of ATP turnvoer

윤태영

한국과학기술원(KAIST) 물리학과

N-ethylmaleimide-sensitive factor (NSF) and soluble NSF attachment protein (α-SNAP) disassemble the soluble NSF attachment protein receptor (SNARE) complex using ATP hydrolysis (the 20S particle) for recycling of the SNARE proteins. Despite its fundamental importance for sustained membrane traffic, the molecular mechanism by which NSF disassembles the SNARE complex is largely unknown. In this talk, with the observations using two orthogonal techniques of single-molecule fluorescence resonance energy transfer (FRET) and magnetic tweezers, I will show that NSF disassembles a single SNARE complex in only one round of ATP turnover. To realize such a high energy efficiency, α-SNAP destabilizes the C-terminal part of the SNARE motif and tightly connects the SNARE complex and NSF. Like a spring-loaded machine, the NSF hexamer releases its built up tension in a burst within 20 ms to disassemble the SNARE complex essentially in one step. The disassembled SNARE proteins are immediately released from the 20S particle. Our observations unravel how an AAA+ ATPase induces global unwinding of the substrate protein complex, which turns out to be a much more efficient mechanism than processive unwinding.

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발표코드: **BIO1-5**
발표분야: Neurodegenerative Diseases in Life Chemistry
발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 최수혁

Are Metal-Associated Misfolded Proteins Involved in Alzheimer’s Disease?

임미희

울산과학기술대학교(UNIST) 자연과학부/화학과

Neurodegenerative disorders impose an enormous financial and emotional burden onpatients, their families, and communities. More than 36 million people worldwide haveAlzheimer’s disease (AD), a devastating and fatal neurodegenerative disease thatremains poorly treated due to an incomplete grasp on the disease etiology. A keyneuropathological hallmark of AD is amyloid-β (Aβ) plaques in the brain. Themechanisms driving formation of these protein aggregates and their causal link todementia are still unclear. An additional observation in the AD brain is the accumulationof metal ions, which has been proposed to be associated with Aβ aggregates andneuronal death, yet relatively little is known, further sustaining the controversysurrounding this aspect of the disease. Even through a large body of continuouslyreported literature regarding metal ions and Aβ species, direct connection of metal-Aβ interaction with AD onset and development has been neglected in this field due tolack of appropriate tools and/or tactics. Therefore, we have developed chemical toolsand/or tactics that are capable of specifically targeting metal-associated Aβ speciesand modulating their interaction and reactivity. Using our chemical tools, we have beenable to regulate metal-induced Aβ aggregation and neurotoxicity in vitro, in living cells,and in primary neurons, along with cognition improvement in the AD mouse model.Here, our rational structure-based design principle and recent findings for chemicaltools and tactics for investigating metal-Aβ chemistry and biology in AD and/orpotential therapeutic agents for AD will be discussed.

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장소: 광주 김대중컨벤션센터

발표코드: **BIO1-6**

발표분야: Neurodegenerative Diseases in Life Chemistry

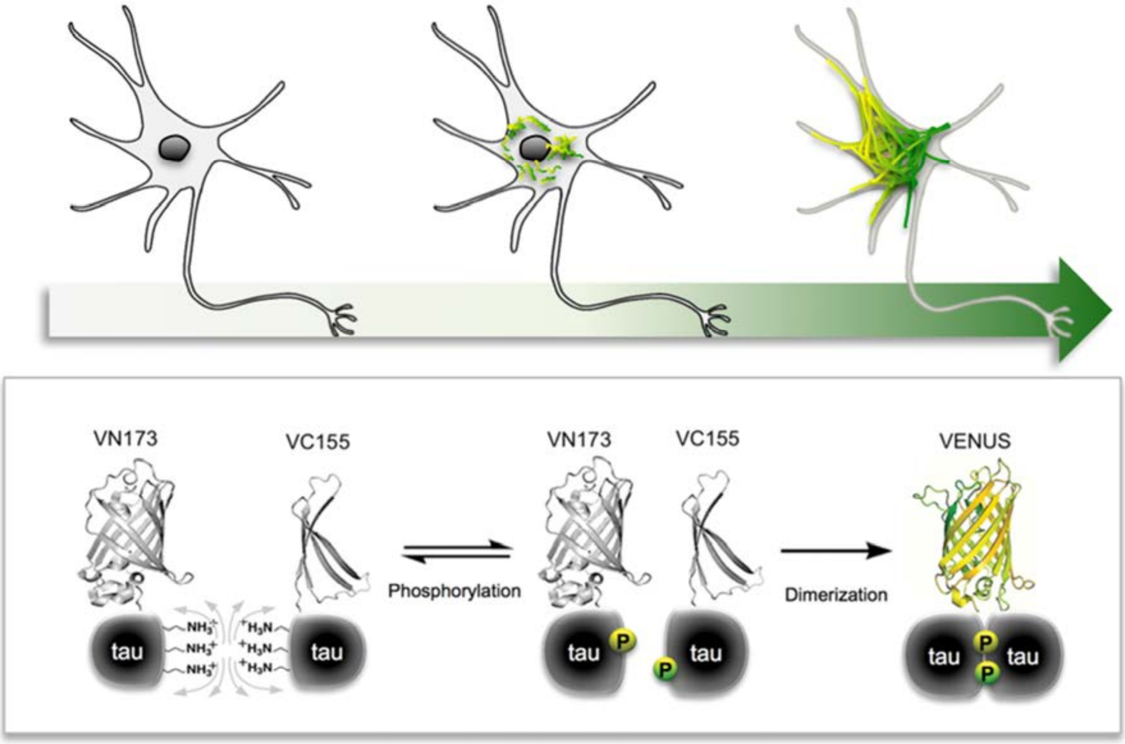
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 최수혁

Cell-based Sensors to Investigate Tau Pathology

김윤경

한국과학기술연구원(KIST) 뇌과학연구소/뇌의약연구단

Tau is a neuron-specific microtubule-binding protein that stabilizes microtubules. When pathologically modified, tau dissociates from microtubules and becomes insoluble aggregates called neurofibrillary tangles (NFTs). Abnormal tau aggregation is a pathological hallmark of many neurodegenerative disorders and it is becoming apparent that soluble tau aggregates play a key role in neuro-degeneration and memory impairment. Therefore, preventing tau aggregation becomes an important therapeutic strategy to cure tauopathies. However, progress has been slow due to the lack of a reliable method to investigate tau aggregation. In this regard, we developed a cell-based sensor that visualizes tau self-assembly. By introducing bimolecular fluorescence complementation (BiFC) technique to tau, we were able to achieve spatial and temporal resolution of tau-tau interactions in a range of states, from soluble dimers to large aggregates. In this presentation, we will introduce our cell-based sensors to monitoring tau assembly and its applications to investigate various tau modifications responsible for tau aggregation.


VN173
VC155
tau
NH3+
+H3N
Phosphorylation
VN173
VC155
tau
P
Dimerization
VENUS
tau
P

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **BIO1-7**

발표분야: Neurodegenerative Diseases in Life Chemistry

발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 최수혁

Distinct Role of Water in Protein Aggregation

함시현

숙명여자대학교 화학과

Understanding the molecular determinants of the relative propensity for proteins to aggregate in a cellular environment has been a central issue in attacking protein-aggregation diseases and in the development of human therapeutics. Despite the expectation that the protein aggregation can largely be attributed to the direct protein-protein interactions within an aggregate or in solution, we here unveil a crucial role of hydration water in ruling the aggregation propensity of proteins both in vitro and in vivo. The protein overall hydrophobicity, defined solely by the hydration free energy of a protein in its monomeric state sampling its equilibrium structures, was shown to predominantly dictate the protein aggregation propensity in aqueous solutions. We also find striking discrimination by the hydration water of positively and negatively charged residues depending on the protein net charge in regulating the solubility of a protein, which establishes novel design strategies for the biotechnological generation of aggregation-resistant proteins as biotherapeutics.

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발표코드: **BIO2-1**
발표분야: Biological Chemistry of Nucleic Acid and Its Derivatives
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이연

Design and Construction of Fluorescent Nucleic Acid Systems

김병현

포항공과대학교(POSTECH) 화학과

Fluorescent nucleic acid systems are widely applied in various fields, from fundamental biological probes to nano-construction, Nucleic acids are used as a scaffold for arranging aromatic fluorophore assemblies, either by insertion into the DNA base pairs or by stacking via the duplex. Moreover, chemical modifications of nucleic acids are accessible by the modified DNA phosphoramidites or postsynthetic approach, and provide with new and interesting fluorescent nucleic acids systems. Fluorescent nucleic acid systems represent an extensive and exciting research area in chemistry as well as in biotechnology and photophysics. We have synthesized and investigated new fluorescent nucleic acid systems for probing single nucleotide polymorphisms (SNPs), structural changes of DNA and ligand interaction with RNA bulge. We have developed the new type of molecular beacon, quencher-free molecular beacon (QF-MB), that exhibits several advantageous features, including a high level discrimination between the target and its single-mismatched congeners and an economical device set-up due to the absence of the quencher. We have also designed and synthesized the probing system for quadruplex structures of DNA (G-quadruplex and i-motif) and B-Z transition. Strong π-π stacking interactions in nucleic acids can be used to generate novel secondary structures. We have investigated the fluorescent phenomena and structures of pyrene modified oligodeoxyadenylate and oligodeoxyguanylate. The covalently linked pyrenes induced the formation of a self-assembled olgiodeoxyadenylate duplex and various secondary structures with interesting fluorescence phenomena. These fluorescent nucleic acid systems can be useful tools for biosensors and biodiagnostics in the area of nucleic acids research.

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발표코드: **BIO2-2**

발표분야: Biological Chemistry of Nucleic Acid and Its Derivatives

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이연

Elasticity-driven single stranded gap creation by exonuclease III during base excision DNA repair

이광록

광주과학기술원(GIST) 생명과학부

DNA damage occurs as many as 1 million individual molecular lesions per cell per day. One of the most frequently occurring DNA lesions is base damage. The damaged bases are quickly processed into AP (apurinic/apyrimidinic) sites, resulting in “missing base” in DNA. AP endonuclease catalyzes them for the Base Excision Repair (BER) process. Exonuclease III (exoIII) in E.coli functions as not only an AP endonuclease but also a 3’->5’ exonuclease exonuclease. We used single molecule FRET to examine how the multifunctional enzyme plays a physiological role during the BER process. When the substrate is a blunt-ended DNA, the enzyme works as a distributive exonuclease, performing multiple binding and dissociation events during the cleavage reaction. However, in the presence of an AP site, exoIII cuts the AP site as an AP endonuclease, and then transforms into a processive exonuclease, performing a continuous digestion by strongly anchoring to the AP site. The strong binding affinity onto the AP site is the origin of the transformation mechanism, allowing the enzyme to digest a series of nucleotides without dissociation from the substrate. The close examination of the enzyme behavior reveals an elasticity-based gap creation mechanism where exoIII forms a single stranded intermediate loop during the creation of a DNA gap for BER process. We found that the size of gap depends on the physiological salt concentration due to the polymer property of singe stranded loop.

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장소: 광주 김대중컨벤션센터

발표코드: **BIO2-3**

발표분야: Biological Chemistry of Nucleic Acid and Its Derivatives

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이연

Nucleic Acid Conjugates for Biomedical Applications

목혜정

건국대학교 특성화학부

Nucleic acids have been used as informative building blocks to allow superior biomedical applications like drug delivery, biosensors, and imaging. Through complementary hybridization, ligation, and chemical conjugation, diverse geometric structures have been created in a micro- and nanoscale. In this presentation, several bio-conjugates based on nucleic acids, particularly short chain RNAs like small interfering RNA (siRNA) and microRNA (miRNA), will be covered. Short chain RNAs are biological molecules which possess great potential not only as regulators of translation but also as therapeutics of diseases like cancers and genetic disorders. One of big challenges in RNA therapeutics is still delivery efficiency. This presentation will outline recent results related to delivery of short chain RNAs. Multivalent aptamer-RNA conjugates will be discussed as an simple, efficient, and targeted delivery systems for siRNAs into target cancer cells. Those multivalent aptamer-RNA conjugates were shaped like a rod with high aspect ratios, which exhibited greatly enhanced intracellular delivery for target cancer cells compared to common Aptamer-siRNA conjugates. It is likely that multivalent ligands of the Comb-type aptamer siRNA conjugates allowed efficient internalization via clustering effects. In addition, delivered Comb-type aptamer siRNA conjugates successfully suppressed target genes and reduced cancer cell proliferation. The newly designed bio-conjugates might have great potential to serve as a carrier for intracellular delivery of short chain RNAs.

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장소: 광주 김대중컨벤션센터

발표코드: **BIO2-4**

발표분야: Biological Chemistry of Nucleic Acid and Its Derivatives

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 유재훈

Transcriptome-wide Analysis of Protein-RNA Interactions in Human Embryonic Stem Cells

권영수

세종대학교 생명공학과

Based on the motif analysis of the human genome, there are more than a thousand RNA binding proteins. RNA binding proteins play essential roles in gene expression and are associated with a number of human diseases. Although functions of a few biologically important RNA binding proteins have been extensively studied in biochemical and/or molecular genetic approaches, relatively little is known about biological function of RNA binding proteins and their RNA partners within the context of intact cells. To study in vivo functions of RNA binding proteins, we analyze transcriptome-wide RNA binding protein-RNA interactions in human embryonic stem cells by coupling UV crosslinking immunoprecipitation (CLIP) with next-generation sequencing. Here, I present RNA targets of DGCR8, Drosha, TLS/FUS, EWS and TAF15. With this technology, we determine not only binding partners but also exact binding sties in the cell. This information provides a framework for identification of biological roles of RNA binding proteins in the cell.

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발표분야: Biological Chemistry of Nucleic Acid and Its Derivatives
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 유재훈

MicroRNA Regulation

김빛내리

서울대학교 생명과학부

MicroRNAs (miRNAs) are non-coding RNAs of ~22-nt in length, which act as key players in gene silencing. Hundreds of miRNA genes have been discovered in animals, plants, and viruses, constituting one of the largest gene families. By targeting many different protein-coding genes, miRNAs are involved in almost all biological processes, such as embryonic development, cell differentiation, cell death, proliferation, metabolic regulation, cancer development, and anti-viral defense. My research on miRNA began with a simple question as to how these unusual small molecules are made in cells. We found that miRNAs are transcribed by RNA polymerase II as long primary transcripts (termed ‘pri-miRNAs’). Pri-miRNAs are processed through two sequential events: the nuclear processing of the pri-miRNAs into stem-loop precursors of ~70-nt (pre-miRNAs) and the cytoplasmic processing of pre-miRNAs into mature miRNAs of ~22-nt. Dicer, a member of the Ribonuclease III (RNase III) superfamily of bidentate nucleases, mediates the latter step. By characterizing the nuclear processing in detail, we identified an RNase III type protein, Drosha, as the nuclease that executes the initiation step of miRNA processing in the nucleus and found that Drosha forms a complex called Microprocessor together with an RNA-binding protein called DGCR8. Recently we have been investigating how miRNAs are regulated. Regulation of miRNA biogenesis can be achieved at either transcriptional or post-transcriptional level. Post-transcriptional control is widespread and can take place at multiple steps including Drosha processing, nuclear export, Dicer processing, RNA editing, uridylation, and decay. We have been investigating the regulatory mechanisms of miRNAs associated with cancer and stem cells. We identified several specific RNA binding proteins that post-transcriptionally regulate miRNA biogenesis. This talk will focus on the roles of miRNAs and its associated proteins in cancer and stem cells.

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장소: 광주 김대중컨벤션센터

발표코드: **ORGN1-1**

발표분야: Current Trends in Organic Chemistry I: Organic Supramolecular Chemistry

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이희승

Development of Small-Molecule Probes for Diagnosis and Imaging of Disease

안교한

포항공과대학교(POSTECH) 화학과

For bioimaging of tissue, two-photon excitation microscopy (TPM) has drawn keen interest in recent years for its several advantageous features in tissue imaging where scattering of light becomes a serious issue. These promising features of TPM for live tissue imaging have inspired our quest for two-photon absorbing molecules with desirable photophysical properties for bioimaging. Small-molecule probes enable noninvasive imaging of biological substances. Such molecular probes can provide indispensible tools for the diagnosis and imaging of disease. In this symposium, also I like to disclose some of our recent works on the development of two-photon fluorescence probes for disease biomarkers including cancer.

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장소: 광주 김대중컨벤션센터
발표코드: **ORGN1-2**
발표분야: Current Trends in Organic Chemistry I: Organic Supramolecular Chemistry
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 이희승

Synthetic Chloride Transporters across Lipid and Cell Membranes

정규성

연세대학교 화학과

There have been known a variety of proteins functioning as chloride transporters and channels in biological systems, which play crucial roles to regulate ionic concentrations, to maintain cellular volume and pH, to transmit electrical signals, etc. In recent years, much effort has been devoted to the design and synthesis of small synthetic molecules that can facilitate anion transport across lipid membranes, in order to help gain insight into the underlying principles of ion transport in biological systems and to find suitable compounds for biomedical applications. It will be discussed our own efforts including a) synthesis and optimization of synthetic chloride transporters, b) development of synthetic salt transporters via cation/anion symport, and c) stimuli-responsive chloride transporters with the controlled activities in response to enzymes or light.

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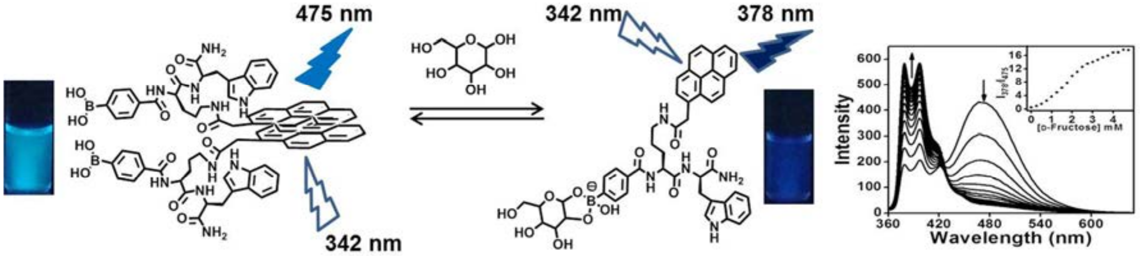
발표코드: **ORGN1-3**
발표분야: Current Trends in Organic Chemistry I: Organic Supramolecular Chemistry
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 이희승

Detection of carbohydrates in aqueous solution using fluorescent chemosensors based on amino acid and peptide

이건형

인하대학교 화학과

During the last decade, there have been many advances in the development of fluorescent chemosensors for sugar using arylboronic acid as a receptor. As the covalent interactions of arylboronic acid with sugar did not considerably change the fluorescence of the fluorophore, fluorescent chemosensors based on arylboronic acid have required certain processes for the change of fluorescence depending on the boronic acid-carbohydrate interactions such as an internal charge-transfer (ICT) process and a photoinduced electron transfer (PET) process. In recent years, we have focused on the development of chemosensors based on peptides because of hydrophilicity, biological compatibility, and binding affinity for biomolecules. We synthesized a new ratiometric sensing system based on peptides for sugars capable of controlling the pyrene monomer and excimer emissions. Amphiphilic dipeptide containing phenylboronic acid aggregated in the absence of sugars in aqueous solutions resulting in a considerable excimer emission. The covalent bonding of the phenylboronic acid of the peptide with sugar converted the aggregates into a monomer form of the complex, resulting in a decrease of excimer emission and a concomitant increase of monomer emission intensity. Fluorescent chemosensors for heparin among polysaccharides were synthesized based onheparin-binding peptides. The fluorescent peptidyl chemosensor showed a highly sensitive ratiometric response to nanomolar concentrations of heparin in aqueous solutions and in biological samples containing human serum. The detection limit was 34 pM for heparin in an aqueous buffer solution containing 5% human serum. The results indicated that peptide-base chemosensor provided a potential tool for monitoring sugar in aqueous buffered solutions.


475 nm
342 nm
342 nm
378 nm
Intensity
Wavelength (nm)
360
420
480
540
600
0
100
200
300
400
500
600
I378/I475
[D-Fructose] mM

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장소: 광주 김대중컨벤션센터

발표코드: **ORGN1-4**

발표분야: Current Trends in Organic Chemistry I: Organic Supramolecular Chemistry

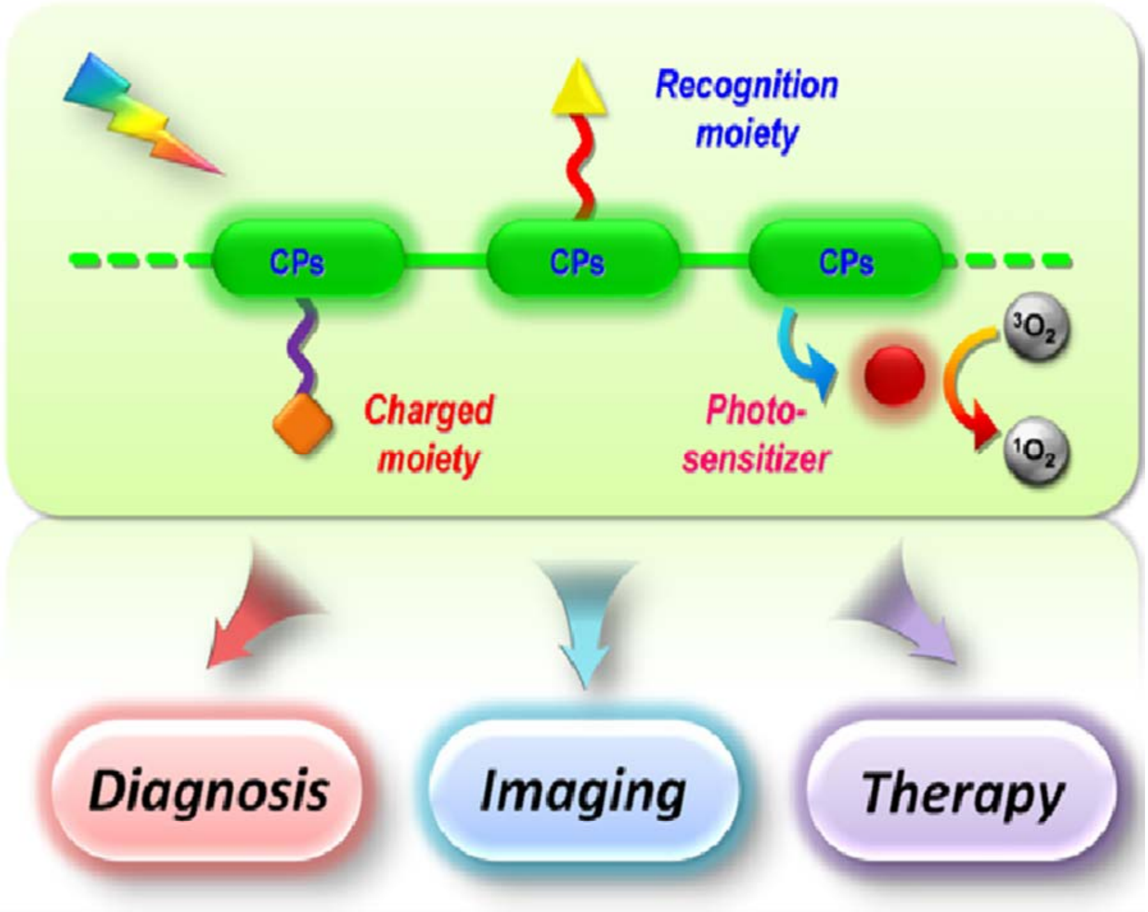
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 윤주영

Optical Self-Assembly Conjugated Polymers Materials for Sensing and Biomedical Application

Shu Wang

Chinese Academy of Sciences, Beijing

Water-soluble conjugated polymers (CPs) provide a unique platform for chemical and biological sensors in view of their optical signal amplification effect. Water-soluble conjugated polymers (CPs) provide a unique platform for chemical and biological sensors in view of their optical signal amplification effect. Our studies showed that the mesoscale macromolecular assemblies of cationic water-soluble conjugated polymers with biomacromolecules can be used to design and develop conjugated polymers-based biosensors for DNA, RNA, protein as well as metal ions. Very recently, we have developed a new technique for preparing multicolor microparticles based on the self-assembly of bacteria and conjugated polymer nanoparticles (CPNs). They can be successfully applied for cell imaging and optical barcoding. A polythiophene-porphyrin dyad was also prepared for effectively killing neighboring cells. This multifunctional material that simultaneously provides therapeutic action and image the results provide new strategies for the treatment of various diseases. A cationic poly(p-phenylene vinylene) derivate bearing polyethylene glycol (PEG) side chains was also synthesized and used for selective recognition, imaging and killing of bacteria over mammalian cells. These results exhibit that the multi-functional conjugated polymers are ideal platforms for recognition, imaging and disease therapy.


Recognition moiety
CPs
CPs
CPs
$^3O_2$
$^1O_2$
Charged moiety
Photo-sensitizer
Diagnosis
Imaging
Therapy

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN1-5**
발표분야: Current Trends in Organic Chemistry I: Organic Supramolecular Chemistry
발표종류: 심포지엄, 발표일시: 목 11:20, 좌장: 윤주영

Toward Functional 3D Molecular Architectures Based on Controlled Self-Assembly of Foldamer

이희승

한국과학기술원(KAIST) 화학과

It has been well known that creatures in nature, even very small living organisms such as bacteria and diatoms, have various shapes of 3D structures. This means that particular 3D shapes should be closely related to many biological functions, which in turn suggests that 3D shapes are necessary tools to recognize or communicate each other for maintaining their living systems. We have recently discovered a strategy to mimic the natural process in a flask. We demonstrated that artificial protein fragments (helical β-peptide foldamers) self-assembled in aqueous solution to form unprecedented 3D molecular architectures (“foldectures”) in a controlled manner. A next challenge in the foldecture research is to find a strategy to install various functional groups in/on the well-defined 3D structures in predictable manner. In this talk, I will introduce our recent efforts toward rational design of fuctional foldectures.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN2-6**

발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction

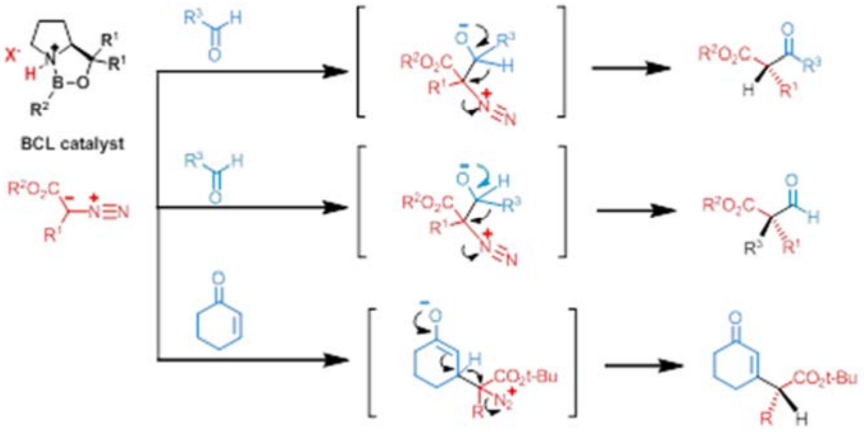
발표종류: 분과기념강연, 발표일시: 목 15:50, 좌장: 박진균

Catalytic Enantioselective C-H and C-C Insertion Reactions with Diazoesters

류도현

성균관대학교 화학과

The chemistry of α-diazocarbonyl compounds has attracted great attention because of its extensive applications in organic chemistry since the first recorded synthesis of ethyl diazoacetate by Curtius in 1883. Recently, we developed highly enantioselective, catalytic cyclopropanation with diazoesters in the presence of chiral oxazaborolidinium ion in high yield (up to 93%) with high to excellent diastereoselectivity (up to 98% de) and enantioselectivity (up to 95% ee).In this talk, we will present that highly enantioselective Carbon-Hydrogen and Carbon-Carbon insertion reactions with diazoesters. Theses methodologies were successfully applied to the synthesis of the natural products, sitophilate, and (+)-epijuvabione. As another application, optically active quaternary α- and β-amino esters were prepared from all carbon α-quaternary aldehydes in good yields and excellent enantioselectivities.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction

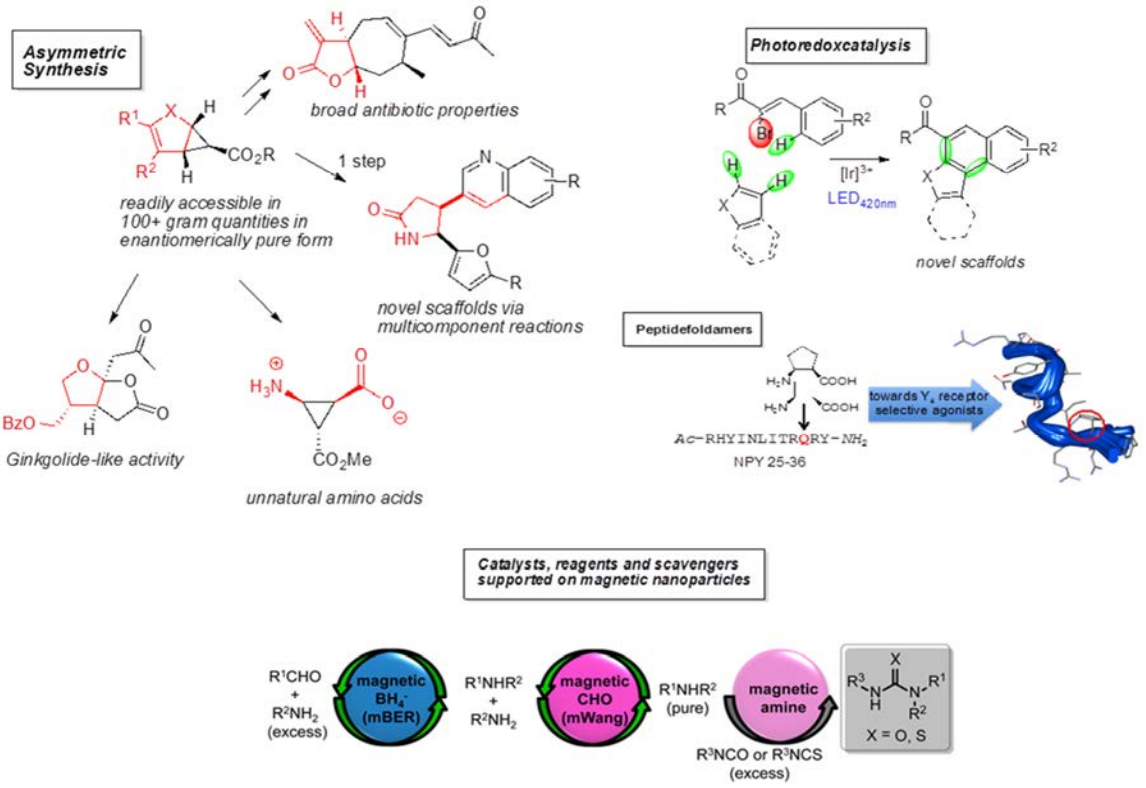
발표종류: 심포지엄, 발표일시: 목 13:10, 좌장: 윤재숙

Mag(net)ic Molecules - Synthesis and Applications

Oliver Reiser

Universität Regensburg, Germany

Sustainability is the edifice for the development of efficient chemical processes. Contributions from our group include transformations mediated by novel transition metal or photoredox catalysts, using renewable resources towards the synthesis of fine chemicals, natural products and drugs, or peptide foldamers. Selected projects from these areas will be presented, involving coworkers from Korea with whom I had the pleasure to work with over the years.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN2-2**

발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction

발표종류: 심포지엄, 발표일시: 목 13:40, 좌장: 윤재숙

Rhodium-Catalyzed Transannulation and Aminoalkenylation Using *N*-Sulfonyl-1,2,3-triazoles

이필호

강원대학교 화학과

Azaheterocycles are a highly important class of compounds due to their biological activities and pharmaceutical usabilities. In particular, dihydroazepines, dihydropyrroles, and pyrroles are constituents of a valuable privileged structure in organic chemistry. For this reason, the development of efficient synthetic methods of multi-substituted azaheterocyclic compounds from simple and easily accessible starting materials has been continuously required. Now, we report an efficient synthetic method of azaheterocycles such as pyrroles, tetrahydrofuranodihydropyrroles, tetrahydropyranodihydropyrroles, dihydropyrroles, and dihydroazepines *via* Rh-catalyzed transannulation of *N*-sulfonyl-1,2,3-triazoles starting from terminal alkynes, sulfonyl azides, and 1,3-dienes in one-pot. Also, the development of rhodium-catalyzed diastereoselective *N*-sulfonylaminoalkenylation of azulenes using *N*-sulfonyltriazoles is described. This procedure can be successfully applied to rhodium-catalyzed diastereoselective *N*-sulfonylaminoalkenylation of azulenes starting from terminal alkynes and *N*-sulfonylazides *via* a three-component semi-one pot process.

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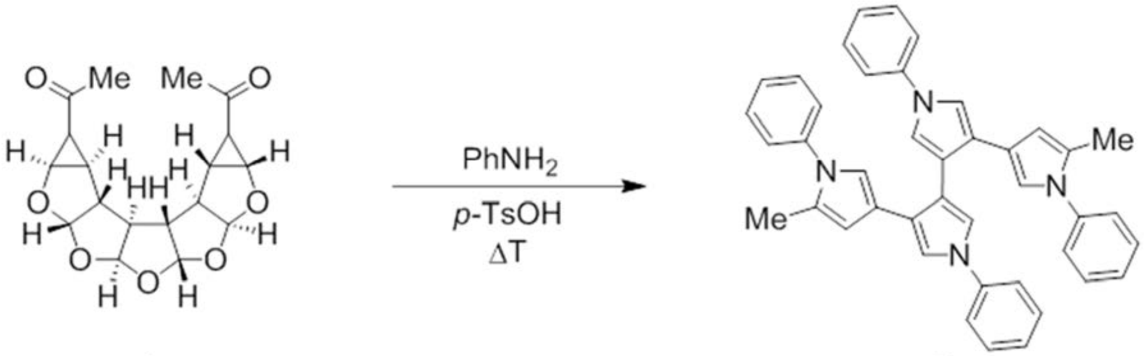
장소: 광주 김대중컨벤션센터
발표코드: **ORGN2-3**
발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 윤재숙

Three-Membered Rings and Triple Bonds as Ideal Starting Materials for Domino Cascades

Daniel B. Werz

Technische Universität Braunschweig, Germany

Cyclopropanes as well as carbon-carbon triple bonds are systems being high in energy. Therefore, both moieties are ideally suited for a cascade of consecutive reactions (domino reactions).In a first part, domino reactions based on ring-enlargement reactions of donor-acceptor-substituted cyclopropanes are discussed. Aldehyde, ketimines and thioketones are utilized as acceptors whereas ether moieties serve as donor. A rearrangement leads to the respective five-membered rings which tend to eliminate water. As a result, aromatic systems are formed. Depending on the substrate domino cascades are initiated which are able to transform the biscyclopropane derivative 1 in one step into the corresponding quaterpyrrol 2. In a second part, Pd-catalyzed domino reactions starting with triple bonds attached to carbohydrate derivatives 4 are reported to construct a variety of chroman- and isochroman-type structures such as 5. Such domino sequences are also employed to a variety of other processes leading to complex scaffolds in a facile and efficient fashion.



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일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN2-4**

발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction

발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 윤재숙

Enantioselective Alkynylation of Trifluoromethyl Ketones Catalyzed by Functionalized-Salen Ni Complexes

홍석원

광주과학기술원(GIST) 신소재공학부

Cooperative catalysis has emerged as a powerful strategy in catalytic asymmetric synthesis. As a part of our program aiming at asymmetric cooperative catalysts, we have developed a series of functionalized salen transition metal catalysts to facilitate challenging bimetallic reactions through the H-bond mediated self-assembly. Recently we also reported that the urea-functionalized-salen Co catalysts could provide an alternative bifunctional activation of an anionic nucleophile (by H-bond) and an aldehyde (by Lewis acid metal center). Herein we wish to report that novel functionalized-salen Ni complexes are highly efficient catalysts for the enantioselective direct alkynylation of trifluoromethyl ketones, affording enantioenriched propargyl alcohol products in high yields and enantioselectivities. The current methodology is operationally simple and allow for the use of substoichiometric amount of base. Ligand synthesis, catalyst/reaction optimization, substrate scope study results will be discussed in detail in the presentation.

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장소: 광주 김대중컨벤션센터
발표코드: **ORGN2-5**
발표분야: Current Trends in Organic Chemistry II: Metallo-Organic Reaction
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 박진균

Collaborative Approach to C-H Functionalization

Huw M. L. Davies

Emory University, USA

This presentation will describe a collaborative approach towards achieving new C-H functionalization strategies and our recent advances in the chemistry of donor/acceptor-substituted carbenoids. This class of carbenoids is capable of a range of highly stereoselective C-C bond-forming reactions, such as cyclopropanation and C-H functionalization. A series of chiral dirhodium catalysts have been developed for this chemistry and they are capable of very high turnover numbers and can induce high enantioselectivity in a wide range of reactions. The application of these new synthetic methodologies to the synthesis of natural products and pharmaceutical targets will be described.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **MEDI-1**
발표분야: The Era of Open Innovation: Recent Trends in Drug Discovery
발표종류: 심포지엄, 발표일시: 목 13:35, 좌장: 남기엽

Synthetic Immunology: Engineering Human Immune System to Fight Cancer

김찬혁

California Institute for Biomedical Research

Despite decades of clinical efforts and research, cancer still remains incurable disease with poor survival rates. Current treatment options for cancer, such as cytotoxic drugs and radiotherapy, largely depends on the differential proliferation and metabolism rate of cancer cells relative to normal cells. However, most of these anti-cancer agents are also toxic to normal cells to some extent, which results in serious systemic toxicity in patients, or eventually succumb to the various escape mechanisms of cancer cells resulting in tumor relapse. Recently, cancer immunotherapy has been drawing growing attention as a novel promising therapeutic modality for cancer. Particularly, the highly encouraging results were released from recent clinical trials using immune-checkpoint blockers (anti-CTLA-4 and anti-PD-1 IgGs), T-cell recruiting bispecific antibodies, and adoptive transfer of chimeric antigen receptor (CAR)-modified T cells. Remarkably, all of these approaches share the same purpose of unleashing the suppressed activity of the patient's own immune system, and harness its power to fight cancer.Notably, this early success of the cancer immunotherapy coincides with the recent progress in a rapidly emerging, multi-disciplinary research area "synthetic immunology", where researchers engineer the human immune system using a variety of chemical and biological tools to ultimately control and create human immunity. In this talk, I'll discuss recent examples of how these tools from different research areas - including synthetic organic chemistry, protein biochemistry, antibody engineering, and cell therapy - are being unified to seek a novel way to modulate human immune cells in the context of developing potent cancer immunotherapeutics.

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장소: 광주 김대중컨벤션센터
발표코드: **MEDI-2**
발표분야: The Era of Open Innovation: Recent Trends in Drug Discovery
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 남기엽

글로벌신약개발의 지름길

KIM DOOSEOP

(주)한독약품 신약연구소

급변하는 시장에 신속대응하고, 경쟁력을 높이기 위해, 많은 글로벌 Major Pharma, 중견기업, small venture 들이 M&A, strategic alliance, partnership/collaboration, outsourcing 형태로 외부와의 협업을 해왔고, 근래에 와서는 open innovation 이라는 이름으로 외부 기관과의 시너지 창출, 또는 그 이상의 activities 에 더욱 더 활발한 박차를 가하고 있다. 본 발표에서는 이들 기업체/연구소/학교 간 Open Innovation 의 성공/실패 사례와 그것들에 대한 중요한 Factor 들을 논의하고자 한다.

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장소: 광주 김대중컨벤션센터
발표코드: **MEDI-3**
발표분야: The Era of Open Innovation: Recent Trends in Drug Discovery
발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 황종연

Humanized-Knockout zebrafish for Disease models

김철희

충남대학교 생물과학과

The zebrafish is a vertebrate model system suitable for fishing novel genes in post-genome era. We challenged a genome-wide screen against the human UniGene collections. We performed microinjections more than 2,700 human genes and identified 64 functionally active genes. I will present the prospect of new technology of targeted KO based on ZFN, TALEN and now RGEN. We have executed a pilot study with more than 100 genes requested from various laboratories. After the first round of injections, we had identified stable mutations in F1 embryos at a very high efficiency. So far, we generated stable knockouts in 70 genes, with additional genes currently under screening. I will show the surprising results of the analysis of some of our mutant lines, each having phenotype with swimbladder-less, thymus-less, and anxiety behavior, respectively. Among these, a novel chemokine-like family member, samdori-2 (sam2), is specifically expressed by neurons in the dorsal habenula (Hb) of zebrafish. The Hb is a structure in the epithalamus highly conserved during vertebrate evolution, and mediates behavioral responses to stress, anxiety, and fear. Dysfunction of Hb is associated with depression, post-traumatic stress disorder, and schizophrenia in humans. Targeted knockout (KO) of the sam2 gene did not affect viability, fertility, or general morphology. Furthermore, sam2 KO fish showed normal development of neural circuits including Hb to interpeduncular nucleus (IPN) pathways. However, sam2 KO fish exhibited strikingly elevated anxiety-like behaviors in the novel tank and scototaxis tests and showed increased social cohesion. With the power of this new genome editing and/or KO technology, we will have a turning point in the biomedical research, such as “Designer Genomics & Bioinnovation”.

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장소: 광주 김대중컨벤션센터
발표코드: **MEDI-4**
발표분야: The Era of Open Innovation: Recent Trends in Drug Discovery
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 황종연

혁신 신약개발을 위한 한국형 오픈 이노베이션 전략: 혁신형 신약 개발에 있어서 연구중심병원의 역할

백태곤

서울아산병원 글로벌임상선도센터

지난 10 년간 신약개발의 투자 비용은 두배이상 증가되었지만 이에 따른 새로운 신약 허가는 오히려 감소하는 경향을 보이고 있다. 다국적 제약사들은 어려운 신약개발 환경을 극복할 방안으로 그들만의 다양한 신약 개발관련 전략들을 구축하였으며 이러한 전략중 "오픈 이노베이션"전략을 신약 개발에 있어서 핵심 전략으로 다국적 제약사들은 채택하고 있다.국내 제약업계에서도 이러한 다국적제약사의 영향으로 오픈 이노베이션 전략을 제약사들의 신약 및 제품개발등에 활용하고 있는 실정이다. 다국적제약사와 국내 제약사들이 똑같이 오픈 이노베이션이라는 전략을 신약 및 제품 개발에 적용하고 있지만, 분명 오픈 이노베이션 전략과 오픈 이노베이션의 개념을 이해하는것에서는 다국적제약사와 국내 제약사들간에는 많은 차이라 있을 것으로 여겨진다. 이러한 차이를 인지하고 신약 및 제품개발에 있어서 국내제약 여건에 충실하고 걸맞는 한국형 오픈 이노베이션 전략을 구축하고 실행해 봄도 의미있는 일이 될것이다.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **MAT1-1**
발표분야: Plasmonic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이기라

고효율 유기태양전지를 위한 플라즈모닉 물질 설계

이정용

한국과학기술원(KAIST) EEWS대학원

유기태양전지의 효율을 극대화하는 방법중의 하나로 플라즈모닉 성질을 갖고 있는 물질을 설계하는 방법에 대해서 논의한다. 우리는 금속나노입자의 크기와 모양을 제어함으로써 유기태양전지의 외부양자효율과 흡수를 증가시킬 수 있었다. 이 연구를 통해서 금속나노입자에 의한 전방 산란효과가 매우 중요하다는 것을 밝혀내었다. 또한, 장파장 영역의 효율을 올리기 위해서 금@은 코어-쉘 구조의 나노큐브(NC) 입자를 제안하였는데, 얇게 코팅된 은 코팅이 산란효과를 올리는데 매우 중요한 역할을 한다는 것을 밝혀내었다. 금@은 코어-쉘 나노큐브가 PEDOT:PSS 층에 삽입되었을때 유기태양전지의 효율을 증대시킨 결과를 보여줄 것이다.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **MAT1-2**

발표분야: Plasmonic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 이기라

Ultrasmall plasmonic lasers

박홍규

고려대학교 물리학과

I present the experimental demonstration of an optically pumped silver-nanopan plasmonic laser with a subwavelength mode volume of 0.56 (lambda/2n)^3. The lasing mode is clearly identified as a whispering-gallery plasmonic mode confined at the bottom of the silver nanopan from measurements of the spectrum, mode image, and polarization state, as well as agreement with numerical simulations. In addition, the significant temperature-dependent lasing threshold of the plasmonic mode contrasts and distinguishes them from optical modes. Our demonstration and understanding of the subwavelength plasmonic lasers represent a significant step toward faster, smaller coherent light sources.

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장소: 광주 김대중컨벤션센터
발표코드: **MAT1-3**
발표분야: Plasmonic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 이기라

Nanogap-Enhanced Raman Spectroscopy (NERS) controlled by DNA

서영덕

한국화학연구원 나노기술융합연구단, 성균관대학교 화학공학부

Since smSERS (single molecule Surface-Enhanced Raman Scattering) was independently reported by S. Nie group and K. Kneipp group in 1997 [1][2], tremendous amount of interest has been shown to this field because Raman spectroscopy can provide molecular fingerprint together with multiplexing capability in bioassay. Regarding to the origin of this smSERS phenomena, so called “SERS hot spot”, Nie group argued sharp edges in nanostructure, such as corners of a silver nanorod or even of a single nanoparticle, can play as a hot spot of smSERS, while Kneipp group argued they could observe smSERS signal only from colloidal aggregation in solution. Later on, Brus group and others showed that SERS hot spots, formed at the junction of two nanoparticles, likely play a major role in smSERS [3][4]. Theoretical calculations also support that SERS electromagnetic enhancement factors can approach up to $\sim 10^{11}$ when inter-particle spacing reaches down to a few nanometer or less at the junction between two nanoparticle pair. However, formation of these smSERS-active nanostructures with a nano-gap at the SERS hot-spot junction, mostly dimer or colloidal aggregation of Ag or Au nanoparticles adsorbed with Raman active molecules (e.g., Rhodamine 6G), is a random process driven by salt-induced non-specific aggregation. This fact has been a main hurdle for smSERS toward advanced applications.Based on the idea that controlling this < 1 nm nanogap between two noble metal nanoparticles is the key to realize reliable smSERS, we have designed a gold-silver nano dumbbell (GSND) and Gold Nanobridged Nanogap Particles (Au-NNP) to exhibit Nanogap-Enhanced Raman Scattering (NERS) controlled by DNA. As for GSND, two gold nano particles with different sizes were linked to each other by double helix DNA (30mer), with a single Raman dye molecule at the center position, to fix the two at a known gap distance (~10 nm). Then we narrowed the gap down to < 1 nm by standard silver staining method to endow the GSND with single molecule sensitivity. We have successfully detected smSERS signals, as well as typical single molecular blinking and polarization behaviors, from each GSNDs by homemade Nano

Raman spectroscopy instrument on the single molecule and single particle level [5-7]. As for Au-NNP, hollow spherical gap (~1 nm) between the gold core and gold shell can be precisely loaded with quantifiable amounts of Raman dyes labeled on DNA backbone which is anchored at the gold core and then covered by gold shell [9].

[1] S. Nie and S.R. Emory, *Science* 275, 1102 (1997).

[2] K. Kneipp, Y. Wang, H. Kneipp, L.T. Perelman, I. Itzkan, R.R. Dasari, and M.S. Feld, *Phys. Rev. Lett.* 78, 1667 (1997).

[3] A.M. Michaels, M. Nirmal, and L.E. Brus, *J. Am. Chem. Soc.* 121, 9932 (1999).

[4] Y.D. Suh, G.K. Schenter, L. Zhu, and H.P. Lu, *Ultramicroscopy* 97, 89 (2003).

[5] D. Lim, K.-S. Jeon, H.M. Kim, J.-M. Nam*, and Y.D. Suh*, *Nature Materials* 9, 60 (2010).

[6] J.-H. Lee, J.-M. Nam*, K.-S. Jeon, D.-K. Lim, H. Kim, S. Kwon,.H. Lee, and Y.D. Suh*, *ACS Nano* 11, 9574 (2012).

[7] H. Lee, J.-H. Lee, S.M. Jin, Y.D. Suh*, and J.-M. Nam*, *Nano Letters*, 13, 6113 (2013).

[8] J.-W. Oh, D.-K. Lim, G.-H. Kim, Y.D. Suh*, and J.-M. Nam*, *J. Am. Chem. Soc.*, in press (2014).

[9] D. Lim, K.-S. Jeon, J.H. Hwang, H.Y. Kim, S.H. Kwon, Y.D. Suh*, and J.-M. Nam*, *Nature Nanotechnology* 6, 452 (2011).

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장소: 광주 김대중컨벤션센터
발표코드: **MAT1-4**
발표분야: Plasmonic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 10:25, 좌장: 박성호

Synthesis of Plasmonic Nanoparticles for Diagnostic Applications

이재승

고려대학교 신소재공학부

Plasmonic nanoparticles exhibit a variety of unique chemical and physical properties, such as distance-dependent intense optical properties and easy fabrication of the surface nature using functional moieties. Conventionally, these plasmonic nanoparticles, when conjugated with DNA (DNA-NPs), can be programmed to assemble reversibly, which has allowed one to build up a number of versatile assay schemes for the colorimetric detection of various targets. Importantly, the interparticle interactions of the DNA-NPs are fundamentally based on (1) the chemical recognition properties of DNA, and (2) the size or shape of the plasmonic nanoparticles. These interesting properties have led to a number of fundamental developments for the assembly formation of the nanoparticles. In addition, new assay schemes utilizing the catalytic properties or shape-dependent optical properties of the plasmonic nanoparticles have been recently reported for the highly sensitive and selective colorimetric detection of physiologically important targets. Based on these properties, the synthesis and diagnostic applications of plasmonic nanoparticles with various sizes, shapes, and materials will be discussed in this presentation.

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Controlled Assembly of Plasmonic Nanoparticles: How-tos and What-to-dos

윤상운

단국대학교 화학과

The assembly of noble metal nanoparticles offers an appealing means to control and enhance the plasmonic properties of nanostructures. Despite their great advantages, however, making nanoassemblies in a controlled fashion with high efficiency remains challenging. In this talk, I will present our recent attempts to assemble nanoparticles into various structures with high yields, including core-satellites, sphere dimers, and sphere-cube dimers.[1,2] The interparticle distance (*d*) in these assemblies is finely tuned at the molecular level using self-assembled monolayers of alkanedithiol linkers. The controlled interparticle distance and ultrahigh purity of the prepared nanoassemblies allow us to investigate the plasmon coupling between the nanoparticles as a function of the gap distance. We find that the plasmon coupling follows the classical electromagnetic model when the nanoparticles are far apart ($d > 1$ nm); however, quantum tunneling effects play a significant role in the plasmonic response of nanoassemblies in the subnanometer gap region.[1-3] I also discuss the applications of nanoassemblies as a plasmon ruler and a surface-enhanced Raman scattering (or fluorescence) substrate.[2,4]

[1] Cha, H.; Yoon, J. H.; Yoon, S. *ACS Nano* 2014, *8*, 8554.
[2] Yoon, J. H.; Lim, J.; Yoon, S. *ACS Nano* 2012, *6*, 7199.
[3] Yoon, J. H.; Zhou, Y.; Blaber, M. G.; Schatz, G. C.; Yoon, S. *J. Phys. Chem. Lett.* 2013, *4*, 1371.
[4] Yoon, J. H.; Yoon, S. *Langmuir* 2013, *29*, 14772.

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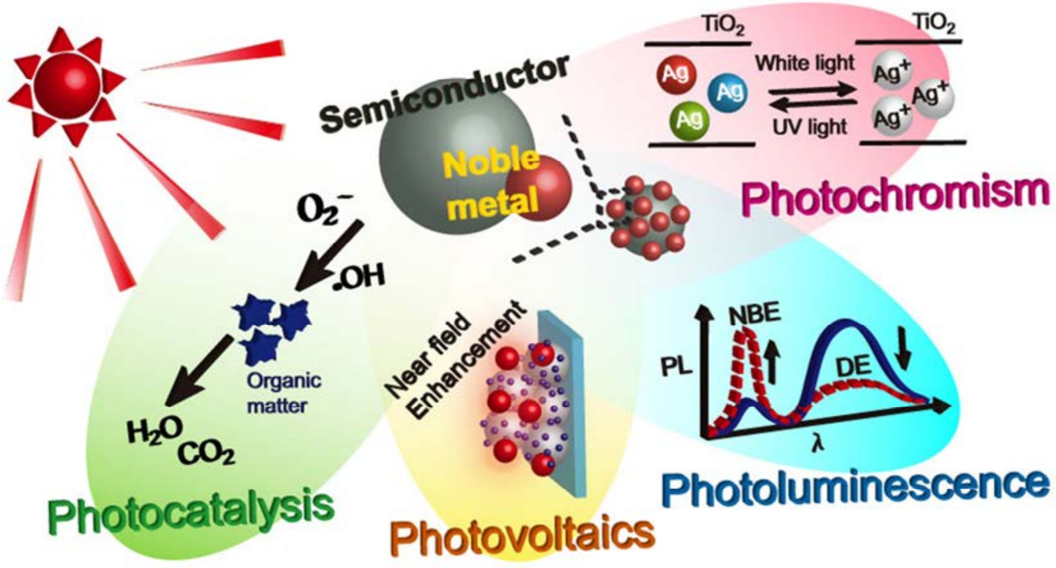
발표종류: 심포지엄, 발표일시: 목 11:15, 좌장: 박성호

Highly Coupled Hybrid Nanomaterials for Plasmonics, with Applications in Energy, Photocatalysis, Sensing and Light Emission

김동하

이화여자대학교 화학나노과학과

In this presentation, a comprehensive approach for the design and synthesis of hybrid plsmonic nanomaterials is discussed to seek their potential applications as key elements in green nano- and bio-technology. Representative subject areas of interest include energy conversion, visible light active photocatalysis, optical (bio-)sensing, and light-emission. Of the numerous methodologies to develop useful nanomaterials for diverse applications, we pay special attention to surface plasmons as a versatile platform based on which target-oriented properties can be obtained by integrating plasmonic nanostructures into the elements of optical (bio-)sensors, photovoltaic devices, photocatalysts, and light-emitting materials. Our recent activities with a special focus on the synthesis and applications of active nanomaterials for highly selective/sensitive sensing, plasmonic dye-sensitized solar cells, visible light active photocatalysis for solar fuel generation, and enhanced optical properties of multi-component fluorophores.


Semiconductor
Noble metal
TiO_2
Ag
White light
UV light
Ag^+
Photochromism
O_2^-
.OH
Organic matter
H_2O
CO_2
Near field Enhancement
NBE
PL
DE
λ
Photocatalysis
Photovoltaics
Photoluminescence

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Graphene-Coated Gold Nanoparticles for Enhanced Photothermal Effect, Highly Sensitive Bio Imaging Agent, and Efficient Plasmonic Photocatalyst

임동권[*] KumarDinesh[1]

전북대학교 BIN 융합공학과 [1]Chonbuk National Uni BIN Fusion Tech.

Plasmonic nanomaterials have been extensively investigated for highly sensitive in-vitro, in-vivo biosensing and therapeutic applications based on the tunable optical properties in the visible and NIR region of light as well as the biocompatibility, colloidal stability, and straightforward chemistry on gold nanoparticles. Varieties of plasmonic nanostructures such as gold nanorod, nanoshell, and nanocage were developed for the therapeutic applications because of excellent light absorption properties in NIR region and subsequent strong photothermal effect. Since the hyperthermia-based anticancer therapy with gold nanoshell (AuNS) is already in the clinical trial stages to treat lung cancer patients, the photothermal effect of plasmonic nanoparticle would be of great interests for the future cancer therapy. Achieving improved light absorption properties is one of important issues in this area, because the nanomaterial with strong photothermal effect can greatly reduce the effective dose of light-absorbing agents and power density of NIR light required for the stimulation of the light-absorbing agents. For this reason, new types of plasmonic hybrid materials have been widely investigated to obtain improved photothermal effect. In this talk, I would like to introduce new type of plasmonic hybrid material investigated for improved photothermal effect, which is useful property for hyperthermia-based photothermal therapy and excellent imaging agent for photoacoustic imaging technology. The synthetic method, underlying mechanism, and applications for improved hyperthermia-based therapy and sensitive photoacoustic imaging will also be discussed including the photocatalytic activity of plasmonic nanoparticles for visible-light induced preparation of reduced graphene oxide.

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발표분야: Advanced Energy Materials
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Nanostructured Carbon-Based Non-Precious Metal Electrocatalysts for the Oxygen Reduction Reaction

주상훈* 천재영[1] 사영진[1] 서보라[1]

울산과학기술대학교(UNIST) 에너지화학공학부 [1]울산과학기술대학교(UNIST) 화학과

Polymer electrolyte fuel cells (PEFCs) have long been considered promising energy conversion devices, owing to their high energy conversion efficiency and environmental benignity. In PEFCs, tremendous recent efforts have been devoted to replacing expensive, scarce Pt-based electrocatalysts with non-precious metal or metal-free materials for the oxygen reduction reaction (ORR). In this talk, we present two examples of new electrocatalysts based on nanoporous/nanostructured carbons, which are desinged to exhibit very high ORR activity as well as long-term durability: transition metal-doped ordered mesoporous porphyrinic carbon (M-OMPC) catalyst [1] and carbon nanotube cores and heteroatom-doped carbon sheath layer (CNT/HDC) catalyst [2]. We also present our efforts to identify critical factors that govern the ORR activity in metal-free, heteroatom-doped nanocarbon catalysts [3]. [1] J. Y. Cheon et al., *Scientific Reports* 3, 2715 (2013).[2] Y. J. Sa, et al., *Angew. Chem. Int. Ed.* 53, 4102 (2014).[3] J. Y. Cheon, et al., *J. Am. Chem. Soc.* 136, 8875 (2014).

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발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 방진호

Rational design of highly active nanocatalysts by understanding nanoparticle reactivity and metastability

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 of our group to improve the catalytic activity of nanoparticles and their implications for future research.

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발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 방진호

Strategy Toward Artificial Photosynthesis

강영수

서강대학교 화학과

In this talk, the basic concept and fabrication technology for the nanodevices for artificial photosynthesis were introduced. Based on the solvothermal and hydrothermal synthesis and alignment of the photocatalytic nanocrystals and its assembled nano-sized monolayers of photocatalytic materials, vectorial electron transport from the higher conduction band energy to lower conduction band energy could be accelerated by suppressing the defect and optimizing the electron transport distance and diffusion capacity. The fabrication of the photocatalysts was done to get the largest exposed surface area of the most photoactive facets for nanocrystals of TiO_2, Cu_2O, α-Fe_2O_3 and ZnO. Especially, α-Fe_2O_3 nanocrystal assembled monolayer fabrication for the visible light sensitive layer on FTO and the measurement of the photocurrent density are the basic approach for the artificial photosynthesis through water splitting and CO_2 reduction. For the efficient electron transport through the TiO_2 nanotubes, $SrTiO_3$, Fe_2O_3, Cu_2O were filled into the pores of the TiO_2 nanotubes and photocurrent was measured.

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발표코드: **MAT2-4**
발표분야: Advanced Energy Materials
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 주상훈

Artificial Photosynthesis: Photocatalytic Conversion of CO2 into Hydrocarbon Fuels

인수일

대구경북과학기술원(DGIST) 에너지 시스템 공학 전공

Photoreduction of CO_2 into hydrocarbon fuels on the surface of photocatalyst is one of the breakthroughs in the field of photocatalysis. At present various approaches have been investigated with the aim of increasing the CO_2 conversion efficiency. The reactor for photoconversion of CO2 plays a vital role in experimental setup. In this work an attempt was made to testify a newly designed the photoreactor for conversion of CO_2 into useful products. The photoreactor was specifically designed for simple operation bearing features of temperature and pressure control.[1] Columnar Cu nanostructures with tunable lengths are formed directly on porous TiO_2 by oblique-angle electron beam evaporation and used as a cocatalyst for photocatalytic conversion of CO_2 to methane. A remarkable enhancement in methane production rate is measured using the sculptured copper films with a maximum of 124.3 ppm · cm^{-2} ·h^{-1} for 160 nm long Cu columnar structures under AM 1.5 illumination. This high methane production rate is attributed to a plasmonic enhancement effect due to the columnar Cu nanostructures.[2][1]Rapid Communicationin Photoscience, 2013, 2, 64-66.[2]Thin Solid Films, 2014, 565, 105-110.

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장소: 광주 김대중컨벤션센터

발표코드: **MAT2-5**

발표분야: Advanced Energy Materials

발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 주상훈

Syntheses of compound semiconductors for thin film solar cells

정덕영* 차지현

성균관대학교 화학과

Chalcopyrite Cu(In,Ga)(S/Se)$_2$ has been promising materials for highly efficient thin film solar cells. However, vacuum-based processes for making of these absorber layers raise cost and technical limitation on the fabrication of photovoltaic devices. We report the non-vacuum syntheses of precursor materials for CIGS absorber layers: the syntheses of copper-gallium bimetallic nanoparticles and core-shell particles of Ga@CuS by ultrasound-assisted chemical reduction method in alcohol solutions to prepare CuGaS$_2$ thin films. A liquid gallium emulsion was prepared as a starting material using ultrasound treatment in ethylene glycol. The chemical reduction of copper sulfate into copper metal by NaBH$_4$ at the surface of the Ga droplets enabled the formation of Ga-Cu core-shell structure. The Ga droplets with submicrometer size were homogenously coated with ~40nm Cu nanoparticles. The exothermic transition of the Ga-Cu core-shell nanocomposite materials occurred below 500°C, which corresponds to the crystalline phase formation of Cu$_9$Ga$_4$. Ga-Cu nanocomposites with a 1:1 ratio were deposited onto molybdenum substrate via electrophoretic deposition method as a precursor of CuGaS$_2$, a p-type semiconductor. The core and shell of Ga@CuS products were composed of amorphous gallium metal and covellite phase CuS, which transformed into chalcopyrite CuGaS$_2$ hollow spheres after sulfurization at 450°C, which was the lowest crystallization temperature. The formation of hollow nanostructures was ascribed to the Kirkendall mechanism, in which liquid gallium particles play an important role as reactive templates.

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발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 주상훈

Tailoring of TiO2 Nanostructures for Several Mesoscopic Solar Cells

이완인

인하대학교 화학과

Monodispersed nanoporous TiO2 spheres were synthesized by controlled hydrolysis of titanium tetraisopropoxide (TTIP) and subsequent hydrothermal treatment. Diameters of the TiO2 spheres were selectively controlled in the range of 100?1,000 nm. The sizes of sphere were inversely proportional to the ratio of TTIP to water during the hydrolysis reaction. The prepared TiO2 spheres, in the pure anatase phase with a crystallite size of ~15 nm, were highly porous structures with the surface areas of 110?125 m2g-1 and pore diameter of 10-15 nm. In this work, the prepared TiO2 spheres were successfully applied as photoanode of dye-sensitized solar cells (DSSCs) and quantum dot sensitized solar cells (QDSSCs). In application to DSSCs, Jsc of 17.8 mA/cm2, a Voc of 845 mV, a FF of 70.4%, and a PCE of 10.54% were obtained under one sun light intensity at AM 1.5G condition. PbS quantum dot-sensitized solar cells (QDSCs) with photovoltaic conversion efficiency of 5.73% has also been fabricated by applying nanoporous TiO2 spheres as photoanode. 100 nm-sized TiO2 spheres were also successfully applied for the perovskite-based solid-state solar cells, suggesting that the assembled TiO2 structure is highly useful material for the QDSSCs or solid-state solar cells. For the application to Co-electrolyte based DSSC, average nanopore sizes of TiO2 spheres were enlarged to from 15 nm to 35 nm. It was found that the TiO2 spheres with 35 nm-sized internal pores provide significantly enhanced photovoltaic properties than the commercial nanoparticles. It was also found that nanoporous spherical TiO2 structures are an essential material for the fabrication of photoanode of the flexible DSSCs.

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발표코드: **ELEC1-1**
발표분야: Symposium for Young Electrochemists
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 박준희

New Insight into Copper Sulfide Electrocatalysts for Quantum Dot-Sensitized Solar Cells

김청수 방진호*

한양대학교 응용화학과

Despite recent significant strides in understanding various processes in quantum dot-sensitized solar cells (QDSSCs), little is known about the intrinsic electrocatalytic properties of copper sulfides that are the most commonly employed electrocatalyst for the counter electrode of QDSSCs. Given that the physical properties of copper sulfides are governed by their stoichiometry, the electrocatalytic activity of copper sulfides toward polysulfide reduction may also be dictated by their compositions. Using a new, simple approach to prepare robust copper sulfide films based on chemical bath deposition, we were able to delicately control the compositions of copper sulfides, which allowed us to perform a systematic investigation to gain new insight into copper sulfide-based electrocatalysts. The electrocatalytic activity is indeed dependent on the compositions of copper sulfides, and Cu-deficient films (CuS and Cu1.12S) are superior to Cu-rich films (Cu1.75S and Cu1.8S). In addition, the stability of the Cu-deficient electrocatalysts was substantially better than that of the Cu-rich counterparts.

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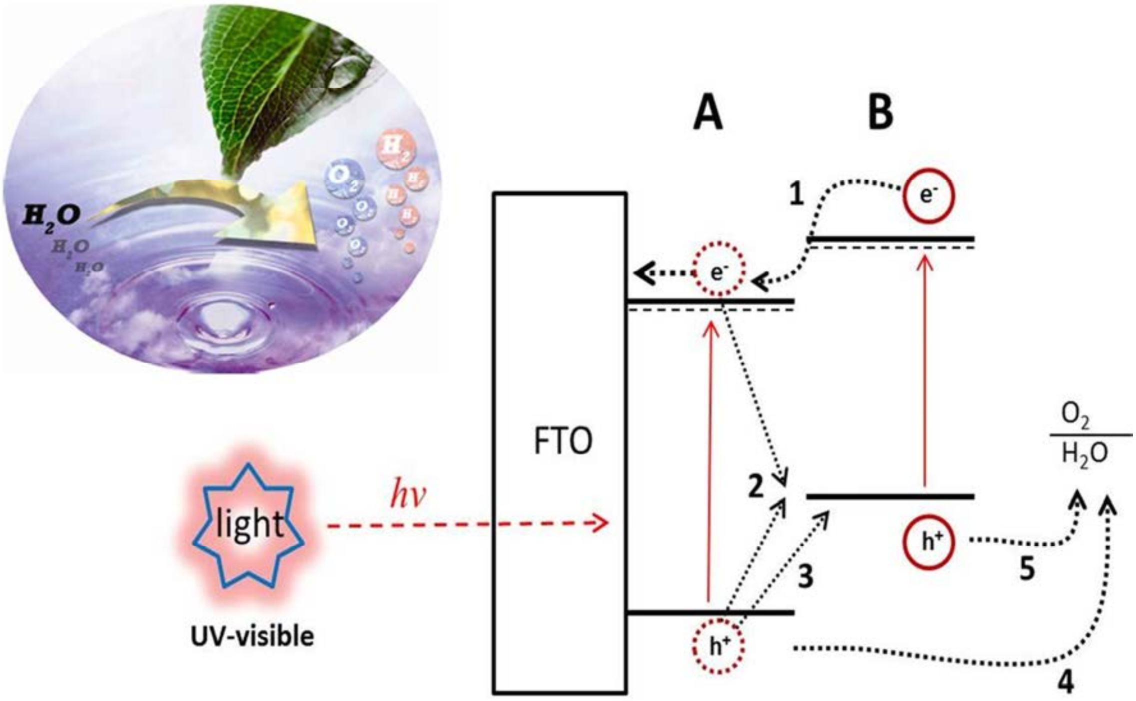
Metal Oxide Composites for Photoelectrochemical Water Splitting

남기민

목포대학교 화학과

Artificial photosynthetic systems are promising approaches to convert sunlight into chemical fuels.The most popular strategy is photoelectrochemical (PEC) water splitting to produce hydrogen sustainably.Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary semiconductor that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through the composite. These composite structures are divided into four different configurations depending on the possible electron-hole separation mechanism. These systems elucidate the effect of conduction and valence band positions of the individual components of composite materials. Finally, we demonstrate and discuss a prospective method for the discovery of new composite photocatalysts based on scanning electrochemical microscopy (SECM) techniques.


H2O
H2O
H2O
O2
H2
A
B
1
e-
FTO
e-
2
3
h+
h+
4
5
O2
H2O
light
hv
UV-visible

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발표코드: **ELEC1-3**

발표분야: Symposium for Young Electrochemists

발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 박준희

Cyclic Voltammetric Study of the Transport of Ionic Species through Three-Dimensional Pore Structures of Mesoporous Zirconia Films

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The transport of ions and molecules in confined nanopores is one of the fundamental studies in many potential fields such as energy conversion devices, membranes for molecular separations, electrochemical sensors, and biological detection. Recent advances in nanotechnology allow us to fabricate the nanopores and their arrays for transporting and analyzing target species. One of them is the film type of mesoporous materials with a uniform pore size, serving as a nanofluidic system for transported species. Here, we modified the electrode surface with mesoporous zirconia films (MZFs) and used them for studying transport behavior of ionic species. The films' pore structures were identified by two distinct ones with the *Fmmm* structure and the $P6_3/mmc$ structure, characterized by grazing incidence small-angle X-ray scattering, electron microscopy, and N_2 sorption measurement.The transport study was carried out with cyclic voltammetry. Ferricyanide anion was chosen as the target species because of its simple one-electron transfer reaction, being easy to analyze behavior changes. To study the transport of the ions in the MZFs, we changed two experimental parameters, the concentration of electrolyte solution and the solution pH value, affecting pore wall-ion interactions. We found that those two parameters could influence the shape of cyclic voltammograms and the position of the formal reduction potential, which means that the transport behavior was changed. Our results demonstrate that the transport of ions inside the pores could be modulated and be distinguished from that on the non-porous electrode surface. Therefore, it is expected to provide comprehensive insights into transport behavior of confined fluid.

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장소: 광주 김대중컨벤션센터

발표코드: **ELEC1-4**

발표분야: Symposium for Young Electrochemists

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 박준희

Dye Stabilization and Performance Enhancement in Dye-Sensitized Solar Cells through Post-Assembly, Atomic Layer Deposition of Metal Oxides (TiO2, Al2O3, and SiO2)

손호진

고려대학교 신소재화학과

Recombination at the TiO2/electrolyte interface, detachment (desorption) of molecular dyes from photo-electrodes, and detachment (desorption) of molecular dyes from photo-electrodes are the major limitations for the operation of dye-sensitized solar cells (DSCs). Here we demonstrate a method to greatly inhibit these losses by growing transparent metal oxides (TiO2, Al2O3, and SiO2) on the dye-coated photo-electrode via atomic layer deposition (ALD) or cross-linking beween metal precusors. The post-metal oxide coating covers the highly convoluted surface of the TiO2 conformally and with a uniform thickness throughout the thousands of layers of nanoparticles. The subsequent coverage by metal oxides could provide a means to not only efficiently reduce the intermolecular interaction of dyes, but also to retard the interfacial charge recombination dynamics. DSCs incorporating these selective and self-aligned metal-oxide layers achieved a 30-40% increase in relative efficiency versus control uncoated cells. A detailed photophysical study using time-resolved fluorescence (TRF) spectroscopy is used to obtain a better understanding of the mechanism by which the post ALD treatment alters the performance of DSSCs. Additionally, the TiO2-enshrouded sensitizers largely resist detachment, even in pH 10.7 ethanol, a standard solution for intentional removal of molecular dyes from photo-electrode surfaces. The ALD post-treatment renders the otherwise hydrophobic dye-coated surface hydrophilic, thereby enhancing photo-electrode pore filling with aqueous solution. When subsequently operated in water, the ALD-treated DSC yielded a 42% increase in relative efficiency versus an untreated cell, with the improvement coming chiefly from increased photocurrent.

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발표코드: **ELEC1-5**

발표분야: Symposium for Young Electrochemists

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 박준희

전기화학법을 이용한 진성, 불순물 실리콘 반도체 성장

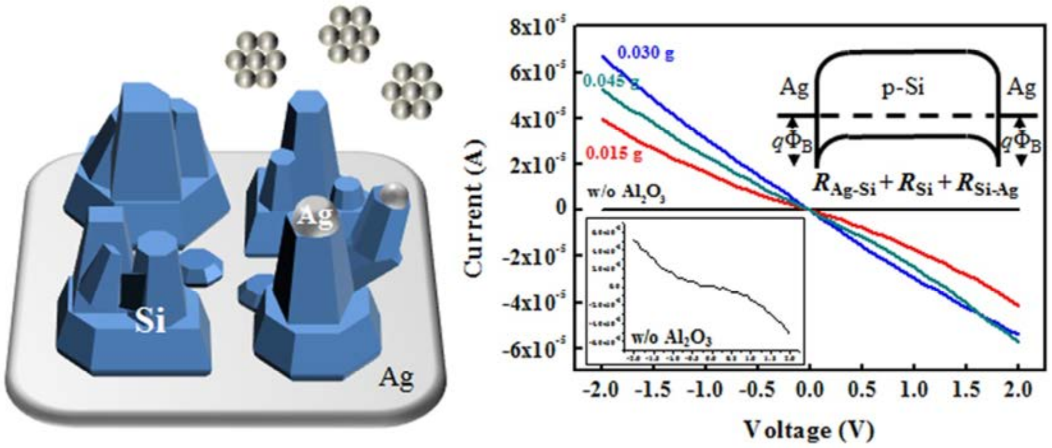
(Electrochemical Growth of Intrinsic and Extrinsic Silicon Semiconductor)

조성기

금오공과대학교 에너지화학공학과

현재 전자 산업 분야에서 Si 은 MOS transistor 기반 Microprocessor 와 태양전지 두 분야에서의 핵심 소재로써 매우 중요하게 이용되고 있다. Si 이 반도체 소자에 적용될 수 있었던 가장 큰 특징으로 도핑 (Doping) 을 들 수 있다. 즉, Si 결정 내에 소량 (ppm level) 의 제 2 원소 주입을 통해 전기적 특성 변화가 가능하며, 이 때문에 하나의 Si 물질상에 다양한 전자 회로 성분을 구현할 수 있게 되었다. 물론 이를 위해선 기본적으로 고순도의 Si 이용이 필수적이다. 그로 인해 고순도 Si 은 높은 원료 가격을 나타내며, 이는 이후 제품 가격에도 영향을 미치고 있다.현재 고순도 반도체 Si 은 Czochralski 법, Chemical Vapor Deposition 등 소수의 공정에 의해 형성되고 있으며, 도핑은 Si 성장 중 도핑 원료를 함께 넣거나, 개별적인 diffusion, implantation 공정을 의해서 수행되고 있다. 여기서 언급된 공정 모두 많은 에너지를 소모하며, 극한 환경에서의 매우 높은 수준의 공정 제어가 요구된다. 본 연구에서는 고순도 Si 의 전기화학적 형성 뿐만 아니라 동시에 도핑 조절을 통해 intrinsic Si 또는, extrinsic Si 형성을 조절할 수 있는 도금법을 소개한다. 전기화학적 실리콘 성장은 고온 용융염상에 분산된 고체상 나노 SiO2 입자를 직접 환원시켜 이루어진다. 도핑의 경우, 전기화학적 환원 동안에 제 2 의 산화물을 추가해 동시적 환원을 일으키고, 이를 통해 doping level 이 조절된 extrinsic Si 을 얻는다. Nanoprobe 를 이용해 성장된 Si 의 전도성을 측정한 경우, 도핑 원료를 추가하지 않은 경우 높은 비저항을 나타내었으며, 이를 바탕으로 형성된 Si 이 intrinsic 조건에 가까운 것을 확인할 수 있었다. 반면, 도핑 원료를 추가함에 따라 전도성이 점차 증가하는 것을 알 수 있었으며, 측정된 전도성으로부터 doping level 를 유추할 수 있었다. Mott-Schottky plot 분석을 통해서도 전기화학적으로 형성된 Si 이 도핑

되었음을 확인할 수 있었으며, 측정된 doping density 도 앞서 언급한 전도성 측정 결과와 일치하였다. 뿐만 아니라, 도핑 원료 선택에 의해 성장된 Si 의 극성 (n-type 또는 p-type) 또한 조절할 수 있음을 photoelectrochemical analysis 상 광산화반응 및 광환원반응 관찰을 통해서 확인할 수 있었다. 최종적으로, 전기화학법을 이용해 형성된 n-type Si 의 경우, single crystalline Si 대비 최대 40% 의 광반응성을 내었으며, 이를 바탕으로 전기화학적으로 성장된 Si 의 태양 전지 소재로써의 높은 적용 가능성을 확인하였다.



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장소: 광주 김대중컨벤션센터
발표코드: **ELEC1-6**
발표분야: Symposium for Young Electrochemists
발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 박준희

Li-Air Battery: Beyond Geometrical Optimization

이홍찬

삼성종합기술원 Energy Lab

Detailed physical and electrochemical understanding of a Li-air battery system is a prerequisite to design optimized cell geometry and to achieve a system close to its theoretical capacity, 3000 Wh/kg. Here, finite element models of the Li-air battery cathode were constructed and analyzed by the COMSOL multi-physics with electrodeposition module. This meso-scale model includes dynamic electrodeposition of reaction products, Li_2O_2, with electron tunneling effect that dominates the limitation of the cell capacity in cathodes less than 80 μm thick. Good agreement in trends between the simulation results and experimental values validates the model. The simulation results suggest the ranges of optimized dimensions for the optimized performance in the discharge capacity. The cells with void structures were also simulated and informed that voids in the cathode could be helpful for cathodes thicker than 80 μm.

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발표코드: **ELEC2-1**

발표분야: Electrochemistry for Energy Conversion

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이호춘

Highly rechargeable Li-O2 battery

강기석

서울대학교 재료공학부

The lithium?oxygen battery has the potential to deliver extremely high energy densities; however, the practical use of Li-O2 batteries has been restricted because of their poor cyclability and low energy efficiency. In this work, we report a novel Li-O2 battery with high reversibility and good energy efficiency using a soluble catalyst combined with a hierarchical nanoporous air electrode. Through the porous three-dimensional network of the air electrode, not only lithium ions and oxygen but also soluble catalysts can be rapidly transported, enabling ultra-efficient electrode reactions and significantly enhanced catalytic activity. The novel Li-O2 battery, combining an ideal air electrode and a soluble catalyst, can deliver a high reversible capacity (1000 mAhg_1) up to 900 cycles with reduced polarization (about 0.25 V).

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발표코드: **ELEC2-2**
발표분야: Electrochemistry for Energy Conversion
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이호춘

Electrochemical intercalation of divalent magnesium and zinc ions into transition metal compounds for post Li ion batteries

홍승태

대구경북과학기술원(DGIST) 에너지시스템공학

Li ion batteries (LIB) are one of the most successful energy storage devices for portable electronics application, electrical vehicles, and utility grids. However, there are still strong needs for higher energy density and lower price materials than what the LIB systems can provide. A rechargeable battery utilizing intercalation of divalent ions such as Mg^{2+} and Zn^{2+} could be one of the good strategies to overcome capacity limit of LIB, and to produce lower price batteries. However, only a few materials have been reported for the electrode materials that can intercalate multivalent ions reversibly. Mg rechargeable batteries have received attention since the reversible Mg intercalation into the Chevrel phase, Mo_6S_8, was demonstrated in 2000. Environmental friendliness and plentiful sources of the magnesium are typical advantages of Mg material over the lithium. Zinc ion batteries can be environmentally friendly, reliable, safe, and particularly low-cost power sources. In this symposium, some recent progress in exploration of electrochemical intercalation of divalent magnesium and zinc ions into various transition metal compounds will be presented, utilizing aqueous electrolytes as well as non-aqueous electrolytes.

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발표코드: **ELEC2-3**
발표분야: Electrochemistry for Energy Conversion
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이호춘

Aqueous Lithium-Iodine Battery

변혜령

Byon Initiative Research Unit, RIKEN, Japan

Higher energy density and cycling efficiency are required for the next generation of batteries. Iodine is an attractive material towards the high energy density battery thanks to its high theoretical energy density of ~0.74 kWh/kg and 3.7 kWh/L. However, due to the nature of low ionic conductivity of solid lithium iodide, the primary lithium-iodine (Li-I2) batteries can only support for extremely low current rate applications such as a pacemaker. To improve rechargeability and rate capability, we have proposed aqueous cathode with a triiodide/iodide (I3-/I-) redox couple to construct a low-cost, non-flammable, and environmentally friendly Li-I2 battery. The aqueous cathode can contain high concentration of I3-/I- redox couple using I2 and I- ion, which are transformed to I3- in an aqueous medium (I2(s) + I- ↔ I3-, K (equilibrium constant) = 723). The electrochemical reaction of this I3-/I- redox couple in the aqueous cathode leads the total cell reaction of Li-I2 battery: 2Li + I3- ↔ 2Li+ + 3I-. This aqueous Li-I2 battery demonstrates high storage capacity (~98% of the theoretical capacity), Coulombic efficiency (>99.5%) and cycling performance (>99.5% capacity retention for 100 cycles), which are thus far one of the highest performance among current Li-I2 batteries, aqueous cathode batteries, and lithium-ion batteries using aqueous electrolyte. In addition, high solubility of the I3-/I- redox couple and appropriate operating potential (~3.5 V vs. Li+/Li and ~0.5 V vs. SHE) but avoiding the electrolysis of water offer a high energy density of ~0.33 kWh/kg. This energy density can be further improved when equipped with a flow device and aqueous electrolyte reservoir, which allows the aqueous Li-I2 battery to be grid-scale flow battery applications.

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발표코드: **ELEC2-4**

발표분야: Electrochemistry for Energy Conversion

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 이재준

Electrochemical Monolayer Approach for Photoelectrochemical Hydrogen Production

황성필

고려대학교 신소재화학과

Pt monolayer decorated gold nanostructured film on planar p-type silicon is applied for photoelectrochemical H2 generation in this work. First, gold nanostructured film on silicon was spontaneously produced by galvanic displacement of the reduction of gold ion and the oxidation of silicon in the presence of fluoride anion. Second, underpotential deposition (UPD) of copper under illumination produced Cu monolayer on gold nanostructured film followed by galvJavaScript:Register();anic exchange of less-noble Cu monolayer with more-noble PtCl62?. Pt(shell)/Au(core) on p-type silicon showed the similar activity with platinum nanoparticle on silicon for photoelectrochemical hydrogen evolution reaction in spite of low platinum loading. From Tafel analysis, Pt(shell)/Au(core) electrocatalyst shows the higher area-specific activity than platinum nanoparticle on silicon demonstrating the significant role of underlying gold for charge transfer reaction from silicon to H^+ through platinum catalyst.

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발표코드: **ELEC2-5**
발표분야: Electrochemistry for Energy Conversion
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 이재준

Methodologies for High Efficiency Perovskite Solar Cells

박남규

성균관대학교 화학공학부

Perovskite solar cell based on organolead halide has been considered as a promising photovoltaic technology due to its superb power conversion efficiency. In this talk, methodologies for perovskite solar cells with power conversion efficiency (PCE) exceeding 17% are presented. The first version of long-term durable perovskite solar cell was developed by Park’s group in 2012, which demonstrated 9.7%. In 2013, PCE of 15% was achieved by Gratzel and Snaith groups. But, the average PCE was as low as 12%. Deposition method was found to be critical to high efficiency devices. Crystal size of methylammonium lead iodide perovskite was controlled by changing the precursor solution concentration in two-step coating procedure. Photovoltaic performance increased significantly with size mainly due to higher photocurrent and fill factor. Photo-CELIV measurements confirmed that amount of the extracted charge increased with size. The highest PCE of 17% was achieved along with average value of more than 16%. Substitution of formamidinium for methylammonium led to phase-transition-free perovskite, which resulted in PCE of 16% and average PCE of 15.5% with better photostability and negligible I-V hysteresis.

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발표코드: **EDEC-1**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 강석진

과학교사의 수업전문성 향상을 위한 멘토링 연구

남정희

부산대학교 화학교육과

이 연구는 과학교사의 수업 전문성 신장을 목표로 현행 교사교육 프로그램들의 실태를 파악하고 이에 대한 문제점들을 추출하여 멘토-멘티 간의 상호작용을 강조한 협력적 멘토링 프로그램을 개발하고, 새로 개발된 협력적 멘토링 프로그램의 효과를 검증한 후 지역 교육청과의 연계를 통해 학교 현장에 지속적으로 확대 적용하는 멘토링 시스템을 구축하는 것을 목적으로 하였다. 이 연구를 통해서 과학교사의 수업전문성 향상을 위한 협력적 멘토링 프로그램을 개발하였고, 지역교육청과의 MOU 협약을 통해 3 년 동안 지속적으로 과학교사의 수업전문성 향상을 위한 멘토링 연수를 진행하면서 대학의 연구결과가 어떻게 현장과 연결될 수 있는지를 보여준다. 이러한 결과를 바탕으로 초임과학교사 뿐만 아니라 경력교사들의 수업전문성 향상을 기대할 수 있으며 이는 궁극적으로 학생들의 학습의 향상을 가져올 것이라 기대한다.

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발표코드: **EDEC-2**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 강석진

STEAM 교육과 융합 교육

김현경[*] 이양락[1] 심재호[2]

한국교육과정평가원 교육평가본부 [1]한국교육과정평가원 수능본부 [2]부산대학교 생물교육과

1990 년대에 미국과학재단(NSF)은 “science, mathematics, engineering, and technology”를 줄여서 “SMET” 사용하기 시작하였고 NSF 프로그램 관리자로 인해 “STEM” 약어가 탄생하였다(Sanders, 2009). 거의 20 여년 동안 NSF 는 STEM 을 과학, 기술, 공학 및 수학의 4 개의 독립된 분야를 지칭하는 것으로 사용해왔다. 그러나 4 개의 글자를 하나로 묶는 것 이상이어야 한다고 주장하는 Sanders(2008)는 “STEM Education” 대신에 “Integrative STEM Education”을 주장하였다. 그 후 주로 산업의 경쟁력 차원에서 창의적인 인력 양성에서 예술이 과학 못지않게 중요하기 때문에 STEM 에 Arts 가 포함되어야 한다며 STEAM 교육이 주장되었다(Tarnoff, 2010). 그러나 STEAM 교육에 대한 관점과 인식의 스펙트럼이 매우 다양함에도 불구하고 이에 대한 정의 또는 합의된 관점 없이 국내외에서 이를 교육과정, 교수학습, 학생 평가에 도입하려는 다양한 시도들이 진행되고 있다. 특히 우리나라에서는 창조경제란 용어가 등장하기 이전부터 융합 연구의 필요성이 산업현장에서 이미 널리 인식이 되어 왔으나 이제는 이러한 융합 담론이 교육에까지 확대되어 융합 교육이 화두가 되고 있다. 이에 본 연구는 STEAM 교육이 무엇이고, 융합 교육은 무엇인지와 또한 왜 STEAM 교육과 융합 교육을 주장하는지에 대해 살펴보고, STEAM 교육과 융합 교육의 연구 사례들에 대해 발표하고자 한다. 이를 통해 우리나라에서 STEAM 교육과 융합 교육은 합의된 것인지, 우리의 과학 교육과정에 바로 접목될 수 있는지, 과학 교육과정에 도입할 경우 어떤 문제를 해소해야 할 것인지를 논의하고자 한다. 또한 초?중등학교 교육에서 창의?융합 인재 양성을 위한 융합 교육의 가능성에 대해 다양한 사례와 쟁점 및 방향에 대해 논의하고자 한다.

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발표코드: **EDEC-3**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 강석진

STEAM의 융합적 문제해결력의 개념적 정의 및 초·중등학생들의 융합적 문제해결력의 특징 조사

박현주 심재호[1,*]

조선대학교 과학교육학부 [1]부산대학교 생물교육과

이 연구는 STEAM 의 융합적 문제해결력을 개념적으로 정의하고, 그에 따른 문항을 개발하여 초·중등학생들의 융합적 문제해결력의 특징을 조사하는 것으로 목적으로 하였다. 문헌 및 선행 연구를 통해, 과학적 문제해결과 융합적 문제해결을 설계기반의 공학의 본성에 따라 차별화하였다. 그리고 융합적 문제해결력을 '해결하고자 하는 내용이 과학·기술과 밀접하게 관련된 문제이면서 실생활 상황에 기초하고 있으며, 해결 과정이 열려 있는 상태이고, 이를 해결하기 위해 과학의 개념 및 탐구뿐만 아니라 공학적 개념과 실행을 활용할 수 있으며, 이 과정에 분석적, 비판적인 사고, 창의적인 사고, 융합적인 접근을 사용할 수 있는 개인의 능력을 의미하는 것으로 정의하였다. 이러한 정의에 따라 '보행도로 설계'와 '인공연못 설계'의 융합적 문제해결 문항을 개발하여, 초등학생과 중등학생들에게 적용하여, 그 과정에서 나타난 융합적 문제해결력의 특징을 조사하였다.

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발표코드: **ENVR1-1**
발표분야: Development of New Materials for Enhancing Energy Conversion and Storage
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 임동희

Solar Fuel and Hybrid Energy System

인수일

대구경북과학기술원(DGIST) 에너지 시스템 공학 전공

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 MoxSy. Prof. Chorkendorff and et al. showed that the bioinspired molecular co-catalysts such as incomplete cubane-like clusters (Mo3S4) 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%. In addition there will be short introduction about Hybrid Energy System which combines solar energy and Microbial Fuel Cell.

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발표코드: **ENVR1-2**
발표분야: Development of New Materials for Enhancing Energy Conversion and Storage
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p-Si nanowire arrays for solar CO_2 conversion

박현웅

경북대학교 에너지공학부

Solar CO2 conversion has attracted increasing attention not only to reduce anthropogenic carbon emissions but also to convert CO2 to renewable and recyclable chemical fuels. Despite the scientific interest, industrial importance, and even socioeconomic attention, the solar CO2 conversion technology progresses very slowly over the past four decades, particularly because of the limited number of suitable photoelectrodes. Si is one of the most appropriate electrodes because it is an earth abundant element with a narrow band gap of ~ 1.1 eV, high carrier mobility, stability over a wide pH range, non-toxicity, well-established fabrication technique, and commercial availability. Although planar p-Si is promising, charge carrier recombination can occur due mainly to the low diffusion length of the minority carriers in the same absorber thickness. A wire-array geometry, however, possesses long optical paths for efficient photon absorption as well as a higher collection efficiency for the minority carrier. To the best of our knowledge, this is the first report of the fabrication of Sn-coupled p-Si nanowire arrays for solar CO2 conversion. Vertically aligned, free standing p-Si nanowire arrays of varying lengths were grown on p-Si wafers, and coupled with Sn nanoparticles. These heterojunction wire/Sn arrays increased the production of formate dramatically, by more than 10 and 5 times compared to planar p-Si and wire arrays, respectively, with Faradaic efficiencies of ~ 40% in a single cell (88% in an H-type cell). This research was financially supported by the Basic Science Research Program (No. 2012R1A2A2A01004517) and the Framework of International Cooperation Program (No. 2013K2A1A2052901) through the National Research Foundation (NRF), Korea.

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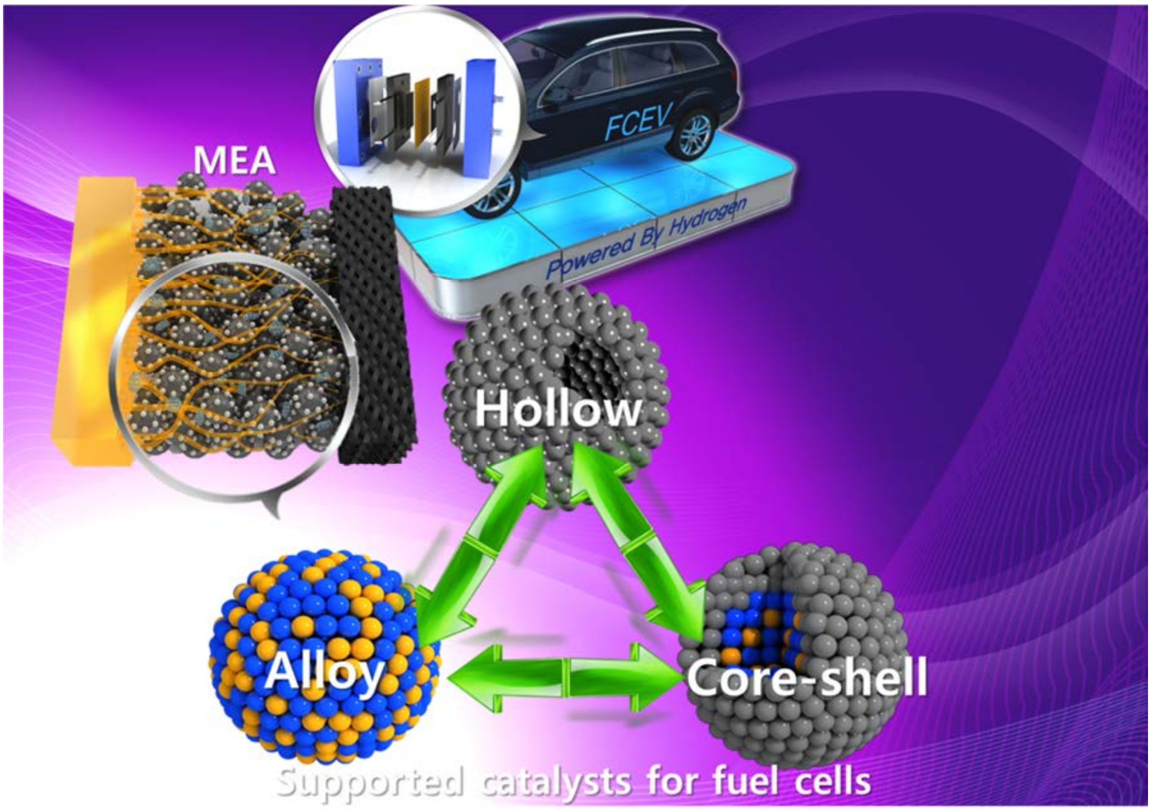
발표코드: **ENVR1-3**
발표분야: Development of New Materials for Enhancing Energy Conversion and Storage
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 임동희

Nanoarchitecture and catalyst designs for fuel cell applications

유성종

한국과학기술연구원(KIST) 연료전지센터

Polymer electrolyte membrane fuel cells (PEMFCs) are promising energy conversion devices, because they can directly convert chemical fuels to electricity with high efficiency, and they are clean. The most important component of a PEMFC is the membrane electrode assembly (MEA), which generates electricity through electrochemical processes, namely the hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR), occurring in the anode and cathode, respectively. The catalyst in the MEA is particularly important in maximizing the fuel cell efficiency. These technical improvements have resulted in PEMFC catalysts suitable for use in commercially available electrochemical energy conversion devices. At this stage, it is necessary to consolidate recent progress in the development of catalysts for PEMFCs. In addition, by examining recent progress in catalyst development, research directions for developing new catalyst concepts in the future can be established. In this symposium, we focus on Pt-based nanocatalysts and support materials with multistructures; they are classified according to their structures and compositions. The nanocatalyst category includes metal alloys, and core-shell and hollow structures. Various carbons (carbon blacks, CNTs, CNFs, and graphenes) and metal oxides are extensively explored as support materials. Although PEMFC reactions include the HOR at the anode as well as the ORR at the cathode, we mainly discuss physical and electrochemical meanings of the nanoarchitectured catalysts and support materials for the ORR, because the ORR is a critical obstacle to high PEMFC performance.


MEA
FCEV
Powered By Hydrogen
Hollow
Alloy
Core-shell
Supported catalysts for fuel cells

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발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 유성종

Universality in Surface Mixing Rule of Adsorption Strength for Small Adsorbates on Binary Transition Metal Alloys

한정우

서울시립대학교 화학공학과

Understanding the adsorption phenomena of small adsorbates that involve in a surface reaction on transition metals is important because their adsorption strength can be descriptors for predicting the catalytic activity. Although density functional theory (DFT) is a fast and economic method to calculate the adsorption energy, tremendous computational efforts are still required to explore it on a wide range of binary transition metal alloys. Using DFT calculations, here we suggest “surface mixing rule” to predict the adsorption energies of H, O, S, CO and OH on binary transition metal alloys, based on the linear interpolation of adsorption energies on each pure surface. We also demonstrate that the 1st layer d-band center of binary transition metal alloys can be predicted from the weighted average of 1st layer d-band center of each pure metal. This can be thought of as an origin of theoretical framework for the surface mixing rule of adsorption energy. As an application, we predict the activity of CO oxidation on bimetallic alloys from the adsorption energies of CO and O easily obtained by the surface mixing rule. Our results provide a useful tool for rapidly estimating the adsorption energies, and furthermore, the catalytic activities on multi-component metal alloy surfaces.

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Nanostructured Elelctrode for Solar to Fuel Production

황윤정

한국과학기술연구원(KIST) 청정에너지 연구센터

태양광 에너지는 그 양이 방대하여 전인류가 사용가능한 앞으로의 신재생에너지원으로 각광받고 있고, 전기에너지로 전환하는 태양전지의 개발이 많이 이루어졌다. 그러나 저장의 문제를 고려하면, 태양광에너지를 직접 화학적 에너지로 변환하여 연료를 생산하는 기술이 매우 유망하다. 아직까지는 촉매와 시스템 개발 연구가 원천 기술 개발 단계로 태양광 연료 전환 효율이 낮다. 대표적인 태양광 연료 전환 반응으로는 물을 분해하여 수소를 생산하는 반응과 이산화탄소를 환원하여 탄소 기반 연료를 생산하는 반응등이 있다. 낮은 태양광 연료 전환 효율을 높이기 위해서는 첫단계로 반도체 물질이 효율적으로 태양광을 잘 흡수 할 수 있어야 하며, 빛의 흡수로 인해 생성된 전하가 분리되어 광전자와 정공이 전극 표면에서 효과적인 촉매반응에 사용될 수 있어야 한다. 태양광의 흡수와 생성된 전하의 분리는 광전극 물질의 개발이 필요하며 특히 가시광 영역의 빛을 잘 활용할 수 있도록 적합한 밴드갭을 가지는 물질의 개발이 중요하다. 또한 일차원 나노구조체가 되면 빛의 흡수와 전화분리에 유리하다는 연구 결과들이 보고 되고 있다. 전극의 표면이 나노구조를 가지면 화학적 산화, 환원 반응이 일어나는 활성자리도 증가할 것으로 기대되므로, 촉매적 특성도 증가될 것으로 기대가 된다. 여기서는 전극 표면의 나노 구조화를 통해서 광전기화학적, 혹은 전기화학적 산화, 환원 촉매 반응의 활성이 증가될 수 있음을 보이고자 한다. 특히, 물분해 광산화 전극의 개발에 있어서, 두가지 서로 다른 반도체 물질을 연결한 (예, WO3/BiVO4, Si/TiO2, Si/InGaN) 이종접합 전극은 각 물질의 나노 형상 제어를 통해 광산화 촉매 활성이 크게 향상될 수 있음을 확인할 수 있었다. 뿐만아니라, 이산화탄소 환원 촉매 전극의 개발에 있어서도 표면의 나노 구조화가 과전압을 줄이고, 선택적 환원 반응에 어떻게 영향을 끼칠 수 있는지에 대해서 논의하고자 한다.

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발표코드: **ENVR2-1**
발표분야: Advances in Solar Fuel Production: Materials and Systems
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 오지훈

Bioinspired Carbon based Catalyst for Hydrogen Evolution Reaction

심욱 남기태*

서울대학교 재료공학부

Hydrogen production by water splitting reaction has especially been widely studied as an environmentally friendly and sustainable energy source. Realization of cost-effective hydrogen production by water splitting requires electrolysis or photoelectrochemical cells decorated with highly efficient co-catalysts. A critical requirement for outstanding catalysts in the photoelectrochemical cell is not only the ability to boost the kinetics of a chemical reaction but also durability against electrochemical and photoinduced degradation. In the race to replace previous noble metal catalyst, the design of carbon-based catalysts can represent an important research direction in the search for non-precious, environmentally benign, and corrosion resistant catalysts. Here, inspired by biomolecular system, we suggest biomimetic carbon based catalysts as a new hydrogen evolution catalyst for photoelectrochemical cell system. A variety of chemical doping processes also generate active sites for hydrogen evolution reaction in carbon based catalysts and these active sites boost their catalytic activity with controllability. Additionally, carbon based catalysts show the passivation effect that suppress the surface oxidation of the photoelectrode, thus enabling the operation of photoelectrode in an aqueous solution. This study shows how the catalysts itself can be applied to photoelectrochemical system as a catalyst with high activity and chemical stability.

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발표분야: Advances in Solar Fuel Production: Materials and Systems

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 오지훈

Development of Bi-based oxide photoanodes using electrodeposition method for solar water splitting

박이슬

대구경북과학기술원(DGIST) 에너지연구부

Development of efficient and practical photoelectrodes for solar energy conversion involves simultaneously satisfying multiple requirements, which remains a challenge. The photoelectrode must absorb visible light, preferably with a direct bandgap transition, and then efficiently separate and utilize the photogenerated carriers to drive desired reactions. In addition, it is important to develop simple and low-cost methods for electrode preparation. One promising photoanode material is bismuth vanadate ($BiVO_4$), an n-type semiconductor with a direct bandgap of 2.4 eV and the appropriate valence band position for O_2 evolution. Its conduction band edge position and flat band potential are fairly negative compared with most other narrow bandgap oxide-based photoanode materials, located just short of the thermodynamic level for H. As a result, complete water splitting with $BiVO_4$ requires only a small amount of external bias. In this study, new electrodeposition route is proposed to produce n-type $BiVO_4$, Mo-doped $BiVO_4$ and other Bi-based oxide (Bi_2WO_6, $Bi_2Mo_6O_{12}$) as well. Electrodeposition has the distinctive advantages of being simple, low cost, and easily scalable while enabling deposition of the material of interest only on the conductive substrate and not on the chamber wall. Various photoelectrochemical properties of Bi-based oxide photoanodes were investigated.

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발표코드: **ENVR2-3**

발표분야: Advances in Solar Fuel Production: Materials and Systems

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 오지훈

Embedding covalency into metal catalysts for efficient electrochemical conversion of CO_2

김형준

한국과학기술원(KAIST) EEWS대학원

CO_2 conversion is an essential technology to develop a sustainable carbon economy for the present and the future. Many studies have focused extensively on the electrochemical conversion of CO_2 into various useful chemicals, which can be eventually coupled with photovoltaic systems towards solar fuel generation. However, there is not yet a solution sufficiently high enough efficiency and stability to demonstrate practical applicability. In this talk, we use high-throughput quantum mechanics (QM) catalyst screening (coupled with continuum description of solvation effects) to discover new catalysts expected improve the performance of the electrochemical CO_2-to-CO conversion by decreasing the overpotential by 0.4-0.5 V. We discovered the covalency-aided electrochemical reaction (CAER) mechanism has a major effect on the modulating reaction energetics, thereby enhancing their catalytic activity. We expect this work to provide useful insights to guide the development of a feasible strategy to overcome the limitations of current technology for electrochemical CO_2 conversion.

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발표코드: **ENVR2-4**
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발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김형준

Nanotextured PEC cells for highly efficient solar-to-hydrogen conversion

이민형

경희대학교 응용화학과

Hydrogen production using photoelectrochemical (PEC) water splitting has gotten great attention as a sustainable and clean ways to convert solar energy to hydrogen energy. However, PEC water splitting is still far from achieving high solar-to-hydrogen efficiency because of several challenges including low absorption of visible light, photo corrosion of PEC cells, and high overpotentials of water splitting. In this talk, we report recent approaches performed in our lab to overcome the challenges and to achieve high-efficiency PEC water splitting. Especially, we focused on developing nano-textured semiconductors to achieve both high current density and a favorable onset potential. We also present various approaches to improve hydrogen evolution reaction by modifying PEC cells with co-catalyst.

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발표분야: Advances in Solar Fuel Production: Materials and Systems
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Efficient and Stable Silicon-based Solar Water Splitting Devices

오지훈

한국과학기술원(KAIST) EEWS

Hydrogen production by solar water splitting has attracted considerable interests as a long-term energy storage system (ESS) to store intermittent solar energy to stable and reusable chemical fuels. In this talk, I’ll present our resent efforts to develop a silicon-based solar water splitting devices, leveraging the existing Si photovoltaic technology. Particularly, I’ll talk about black Si anti-reflection technology to improve hydrogen production rate. In addition, I’ll present our novel strategy for enhanced stability for O_2 evolution reaction which provides electrons for proton reduction reaction during water splitting reaction. Finally, I’ll also present our new device structures based on an integrated Si based water splitting cell for unassisted solar water splitting reaction.

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장소: 광주 김대중컨벤션센터

발표코드: **KCS1-1**

발표분야: [산학심포지엄] 신약개발의 미래지향적 방향: 화학과 생명과학의 융합연구

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 민선준

한국 제약산업 발전을 위한 화학계의 역할

이경호 회장

(사)한국제약협회

미정

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **KCS1-2**

발표분야: [산학심포지엄] 신약개발의 미래지향적 방향: 화학과 생명과학의 융합연구

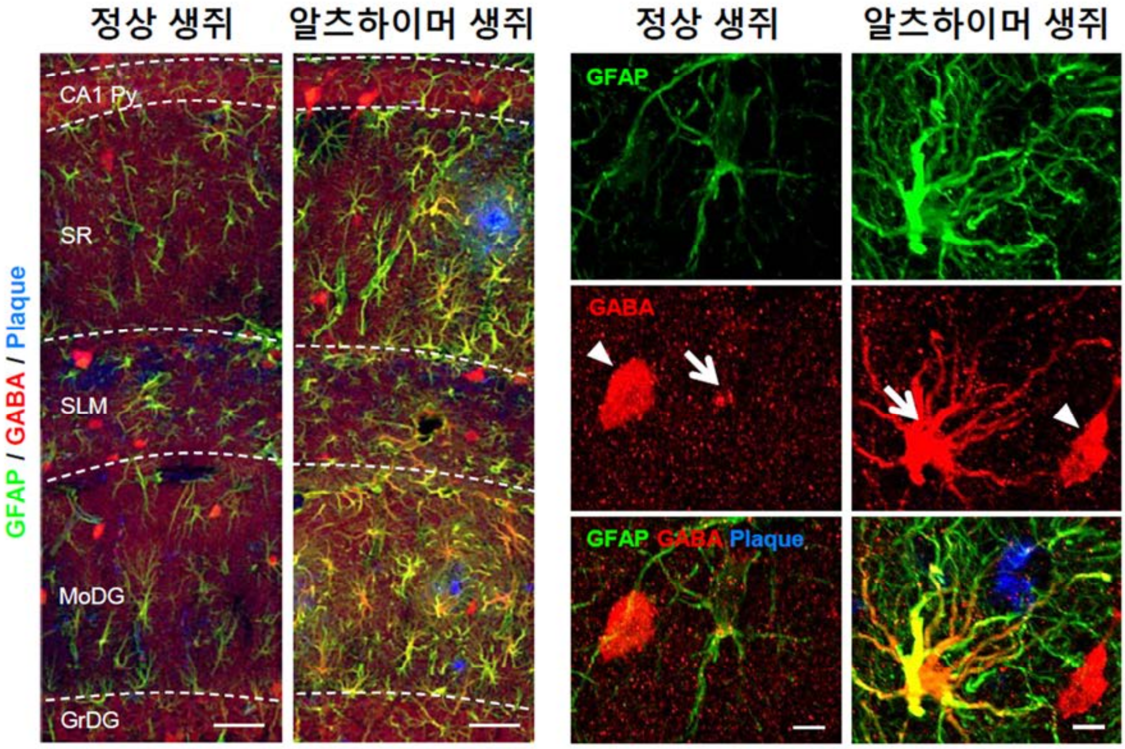
발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 민선준

Glia-targeted drug development for neurodegenerative diseases

<u>이창준</u>

한국과학기술연구원(KIST) 기능커넥토믹스연구단

Traditionally, neurocentric research has been the focus of drug develpment in neurodegenerative diseases. However, recent advances in glia research has led us to re-evaluate the traditional approach. I will present the latest findings of GABA from reactive astrocytes as the cause of memory impairment in Alzheimer's disease and then discuss the potential therapeutic value of such novel findings.



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장소: 광주 김대중컨벤션센터
발표코드: **KCS1-3**
발표분야: [산학심포지엄] 신약개발의 미래지향적 방향: 화학과 생명과학의 융합연구
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 민선준

Molecular Modeling and Computer-Aided Drug Design (CADD) and their Applications in Drug Discovery

최선

이화여자대학교 약학대학

Drug discovery is highly technology-intensive and interdisciplinary process which integrates the various scientific fields such as chemistry, biology, pharmacology, pharmaceutics, and computational sciences. This process is very time- and resources-consuming; therefore, it would be very beneficial to find efficient ways to reduce the cost. Molecular modeling and Computer-Aided Drug Design (CADD) are the interdisciplinary fields which could accelerate the entire drug discovery process and save time, money, and efforts. They are playing more and more important roles in various fields of drug discovery with the increasing information of the small molecules and biomacromolecules. It has been utilized throughout the entire steps of drug discovery including target identification, target validation, lead discovery, lead optimization, and in silico ADME/Tox prediction. This talk will cover our recent applications for drug design and discovery of therapeutically important enzyme, GPCR, and ion channel based on the integrated state-of-the-art technologies. In addition to the drug design and data analysis using target-structure based drug design, ligand-based design, and cheminformatics, applications of novel approaches will be presented such as multiple receptor conformations and network analysis of the protein structures.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **KCS1-4**
발표분야: [산학심포지엄] 신약개발의 미래지향적 방향: 화학과 생명과학의 융합연구
발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: 허정녕

Development of DA-7218(Tedizolid), a Next-Generation Oxazolidinone

임원빈

동아제약(주) 신약연구소

The oxazolidinones represent a novel chemical class of synthetic antimicrobial agents. DA-7218 (Tedizolid) is a second generation oxazolidinone antibacterial prodrug. It is a potent inhibitor of Gram-positive bacterial pathogens such as methicillin-resistant Staphylococccus aureus, penicillin-resistant Streptococcus pneumoniae and vancomycin-resistant Enterococcus spp. DA-7218 is also active against pathogens that have developed resistance to first generation oxazolidinones such as linezolid-resistant S. aureus and linezolid-resistant Enterococcus spp. With a long half-life, high bioavailability and solubility and high potency, DA-7218 will provide clinicians with flexible dosing and a possible shorter course of therapy thereby enabling the early transition of hospitalized patients from IV to oral treatment and subsequent early discharge from the hospital. Tedizolid had successfully completed Phase I ,Phase II and Phase III clinical trials. Sivextro(Tedizolid) has been approved by the FDA on June 20, 2014 for the treatment of acute bacterial skin and skin structure infections (ABSSSI) caused by Gram-positive bacteria. In this presentation, overall progress of the development of DA-7218 will be discussed.

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발표코드: **KCS1-5**
발표분야: [산학심포지엄] 신약개발의 미래지향적 방향: 화학과 생명과학의 융합연구
발표종류: 심포지엄, 발표일시: 금 12:40, 좌장: 허정녕

성공적인 임상연구를 위한 바람직한 비임상연구

김달현

(주)종근당 효종연구소

약으로 허가를 받으려면 다양한 임상 시험을 거친다. 이러한 다양한 임상 시험을 하는 도중에 많은 신약후보물질들이 약효의 미흡, 약동학적인 문제, 부작용의 발생 등으로 시장에 진출하지 못한 채 의약품 개발 트랙에서 사라진다. 임상 시험 도중 약물 개발 실패는 제약사나 이 의약품을 개발하는 많은 연구자 및 허가 당국에 이르기까지 많은 손실과 충격을 준다. 따라서 임상 시험을 성공적으로 이끄는 것은 매우 중요한 일이다. 임상 시험을 성공적으로 이끌기 위해서는 제대로 된 임상 프로토콜이 필수적이라는 것은 말할 필요도 없을 것이다. 이에 못지않게 중요한 것이 완성도가 높은 비임상시험이다. 이러한 비임상시험을 통해 제대로 된 임상프로토콜이 완성되고, 임상 시험에 진입할 수 없는 물질을 조기에 탈락 시킬 수 있기 때문이다.

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장소: 광주 김대중컨벤션센터
발표코드: **KCS2-1**
발표분야: The Secrets of Scientific Publishing
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 하현준

The Secrets of Publishing Success

Richard Threlfall

Managing Editor, Asian Journal of Organic Chemistry

This talk answers some of the most commonly asked questions and also reveals some of the less obvious, but nevertheless important, aspects of publishing scientific papers. As well as what really happens when an editor first receives your paper, I'll discuss the psychology of referees and the concept of "novelty", as well as how an overly complicated writing style might lead to bad reviews. In this context, there will be a step-by-step guide to simplifying your writing and showing your readers the most critical parts of your work concisely. Additionally, I'll examine the idea of "discoverability", that is, how you can write your paper to maximize the chances of people finding it online and in databases, and how what happens to your paper online after publication can be just as important as what happens before. This insider view from the editorial office will help you understand how the publishing process really works and how you can apply this knowledge to get the best outcome for your own papers.

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발표코드: **POLY.O-1**
발표분야: New Trends in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 윤명한

A Benzodithiophene-Based Novel Electron Transport Material for a Highly Efficient Polymer Solar Cell

김홍일 신원석[1] 박태호*

포항공과대학교(POSTECH) 화학공학과 [1]한국화학연구원 에너지소재연구센터

We designed and synthesized a novel conjugated polyelectrolyte (CPE), poly{3-[2-[4,8-Bis-(2-ethyl-hexyloxy)-6-methyl-1,5-dithia-s-indacen-2-yl]-9-(3-dimethylamino-propyl)-7-methyl-9H-fluoren-9-yl]-propyl}-dimethyl-amine (PBN). We employed PBN as an electron-transporting layer on a ZnO layer and constructed a highly efficient, inverted structure device consisting of a mixture of poly({4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b′]dithiophene-2,6-diyl}{3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl}) (PTB7) and PC70BM, achieving a high power conversion of up to 8.6%, constituting a 21.1% improvement over the control device performance (7.1%) prepared without a PBN layer. This result was ascribed to the reduced interfacial resistance and the improved charge transport and collection through the PBN electron transport layer.

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발표코드: **POLY.O-2**
발표분야: New Trends in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 윤명한

Adjustable Peptoid Helices: Minute Control of Peptoid Secondary Structures via Position-Specific Placement of Chiral Monomers

신혜민 서지원[1,*] 윤명한[*]

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

Natural molecules such as proteins, nucleic acids and carbohydrates have specific functions, which are mainly originated from their 3D structures. Hence, many biomimetic molecules such as artificial peptides and peptoids are being investigated to fold into specific secondary structures. Peptoids, oligo-N-substitute glycines, have achirality of backbone and lack of hydrogen bond donors, so difficult to form secondary structures like α-helical structure. Yet, peptoid structures such as α-helix, threaded-loop, beta-sheet and cyclic peptoid have been discovered, which peptoid have specific side-chains to complement peptoid backbone. Peptoids with α-chiral, aromatic side-chains form stable polyproline-like helices in both organic and aqueous solutions. Even though, there is still lack of understanding on the precise control of peptoid structures that lie in between fully helical and unstructured. To expand functional applications of peptoid helices, it is desirable to access more minutely controlled peptoid structures and to understand further the underlying sequence-structure relationship. In this study, we report the structural role of each monomer position collected from 30 comprehensive model peptoid oligomers demonstrating a meticulous manner to fine-tune peptoid secondary structures. We observed that the degree of peptoid helicitiy can be effectively adjustable by incorporation of α-chiral aromatic monomers in position-specific placement. These results will be the foundation of peptoids’ sequence-structure relationships.

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발표코드: **POLY.O-3**
발표분야: New Trends in Polymer Chemistry
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Plasmonic Coupling via Gold/Stimuli-responsive Polymer Hybrid Nanostructures Monitored by Surface Plasmon Resonance Spectroscopy

이지은 김동하*

이화여자대학교 화학나노과학과

Noble metal nanostructures coupled with responsive polymers can be used to probe unique plasmonic properties associated with swelling-shrinking transitions in polymer chains triggered by a specific external stimulus. The phase transition causes changes in the refractive index in the vicinity of the particle surface and induces concurrent changes in the characteristic inter-particle distance. The use of gold nanoparticles (Au NPs) for signal amplification has obtained significantly improved sensitivity in surface plasmon resonance (SPR) sensing. These structures are especially interesting for biological and optical sensing, catalysis and various specialized photonic and electronic devices.Here, we developed a plasmonic-coupling-based sensing device consisting of Au nanoparticles separated from the Au substrate in Kretschmann configuration SPR spectroscopy through a thermo-responsive polymer linker layer. Concretely, the disulfide initiator was immobilized on the surface of Au film. Subsequently, surface initiated atom transfer radical polymerization (SI?ATRP) of N?isopropylacrylamide (NIPAM) was performed on Au film. Next, azidation and click chemistry were performed with propargylamin to generate amine functionality at the other end of the chains. Finally, Au NPs were immobilized using citrate-capped Au NPs, leading to the construction of Au film-PNIPAM-Au NPs assembly. The areal density of the anchored Au NPs was controlled by varying the deposition time of modified Au substrates into the Au NPs colloidal solution. The optical properties of these stimuli-responsive devices were investigated by both in-situ and static SPR analysis.

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발표분야: New Trends in Polymer Chemistry
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Encapsulation of Corrosssion Inhibitors by Urea Formaldehyde (UF) Microcapsules for Enhancing the Anticorrosive Property of Acrylic Based PU Smart Coatings

GITEVIKAS 이호익 이정욱 고재형[1] 유정주 **RAVI MARATHE**[2] **PRAMOD MAHULIKAR**[3] 손대원[*]

한양대학교 화학과 [1]한양대학교 고분자 물리화학 연구실 [2]Department of Polymer Chemistry, School of Chemical Sciences, North Maharashtra University, Jalgaon, India [3]School of Chemical Sciences, North Maharashtra University, Jalgaon, India

Two corrosion inhibitors viz. 2-marcaptobenzimidazole and 2-marcapatobenzothiozole were encapsulated in urea formaldehyde polymeric microcapsules. Enacapsulated inhibitors were added to acrylic polyol based polyurethanes to check effect on corrossion. Microcapsules were characterized for morphology, size and thermal stabilty by FE-SEM, particle size analyzer and TGA respectively. The release rate of inhibitors from microcapsule shell was investigated by UV spectrophotometrically. The anticorrosive study of polyurethane coatings incroporated with microcapsules containing inhibitors was investigated by Tafel plot method, immersion study and FESEM of corrosive panels. The results of corrossion study displayed that presence of encapsulated corrosion inhibition enhanced efficiency of acrylic based PU coatings.

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발표분야: New Trends in Polymer Chemistry
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Scalable and Reusable Polypyrrole Nanocoatings for Highly Efficient Mercury Ion Removal

HanifZahid 윤명한* 홍석원*

광주과학기술원(GIST) 신소재공학부

Mercury is one of the most toxic heavy metals found in various industrial wastes and natural water and its removal from the contaminated water in an effective and economic manner at a practically large scale has been an issue. Herein, we report polypyrrole (PPy)-based nanocoatings fabricated on the various forms of cellulose (i.e., paper and cotton fabric) via an environmentally friendly and cost-effective vapor-phase polymerization. The resultant PPy-cellulose composite exhibits the stable adhesion and mechanical durability in both water and strong acid, and the capability of efficiently removing mercury with a specific adsorption capacity of 2.76 mmol Hg/g PPy and chromium ions either as a suspended adsorbent or a dripper-type membrane within a practically short time scale at the large dynamic range of pH.

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The effect of Flory-Huggins interaction parameter (χ) on the self-assembled patterns of block copolymers containing poly(dimethylsiloxane) (PDMS)

허윤형 정재원 정연식*

한국과학기술원(KAIST) 신소재공학과

The inherent feature-size limitations of optical lithography and the low throughput of electron-beam lithography have demanded the development of practical nanoscale fabrication methods. Directed self-assembly (DSA) based on block copolymers (BCPs) enables a simple, cost-effective, and scalable nanopatterning with a great advantage of good compatibility with optical lithography, which will significantly reduce facility investment cost. Important features of self-assembled pattern from the microphase separation of BCPs are largely determined by the Flory-Huggins interaction parameter (χ), such as the order-to-disorder transition temperature, interfacial width, periodicity, and chain mobility. For example, the equilibrium domain spacing (L), which determines the period, has a dependence on the χ parameter and the degree of polymerization (N), L ~ N2/3 * χ1/6.In this work, we demonstrated the effect of χ parameter on self-assembled patterns of BCPs. First, we selected poly(dimethylsiloxane) (PDMS) as one of two blocks of BCPs to increase etching selectivity because Si moiety can be converted to silica (SiOx) in oxygen plasma process. Second, we varied the other blocks to control the χ parameters and characterized the BCPs synthesized via radical polymerization using 1H-NMR, FT-IR and SEC. The BCPs are then annealed to self-assemble into well-ordered cylinders with 10 - 25 nm feature size. Finally, we investigated the relation between χ and size and quality (line edge roughness and line width roughness) of self-assembled pattern using the scanning electron microscopy (SEM).

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In situ modulation of the vertical distribution in a bulk heterojunction solar cell via the addition of a composition gradient inducer

김관우 이강영 김홍일 박태호*

포항공과대학교(POSTECH) 화학공학과

Bulk heterojunction (BHJ) polymer solar cells (PSCs) became one of the most promising options for alternative energy sources. Especially, organic photovoltaic cells (OPVs) have attracted much interest due to their high possibility for solution processing and flexibility. In OPVs, a large interfacial area and vertically aligned charge pathways should be achieved for high efficiency. A BHJ with above characteristics might be constructed by tuning the interactions between donor and acceptor in a mixed solution. Such interactions could be controlled via the small amount of additives which can selectively interact with donor or acceptor and tune the surface energy of each material. Here, two additives, one is 2,2,3,3,4,4,4-heptafluoro-N-phenyl-butyr-amide (F-ADD) and the other is tetrabromothiophene (Br-ADD), which could selectively interact with donor or acceptor were used to increase the efficiency of bulk heterojunction OPVs. This kind of approach might open the road for general additives which could be applied to various polymers.

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Sulfonated Poly(arylene ether) Membranes containing Perfluorocyclobutyl and Ethynyl groups: Increased Mechanical Strength through Chain Extension and Crosslinking

이수빈 이재석[1,*]

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

Novel extendable and crosslinkable sulfonated poly(arylene ether) copolymers (ESHQx-CMy) were synthesized. These copolymers utilized 4-[trifluorovinyl(oxy)]phenol (TFP) as a linker to extend the polymer and provide better elongation at break and mechanical strength. The extension moiety was successfully synthesized and introduced at the chain end of the sulfonated poly(arylene ether) copolymers to induce a strong interaction of the copolymer while maintaining its flexibility. The extension and crosslinking reactions were performed by thermal curing at 200 °C, and confirmed by FT-IR and chemical resistance testing. The synthesized copolymers (ESHQx-CMy) possessed reasonable thermal and chemical stability. In addition, the elongation at break was improved to 14.2%, with a higher tensile strength (73.6 MPa) than other sulfonated poly(arylene ether) copolymers containing only a crosslinked moiety (CM). Importantly, these novel copolymers also displayed the highest proton conductivity (0.145 S/cm) than Nafion 212 (0.093 S/cm) at room temperature.

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발표코드: **POLY.O-9**
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Characterization Techniques for Thin Polyamide Layer of TFC RO Membrane Prepared via Interfacial Polymerization

박상희 백경열*

한국과학기술연구원(KIST) 물질구조제어연구단

The polyamide-based reverse osmosis (RO) membrane is generally developed on UF membrane via interfacial polymerization is a well-known technique using two kinds of immiscible monomers, MPD and TMC. It is difficult to control the performance of obtained RO membrane because of the random reaction forming the cross-linked polyamide layer on porous ultrafiltration (UF) membrane. Also, the ultrathin polyamide layer (~ 100 nm) is too thin to analyze the physical and chemical properties of the layer by conventional techniques. We need to develop the new technique for obtaining the correct results with the exact interpretation. Here, we demonstrated that a variety of polyamide-based membranes including various performances were prepared with difference concentrations of monomers. SEM analysis was used to confirm the surface morphology of TFC RO membranes, and AFM analysis was used to obtain the surface area and thickness of the polyamide selective layer. Contact angle analysis was also carried out to confirm the water wettability of the polyamide selective layer. The mechanical properties of the polyamide selective layer were measured by nanoindenter equipped with a Berkovich diamond tip. Water flux and salt rejection of TFC RO membranes were measured under 16 bar at 25℃ using cross-flow type test equipment.

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발표코드: **POLY.O-10**
발표분야: New Trends in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 11:50, 좌장: 윤명한

Bistable Reversible Electrochemical Mirrors with Polymeric Electrolyte

박치현 서석재 김은경*

연세대학교 화공생명공학과

An ordinary silver mirror, coated on its back surface with silver, reflects light to produce high quality of images by reflection, owing to the high reflectivity of silver. Recently, tunable mirrors, including liquid-liquid interfacial mirrors started to gather attentions by its high applicability for smart windows, light modulators, and chemical sensors. On the other hands, reversible electrochemical mirrors (REMs) are designed to modulate their reflectance, from a highly reflective state enough to mirror a subject to a highly transparent state, according to external stimuli such as electricity, light, or heat. A number of REMs have been suggested, however, none reached widespread practical application because of critical problems such as the poor stability of the mirror state and lack of bistability in reflectance. Thus, there remain very important challenges to realizing switchable silver mirrors with long memory effect to afford bistable reversible electrochemical mirrors (BREMs). Recently, the BREM was invented by our group which used ionic liquids as electrolyte to enhance its bistibility by introducing electric double layer (EDL) into the device. Herein, we report the electro optical properties of BREM and use of polymeric electrolyte to further enhance its performance.

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발표코드: **POLY.O-11**

발표분야: New Trends in Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 윤명한

Reticulated Nanoporous Organic-Inorganic Hybrid Frameworks

전은경 박지웅[1,*]

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

We synthesized the nanoporous organic-inorganic frameworks by heat treatment of solution mixture comprised of urea network (UN) as template and bis(triethoxysiliyl)ethane (BTESE) as organosilica precursor in dimethylformamide (DMF) solvent. The solvent evaporation induced UN gelation in phase separating mixture of UN sol and inorganic precursors produces reticulated nanoporous organic-inorganic frameworks with the highly open and randomly connected pores that are adjusted by varying the compositions and species of inorganic components. The resultant films show unique hybrid structure consisting of organic skeleton and inorganic crust that brings considerable advantages for their application of selective molecular transport. Also, the nanoporous hybrid films can be easily transformed to the porous silica by organics calcination. This work was supported by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean. [20120008889]

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발표코드: **POLY.O-12**
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Well defined all conducting block copolymer layer by photoelectrochemical polymerization for efficient charge collection

송인영 임종철 박태호*

포항공과대학교(POSTECH) 화학공학과

The photoelectrochemical polymerization (PEP) method is one of the ways to prepare polymer networks under mild operation conditions with environmentally benign processes. In addition, PEP polymers could be easily obtained under illumination of visible light at a room temperature, being attracted to many polymerchemists, since Prof. Yanagida firstly reported in 1997. The polymerization is initiated by excited sensitizing molecules after irradiation and propagated from the initiative sites for the formation of a conducting polymer layer. In spite of the easy process of PEP, still the detailed mechanism is not fully understood. Herein, we present the mechanism of PEP by the careful design of experimental conditions to confirm our assumption. Bis-ethylenedioxythiophenes (bis-EDOT) and its derivative were used for the preparation of conducing polymer membranes depending on the desired functionality. Furthermore, bilayered structures of the polymers could be realized by a sequential polymerization of two different monomers, resulted in the selective positioning of each polymer membrane. The layer composition was characterized by several analysis such as SIMS, contact angle measurements, Raman spectrophotometer, and IMPS/IMVS. Finally, we applied various conducting polymer bilayer membranes to photocells consisting of TiO_2 nanocrystalline nanopaticles and ruthenium dyes. A single layer prepared from different monomers and a double layer prepared from the sequential polymerization of two different monomers were successfully introduced to the cells. The comparison of different polymer membranes and their effects on the photovoltaic performances are described by correlating the function of the layer in terms of charge transfer kinetics at the heterojunctions

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Multi-armed Poly(3-hexyl thiophene) Star Polymers by Atom Transfer Radical Polymerization

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Regioregular poly(3-hexyl thiophene) (rr-P3HT) based star polymers were synthesized by a crosslinking reaction of the linear rr-P3HT macroinitiator and ethylene glycol dimethacrylate (EGDMA) crosslinker through Ru-based atom transfer radical polymerization (ATRP). Relatively high molecular weight of the star polymers were obtained, which consisted of large numbers of the rr-P3HT arm chains radiating from the EGDMA based microgel core. The yield of the star polymers were strongly affected by added amount of the EGDMA crosslinker. Well-defined 3 dimensional structured P3HT such as star polymer and branched polymers have been not examined yet although such 3D structures may exhibit changes. We characterized their thermal and morphologies and so on.

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Synthesis and characterization of low bandgapπ-conjugated copolymers incorporating 4,7-bis(3,3'/4,4'-hexylthiophene-2-yl)benzo[c][2,1,3]thiadiazoleunits for photovoltaic application

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4,7-Bis(3,3'/4,4'-hexylthiophene-2-yl)benzo[c][2,1,3]thiadiazoles (HT?BT?HT) were used as building blocks to construct a series of low bandgap π-conjugated copolymers for photovoltaic applications. The desired copolymers were obtained by incorporating the HT?BT?HT comonomers together with donor or acceptor units, such as 3,4-ethylenedioxythiophene (EDOT), bis-EDOT, thieno[3,4-b]pyrazine (TP), and 2,3-dimethyl-TP, via a palladium-catalyzed Stille cross-coupling method. A facile synthetic method has also been developed for the synthesis of several EDOT- and TP-based copolymers via direct C?H arylation of EDOT,bis-EDOT, and TP derivatives using the commercially available catalyst Pd(OAc)2 under Heck-type experimental conditions (Jeffery method). For all of the synthesized copolymers, moving the hexyl side chains of the HT unit in the HT?BT?HT comonomers from 3,3'-positions (close to BT, as in P1?P4) to 4,4'-positions (away from BT, as in P5?P8) led to a significant red shift of the UV-vis absorption spectrum, a decrease of the energy bandgap, an increase of the glass transition temperature, and more promising photovoltaic performances. The thin-film copolymer P7 incorporating TP units (?TP?HT?BT?HT?)n exhibited the most extended absorption (beyond 1000 nm) and the lowest optical bandgap (1.24 eV) among the synthesized copolymers. According to time-dependent density functional theory calculations, the TP unit, in contrast to EDOT, has its lowest unoccupied molecular orbital (LUMO) at the same level as BT. An extended p-conjugation along the TP and BT units leads to low-lying LUMO levels of the resultingcopolymer P7 and in turn its reduced bandgap. The power conversion

efficiencies (PCEs) of organicphotovoltaic devices employing copolymers P1?P8 were measured in the configuration of ITO/PEDOT:PSS/copolymer (P1?P8) : PC60BM (1 : 1 w/w)/Al. Copolymer P7 in particular showed the highest PCE of 3.32%.

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Fabrication of Nanostructured Surfaces and Their Applications

이진석

숙명여자대학교 화학과

Nanotechnology makes it possible to intentionally modify the properties of surfaces and endow them with any desired function. Nanostructured surfaces have represented important advances in control of wetting, adhesion, and mechanical, thermal, magnetic, electrical, and optical properties and ability to direct cell behavior. A number of promising approaches to fabricate functional micro- and nanostructured surfaces have been stimulated by opportunities to enhance the properties of surfaces and interfaces via the combination of surface structure, morphology, and physical and chemical properties. Such functional micro- and nanostructured surfaces are playing an increasingly important part in a broad range of novel applications.In this presentation, I will introduce our recent experimental results based on chemical reactions on solid surfaces, which are fabrications of nanostructured surfaces including vertically aligned Si nanowire arrays, closely packed beads, porous anodic alumina, and anisotropic graphene domains. Also, I will discuss various surface treatment techniques, such as molecular layer deposition and liquid phase deposition, with the aim of improving their surface properties and functional performance, as well as new insights on physical principles underlying their properties and enormous potential applications.

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Inorganic Material@Microporous Organic Network: New Versatile Composites for Energy Storage and Green Technologies

손성욱

성균관대학교 화학과

This presentation will introduce the recent results on the new inorganic-organic composites which consist of the functional inorganic materials and microporous organic networks (MONs). The MON materials can be prepared by organometallic catalysis such as Sonogashira coupling. Various inorganic materials can be coated with the MONs to form the new composites materials. For example, silica materials, MOF, and metal oxides could be coated successfully with the MONs. The silica can be used as a template for the shape controlled synthesis of MON materials. The resultant MON materials can be further utilized for the synthesis of inorganic green catalysts for the removal of pollutants from water. The MON coating on the MOF changed the hydrophilicity of MOF to hydrophobic character of composites. The composites float on the water and can be used as an adsorbent for the removal of organic pollutants on the water. The MON coating on the metal oxides can be carbonized by heat-treatment under inert gas. The resultant carbon-metal oxides showed the enhanced electrochemical performances as anode materials in lithium ion batteries.

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발표분야: Oral Presentation for Young Inorganic Chemists
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Elucidation of Binuclear Non-Heme Iron Enzyme Intermediates

박기영

한국과학기술원(KAIST) 화학과

Binuclear non-heme iron enzymes perform a wide range of chemistries that are essential for aerobic metabolism. This class of enzymes utilizes a coupled diiron cofactor to activate O_2 to form peroxy or high-valent oxygen intermediates that lead to H-atom abstraction, desaturation, hydroxylation, or electrophilic attack. To understand this diverse reactivity of the diiron cofactor, various spectroscopic techniques, such as nuclear resonance vibrational spectroscopy, circular dichroism (CD), magnetic CD (MCD), variable-temperature, variable-field MCD, and resonance Raman spectroscopies, and density functional theory computations have been applied to define key oxygen intermediates. Specifically, two peroxy intermediates, only one of which is poised for O-O bond cleavage, have been structurally defined, and their differences in spectroscopic properties and electrophilic reactivity have been clarified. This understanding of the peroxy-level intermediates is key to elucidating the mechanisms of class Ia ribonucleotide reductase (RR) and soluble methane monooxygenase (MMO), where the peroxy intermediates further convert to reactive high-valent intermediates that abstract an H atom from Tyr in RR and from CH_4 in MMO.

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Molecular Engineering for efficient light harvesting and collection

손호진

고려대학교 신소재화학과

Part 1.The remarkably efficient exciton migration in DA-MOF is attributed to enhanced π-conjugation through the addition of two acetylene moieties in the porphyrin molecule, which leads to greater Q-band absorption intensity and much faster exciton-hopping (energy transfer between adjacent porphyrin struts). The long distance and directional energy migration in DA-MOF suggest promising applications of this compound or related compounds in solar energy conversion schemes as an efficient light-harvesting and energy-transport component. Part 2.Recombination at the TiO2/electrolyte interface, detachment (desorption) of molecular dyes from photo-electrodes, and detachment (desorption) of molecular dyes from photo-electrodes are the major limitations for the operation of dye-sensitized solar cells (DSCs). Herein demonstrated is a method to greatly inhibit these losses by growing transparent metal oxides (TiO2, Al2O3, and SiO2) on the dye-coated photo-electrode via atomic layer deposition (ALD) or cross-linking beween metal precusors. The post-metal oxide coating covers the highly convoluted surface of the TiO2 conformally and with a uniform thickness throughout the thousands of layers of nanoparticles. The subsequent coverage by metal oxides could provide a means to not only efficiently reduce the intermolecular interaction of dyes, but also to retard the interfacial charge recombination dynamics. DSCs incorporating these selective and self-aligned metal-oxide layers achieved a 30-40% increase in relative efficiency versus control uncoated cells. A detailed photophysical study using time-resolved fluorescence (TRF) spectroscopy is used to obtain a better understanding of the mechanism by which the post ALD treatment alters the performance of DSSCs.

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Position controlled synthesis of fullerene crystal for electronic device applications

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포항공과대학교(POSTECH) 화학과

Recently, morphology controlled organic crystals are attracting great interest not only because they exhibit enhanced optoelectronic properties but also because their well-defined crystal facets can be a good model system for fundamental studies. Although most of organic crystals are obtained either in solution or vapor phase crystallization, no general way to control the position of the organic crystals are available in spite of the necessity for further research or practical applications. Here, we present a simple but efficient method to obtain the morphology controlled fullerene crystals at the desired position of solid substrate. By adopting position control technique, we successfully fabricated array form of electronic devices with fullerene crystals. The detailed photo response and transport behavior will be discussed.

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Discovery of an unexpected, tiny molecular entity, N,N-dimethyl-p-phenylenediamine, for redirection of amyloidogenesis

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N,N-Dimethyl-p-phenylenediamine (DMPD; molecular weight (MW) = 136) hasbeen applied as a vital component to various reactions, such as organic synthesis,electrochemical analysis, and antioxidant assay. Although the use of DMPD as anagent for multiple applications has been indicated, the reactivity of such a tiny,monodentate ligand itself toward peptides or proteins has not been expected andstudied to date. Herein, we present the first report on the molecular-level interactionand reactivity of DMPD with the aggregation-prone peptide employing an in vitromodel system containing amyloid-β (Aβ40/Aβ42) peptides and metal ions, as well asbiochemical/biophysical/molecular dynamic simulation approaches. Unexpectedly,the small structural entity, DMPD, is able to redirect misfolding pathways of Aβ intooff-pathway amorphous aggregates. Even in the presence of metal ions (e.g., Cu(II)and Zn(II)), the ability of DMPD to (i) control the formation of Aβ fibrils and (ii)disaggregate preformed Aβ aggregates is noticeably observed to different extents,compared to metal-free analogues. Based on our investigation in living cells,DMPD's activity toward Aβ/metal?Aβ could be linked to prevention of cell deathinduced by Aβ/metal?Aβ. Considering monodenticity of DMPD, the interaction ofthis ligand with Aβ peptides over metal ions is suggested to be more critical for suchredirection of Aβ aggregation. This ligand is able to interact with Aβ favorably (ΔG =-31 kJ/mol, measured by isothermal titration calorimetry), especially the residuestoward hydrophobic C-terminal (observed by 2D SOFAST-HMQC NMR andmolecular dynamic simulation). Moreover, the redox property of DMPD, previouslyreported, could play a role in the interaction and reactivity with Aβ, which wasconfirmed by optical and mass spectrometric studies. Taken together, for the firsttime, our new observations of the molecular action and effect of the tiny, redox-activeligand, DMPD, toward amyloidogenic Aβ peptides demonstrate its unexpectedversatility.

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Improved Isosteric Heat of Hydrogen adsorption in Porous Metal-Organic Framework

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The lack of fossil fuel supplement and climate change by carbon based energy source require an alternative for energy carrier. Hydrogen has an attractive attention to be a promising energy source due to their high energy density and renewability. Even though it has a lot of advantages as a clean energy source, the use of hydrogen is challenging because of a difficulty of safe and efficient hydrogen storage system development. The storage of hydrogen as a solid state is considered more efficient and safe method than pressurized or cryogenic hydrogen.In order to store of H2 as solid state, porous metal-organic frameworks (MOFs) are potential candidate for hydrogen storage material owing to their high porousity, large surface area and tunable functionality. To date, at low temperature and high pressure, H2 storage capacity of MOFs have achieved up to 9 wt%. However, low interaction energy (Qst, < 8 kJmol-1) in MOF, between the frameworks and hydrogen, results in decrease of H2 storage capacity (less than 1 wt%) at room temperature. Therefore, to extend the hydrogen storage performance of MOFs at room temperature, the heat of adsorption for H2 should be enhanced.To improve the heat of adsorption of H2 in MOF, we try to fabricate Mg nanoparticles in MOF as a hybrid material(Mg@SNU-90) and include various cation into the new type of MOF(K+, NH4+ or MV2+⊂SNU-200), respectively. The hybrid material adsorbs hydrogen by both physi- and chemi-sorption with synergistic effects that increase isosteric heat of the H2 in physisorption and decrease the temperatures for chemisorption/desorp. In various cation inclusion into a new type MOF that incorporates a specific binding sites, K+ increase the Qst value in the H2 adsorption up to 2 kJmol-1 than that of pristine MOF.

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Solution Phase Synthesis of 1D & 2D Bi_2Se_3

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Bismuth selenide (Bi_2Se_3) is an attractive material for both thermoelectric and topological insulator applications. However, it is very difficult to grow high-quality, large 1D and 2D Bi_2Se_3 material in solution phase. In this study, a simple and reliable method for the growth of large (~15-20 ?m) hexagonal disk as well as nanowire of Bi_2Se_3 is reported. We can synthesize 2D Bi_2Se_3 with single grained as well as multiple grained crystals with stacked spirals by controlling the nucleation and growth process. For 1D growth of Bi_2Se_3 we use Se nanowire as a sacrificial template and then gradual addition of Bi precursor. XRD study shows that the hexagonal disk grown by our technique are highly crystalline and oriented along [006] direction. For 2D Bi_2Se_3 more than 4 quintuple-layer is necessary to obtain topological insulator property. Raman spectroscopic analysis as well as AFM studies shows that the synthesized Bi2Se3 hexagonal disks are composed of more than 15 quintuple-layer.

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Mechanistic Insight into Yolk@Shell Transformation of MnO@Silica Nanosphere Incorporating Ni2+ ions: Solid-State Route toward Colloidal Nanoreactor System

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포항공과대학교(POSTECH) 화학과

Annealing of MnO@SiO_2/ Ni^{2+} nanospheres in a reducing gas environment resulted in the transformation of the core?shell structure into a yolk-shell structure. The recent study on the conversion chemistry of manganese oxide nanocrystals inside a silica nanosphere, we had observed the evolution of the hollow structure as a result of outward diffusion of MnO species into a thermodynamically more stable silicate phase of the shell. One interesting phenomenon we have noticed is that the incorporation of Ni^{2+} ions left a single Ni nanocrystal inside the newly generated void space and therefore produced a yolk@shell-type nanostructure. This presentation reports recent findings in our efforts toward a more complete understanding of the pathway of this transformation, which was revealed to involve sequential steps, including formation of a mixed-metal-oxide and segregation of the reduced metallic species, all confined within a silica. Also we discovered MnO@SiO_2/$Co^{2+}$and the MnO@SiO_2/Cu^{2+} nanospheres were transformed into yolk-shell structure. Perhaps it is similar mechanism above described for the formation of the MnO@SiO_2/ Ni^{2+}. It is expected yolk-shell structure nanoparticles offer a possibility to provide a hollow nanoreactor framework for catalyzing the chemical reactions of selected substrate molecules inside the cavity.

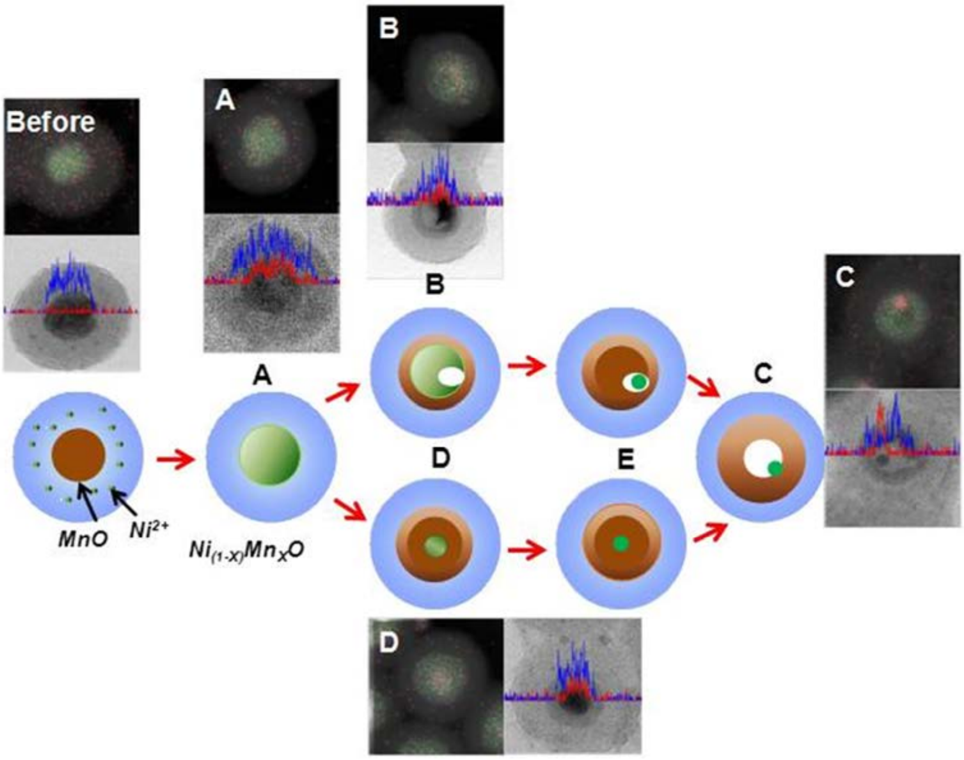

Figure 1. Transformation mechanism of yolk@shell structure.

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Heteroleptic Magnesium Complexes as Precursors for MgO Thin Films Growth by Atomic Layer Deposition (ALD)/Metal Organic Chemical Vapor Deposition (MOCVD)

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Magnesium oxide (MgO) thin films have attracted great scientific and technological interest in recent decades. Because of its distinguished properties such as a wide band gap (7.2 eV), a low dielectric constant (9.8), a low refractive index, an excellent chemical and thermal stability (melting point = 2900°C), it is widely used as inorganic material in diverse areas such as optical materials, protective layers in plasma display panels, buffer layers of multilayer electronic/photonic devices, and perovskite ferroelectric thin films. MgO thin flms have been deposited by several techniques. Among them metal?organic chemical vapor deposition (MOCVD) and atomic layer deposition (ALD) are particularly valuable because they offer the potential for large-area growth and the advantages of good composition control, high film uniformity, and excellent conformal step coverage on nonplanar device geometries.Precursor used in the ALD/MOCVD requires volatility, stability, and low deposition temperature. Various organometallic and coordination compounds have been used as MgO sources, including alkyls, alkoxides, amide, cyclopentadienyls, aminoalkoxide, amidinate, guanidinate, and β-diketonates. In this presentation, we demonstrate synthesis of new heteroleptic magnesium precursors containing combination of β-diketonate/aminoalkoxide and amidinate/aminoalkoxide ligands. The complexes were characterized by NMR, FT-IR, elemental analysis, thermogravimetric analysis (TGA), and single-crystal X-ray diffraction.References1.B. Sedai, M. J. Heeg and C. H. Winter, J. Organomet. Chem. 2008, 693, 3495.2.T. Hatanp??, J. Ihanus, J. Kansikas. I. Mutikainen, M. Ritala and M. Leskel?, Chem. Mater. 1999, 11, 1846.3.A. Sartori, N. E. Habra, M. Bolzan, G. Rossetto, S. Sitran, D. Barreca, A. Gasparotto, M. Casarin, Chem. Mater. 2011, 23, 1113.

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Diffusion Mechanisms of Hydronium and Hydroxide Ions in Amorphous Solid Water

강헌* 이두형

서울대학교 화학부

Diffusion of hydronium and hydroxide ions is one of the most intriguing topics in aqueous chemistry. It is considered that these ions in aqueous solutions move via sequential proton transfer events, known as the Grotthuss mechanisms. Here, we present an experimental study of the diffusion and H/D exchange of hydronium and hydroxide ions in amorphous solid water (ASW) films at < 180 K by using low energy sputtering and temperature-programmed desorption experiments. The study shows that the two species transport via fundamentally different molecular mechanisms. Whereas hydronium ions migrate via efficient proton transfer, hydroxide ions move via Brownian molecular diffusion without proton transfer. The molecular hydroxide diffusion in ASW is in stark contrast to the current view of hydroxide diffusion mechanism in aqueous solution, which involves proton transfer.

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발표종류: 구두발표, 발표일시: 금 10:25, 좌장: 김우연

Quantum Mechanical Modelings of Chemical Reactions on Ice Surface

최철호

경북대학교 화학과

Chemical reactions on ice surface have become one of the most important research subjects recently. The interest in the interactions of gases with ice surface largely prompted by the discovery of the Antarctic Ozone Hole and the recognition that atmospheric ice particles can play a dominant role in determining the chemical composition of the atmosphere. At the temperature of ice, the occurrence of a chemical reaction with an appreciable speed has been considered to be unlikely. However, recent studies show that reactions occur even at substantially low temperatures at the surface of ice. On the other hand, theoretical studies of chemical reactions on ice surface based on ab initio methods predict in general large reaction barriers implying that the surface reactions are not facile, contradicting experimental results. To properly model ice surface, the key features should be carefully investigated. Most importantly, long-range electrostatics by bulk ice should be studied. The electrostatic and polarization interactions play a vital role in various condensed phases containing polar and polarizable molecules. In addition, hydrogen disorders of ice crystal should be taken into account. There is no long-range order in the orientations of the H2O molecules or of the hydrogen bonds, which are summarized by the ice rules. Finally, surface heterogeneity in which oxygen dangling bond as well as hydrogen dangling bond are statistically distributed, needs to be properly modeled. In this talk, we introduce our quantum mechanical modeling efforts to describe such delicate and complex reaction environment of ice surface.

일시: 2014년 10월 15~17일(수~금) 3일간
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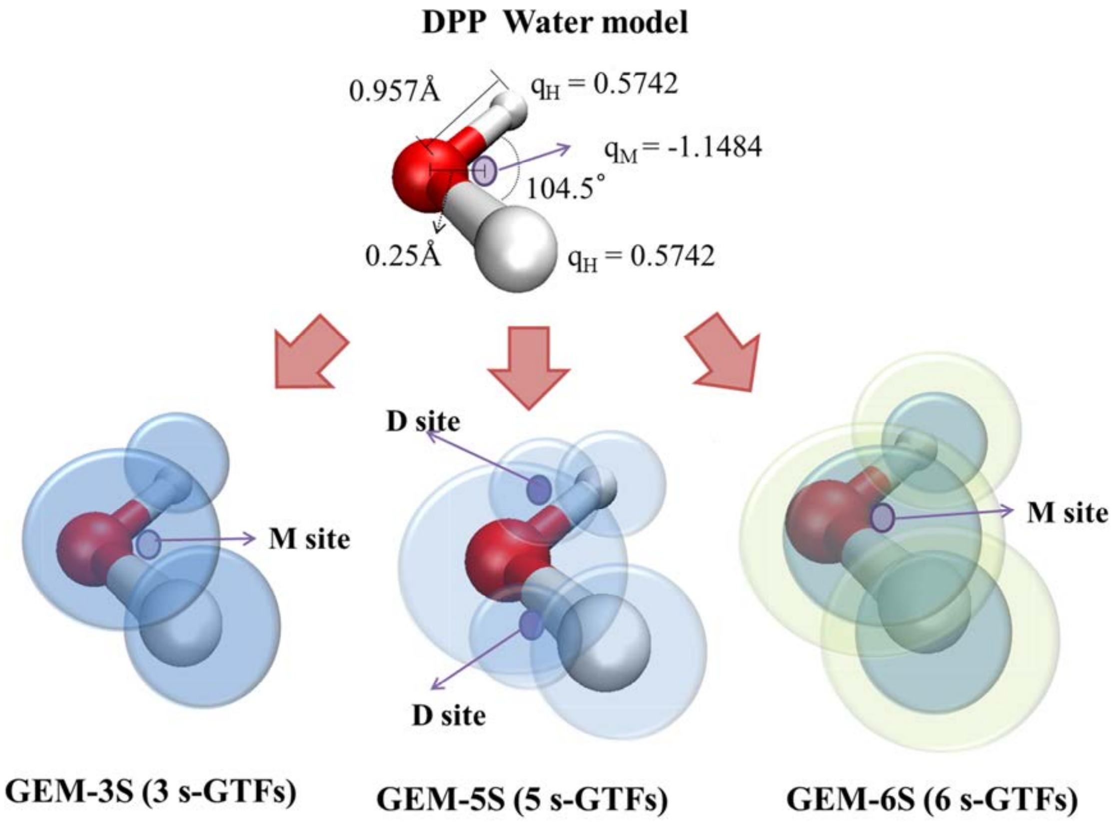
발표코드: **PHYS.O-3**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김동욱

Modeling Charge Penetration Effects in Water-Water Interactions

최태훈

충남대학교 화학공학교육과

This report introduces Gaussian electrostatic models (GEMs) to account for charge penetration effects in water-water interactions, allowing electrostatic interactions to be accurately described. Three different Gaussian electrostatic models, GEM-3S, GEM-5S, and GEM-6S are designed with s-type Gaussian functions. The coefficients and exponents of the Gaussian functions are optimized using the electrostatic potential (ESP) fitting procedure based on that of the MP2/aug-cc-pVTZ method. The electrostatic energies of ten different water dimers that were calculated with GEM-6S agree well with the results of symmetry-adapted perturbation theory (SAPT), indicating that this designed model can be effectively applied to future water models.


DPP Water model
0.957Å
$q_H = 0.5742$
$q_M = -1.1484$
104.5°
0.25Å
$q_H = 0.5742$
D site
M site
D site
M site
GEM-3S (3 s-GTFs)
GEM-5S (5 s-GTFs)
GEM-6S (6 s-GTFs)

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **PHYS.O-4**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:25, 좌장: 김동욱

A Molecular Simulation Study for Multicomponent Bulk Metallic Glasses

성봉준* 김정민

서강대학교 화학과

Multicomponent bulk metallic glasses (BMGs) show both excellent glass-forming ability (GFA) and intriguing dynamic behaviors such as dynamic heterogeneity and decoupling. Both the excellent GFA and the dynamic behaviors have been issues of academic interest. However, how the dynamic heterogeneity and decoupling of BMGs would relate to GFA remains unanswered. We carry out extensive simulations for Pd-Cu-N-P and Pd-Cu-N melts in order to answer questions of how the local atomic order may form and disintegrate, how the dynamic decoupling and heterogeneity would affect the kinetics of the formation and the disintegration of the local atomic order, and how GFA would relate to the dynamic heterogeneity and decoupling. We find that the smallest component of Pd-Cu-N-P melts should account for the dynamic heterogeneity .The dynamically heterogeneous P atoms break down Stokes-Einstein relation and also lead to the dynamic decoupling of P and Pd atoms. When the dynamically heterogeneous P atoms are removed as in Pd-Cu-N melts, the atomic diffusion slows down significantly even though the pair correlation functions of Pd atoms for Pd-Cu-N-P and Pd-Cu-N melts are almost identical to each other. We also employed a common neighbor analysis to estimate the structure and the lifetime of the local atomic orders. Interestingly, the presence of P atoms decreases the lifetimes of both the icosahedral local atomic order and the nucleus of close-packed geometries by orders of magnitude.

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발표코드: **PHYS.O-5**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 최태훈

Theoretical Studies of Structure and Thermodynamic Properties of Electrolytes and Electrolyte Additives Mixture

One Sun Lee

Qatar Environment and Energy Research Institute

It has been reported that fluoroethylene carbonate (FEC) is a promising electrolyte additive with many potential applications including improved passivation of solid electrolyte interphase films, improved reversibility of electrochemical sodium insertion for hard-carbon electrodes, and avoiding the exfoliation of graphite electrodes. However, the atomistic details of the structure of electrolyte liquid with FEC additive are not known. Here we studied the structural and thermodynamic properties of ethylene carbonate and propylene carbonate electrolyte liquids mixed with FEC additive using classical molecular dynamics simulations. The characterization of the electrolyte liquid structure was performed by examining the radial distribution functions, coordination numbers, and dipole-dipole correlation.

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발표코드: **PHYS.O-6**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 12:15, 좌장: 최태훈

The effect of an aqueous phase on phenol hydrogenation over Pt/Ni catalysts : First Principles Study

윤여훈

Pacific Northwest National Laboratory, USA

The effect of an aqueous phase on phenol hydrogenation over Pt and Ni catalysts was investigated using density functional theory-based ab initio molecular dynamics calculations. The adsorption of phenol and the addition of the first and second hydrogen adatoms were explored in both vacuum and liquid water. The major change in the electronic structure of both Pt(111) and Ni(111) surfaces, between a gaseous and liquid phase environment, results from a repulsion between the electrons of the liquid water and the diffuse tail of electron density emanating from the metal surface. The redistribution of the metal's electrons toward the subsurface layer lowers the metal work function by about 1 eV. The lower work function gives the liquid covered metal a higher chemical reduction strength and, in consequence, a lower oxidation strength, which, in turn lowers the phenol adsorption energy, despite the stabilizing influence of the solvation of the partly positively charged adsorbate. At both the solid/vapor and the solid/water interface, H adatom addition involves neutral H atom transfer hence the reaction barriers for adding H adatoms to phenol are lowered a little due to a small stabilizing at the transition state. More importantly, the liquid environment significantly influences the relative energetics of charged, surface-bound intermediates and of proton-transfer reactions like keto/enol tautomerization. For phenol hydrogenation, solvation in water results in an energetic preference to form ketones as a result of tautomerization of surface-bound enol intermediates.

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발표코드: **PHYS.O-7**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 최태훈

IR spectroscopy of cold biomolecular ions embedded in liquid helium nanodroplets

안두식* Ana Isabel Gonz?lez Fl?rez[1] Gert von Helden[1]

Fritz-Haber-Institut Molecular Physics [1]Fritz-Haber-Institute, Germany

Liquid helium nanodroplets are ideal cryostats for the spectroscopic investigation of molecules by means of intrinsic characters of superfluid helium droplets such as isothermality at 0.38 K and a wide spectral window range from far IR to deep UV. We have developed a pulsed liquid helium nanodroplet beam setup coupled with electronic spray ionization source and linear hexapole ion trap for cooling of large biomolecular ions via embedding on helium nanodroplets. IR spectra of the mass-to-charge selected biomolecular ions in liquid helium nanodroplets have been obtained using IR Free Electron Laser (FEL) facility at Fritz-Haber-Institute. In Amide I and II region, the effects of cooling of ions are clearly shown in the narrowed bandwidth of spectra compared to the spectra in the room temperature. We will present the recent results on various peptides and small proteins ions such as protonated Ubiquitin.

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발표코드: **PHYS.O-8**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:45, 좌장: 최태훈

Real-time Imaging of the propagation of RNA polymerase noise in living cells

양소라 임유림[1] 김철희 성재영[1] 이남기[2,*]

포항공과대학교(POSTECH) 물리학과 [1]중앙대학교 화학과 [2]포항공과대학교(POSTECH) 시스템생명공학부/물리학

Cell-to-cell variation in gene expression, or noise, is a general phenomenon observed within cell populations. Transcription is known to be the key stage of gene expression where noise is generated, however, how variation in RNA polymerase (RNAP) concentration contributes to gene expression noise is unclear. Here, we quantitatively investigate how variations in absolute amounts of RNAP molecules affect noise in the expression of two fluorescent protein reporters driven by identical promoters. We find that intrinsic noise is independent of variation in RNAP concentrations, whereas extrinsic noise, which is variation in gene expression due to varying cellular environments, scales linearly with variation in RNAP abundance. Furthermore, by measuring the concentrations of the downstream proteins together with RNAP concentration in real-time at the single-cell level, we confirmed that the fluctuation history of RNAP concentration presented a minimal effect on downstream protein noises. Specifically, the propagation of RNAP abundance variation to expressed protein noise is inversely proportional to the concentration of RNAP, which suggests that the change in noise that results from RNAP fluctuations is determined by the fraction of promoters that is not occupied by RNAP.

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장소: 광주 김대중컨벤션센터

발표코드: **ANAL.O-1**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 신익수

A Surface Sandwich Assay for Protein Biomarker Utilizing Double Nanopartielcs on a SPR Sensing Platform

백승희 이혜진*

경북대학교 화학과

본 발표에서는 서로 다른 모양과 크기를 갖는 두 종류의 금 나노입자에 짧은 서열의 DNA 를 컨쥬게이션하여 SPR (Surface plasmon resonance, 표면 플라즈몬 공명법) 센싱 플랫폼에 도입함으로써 초고감도로 단백질 (예: 트롬빈)을 검출한 결과를 보여주고자 한다. 먼저, SPR 용 금 박막 칩에 트롬빈 항체를 고정하고, 트롬빈을 흘려준 후 트롬빈에 특이적으로 결합하는 트롬빈-앱타머를 주입하여 샌드위치 복합체를 형성하였다. 트롬빈 앱타머에 도입한 여분의 DNA 서열과 상보적 결합을 할 수 있는 짧은 DNA 를 서로 다른 모양과 크기를 가지는 두 종류의 금 나노입자(예; 나노로드와 다각형 나노입자)에 각 각 컨쥬게이션 한 후 이를 이미 형성된 샌드위치 복합체에 순차적으로 결합시켰을 때 트롬빈 농도에 따라 SPR 신호가 변화함을 실시간으로 측정하였다.

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장소: 광주 김대중컨벤션센터

발표코드: **ANAL.O-2**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:25, 좌장: 신익수

A synthetic chemosensor based electrochemical assay of protein kinase on a microchip

CHANDROHITPRADIP

성균관대학교 전자전기컴퓨터공학과

Phosphorylation by protein kinases is a predominant form of protein regulation. Abnormal phosphorylation of protein is linked to several medical states. Mutations in particular protein kinases give rise to a number of disorders and many naturally occurring toxins and the pathogens exert their effects by altering the phosphorylation states of intracellular proteins. Understanding of the specificity and regulation of particular protein kinase is crucial for the development of drugs to treat diabetes or cancers.Tremendous efforts have been devoted to quantify the catalytic activities of these enzymes. Radioactive labelling with [γ-^{32}P]ATP with protein or peptide substrates are the most common method for measuring cellular kinase activities. However, the electrochemical method offers sensitive, cost-effective, and portable assays for kinase activity. Herein, we report an electrochemical assay for protein kinase A activity using a synthetic chemosensor.The synthetic chemosensor comprises of a bis(Zn^{2+}-dipicolylamine) group and a thiol group at the ends of a hydrocarbon chain. The former strongly and selectively captures the phosphorylated enzyme product, forming a bridge between the two Zn^{2+} cations. The thiol group forms a self-assembled monolayer on the gold surface. In the presence of protein kinase, the substrate undergoes phosphorylation, which subsequently binds to the chemosensor, and then the ferrocene tag of the enzymatic product generates strong oxidation current under voltammetry.We performed differential pulse voltammetry to study the electrochemical signal obtained. Upon voltammetry, the mixture produced a well-defined oxidation peak corresponding to that of ferrocene and enabled a very low limit of detection. Our method was successfully applied even in the presence of human blood, and modified to enable single-use, chip-based electrochemical assay for kinase activity.

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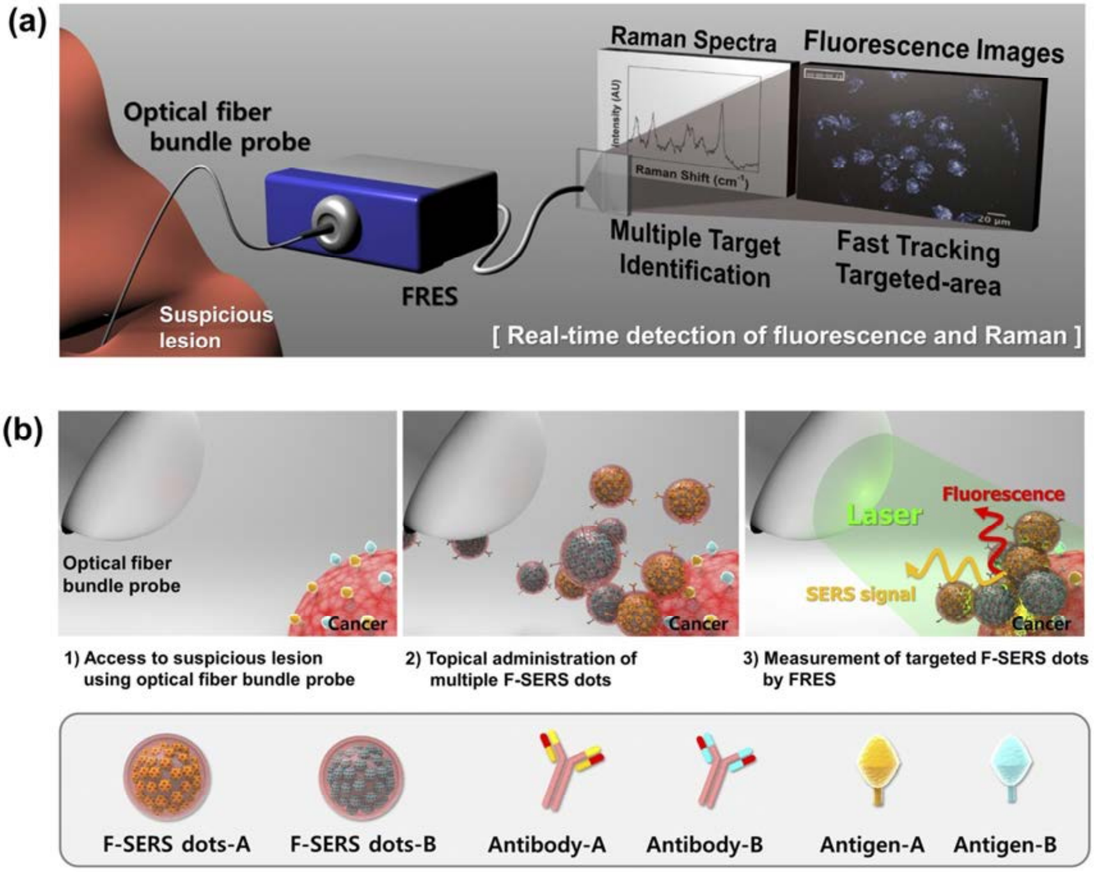
발표코드: **ANAL.O-3**
발표분야: Oral Presentation of Young Analytical Chemists
발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 신익수

Fluorescence-Raman Endoscopic System for *in vivo* Real-time Multiplexed Molecular Diagnosis

정신영 정대홍* 이윤식[1]

서울대학교 화학교육과 [1]서울대학교 화학생물공학부

Optical endoscopic imaging techniques afford access to specific internal organs with minimal invasiveness and real-time detection for the diagnosis of specific cancers and determination of pathological conditions in suspicious lesions. Recently, additional functionalities of bioluminescence, fluorescence, and Raman scattering have been incorporated to the endoscopy with advantages of the conventional white-light reflectance endoscopy in distinguishing morphological changes. To characterize the pathologic lesions in a multiplexed way, we developed a dual modal fluorescence-Raman endoscopic system (FRES) which used fluorescence and surface-enhanced Raman scattering nanoprobes (F-SERS dots). Real-time, in vivo, and multiple target detection of a specific cancer was successful, based on the fast imaging capability of simultaneous detection of dual modal probes with fluorescence and multiplex SERS signals using an optical fiber bundle for intraoperative endoscopic system. The in vitro detection sensitivity of FRES was 1-pM of F-SERS dots. Human epidermal growth factor receptor 2 (HER2) and epidermal growth factor receptor (EGFR) on the breast cancer xenografts in a mouse orthotopic model were detected successfully in a multiplexed way, which illustrated the potential of FRES as a molecular diagnostic instrument that enables real-time tumor characterization of the receptors during routine endoscopic procedures.


(a)
Optical fiber bundle probe
Suspicious lesion
FRES
Raman Spectra
Intensity (AU)
Raman Shift (cm^{-1})
Fluorescence Images
20 μm
Multiple Target Identification
Fast Tracking Targeted-area
[Real-time detection of fluorescence and Raman]
(b)
Optical fiber bundle probe
Cancer
Laser
Fluorescence
SERS signal
1) Access to suspicious lesion using optical fiber bundle probe
2) Topical administration of multiple F-SERS dots
3) Measurement of targeted F-SERS dots by FRES
F-SERS dots-A
F-SERS dots-B
Antibody-A
Antibody-B
Antigen-A
Antigen-B

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ANAL.O-4**

발표분야: Oral Presentation of Young Analytical Chemists

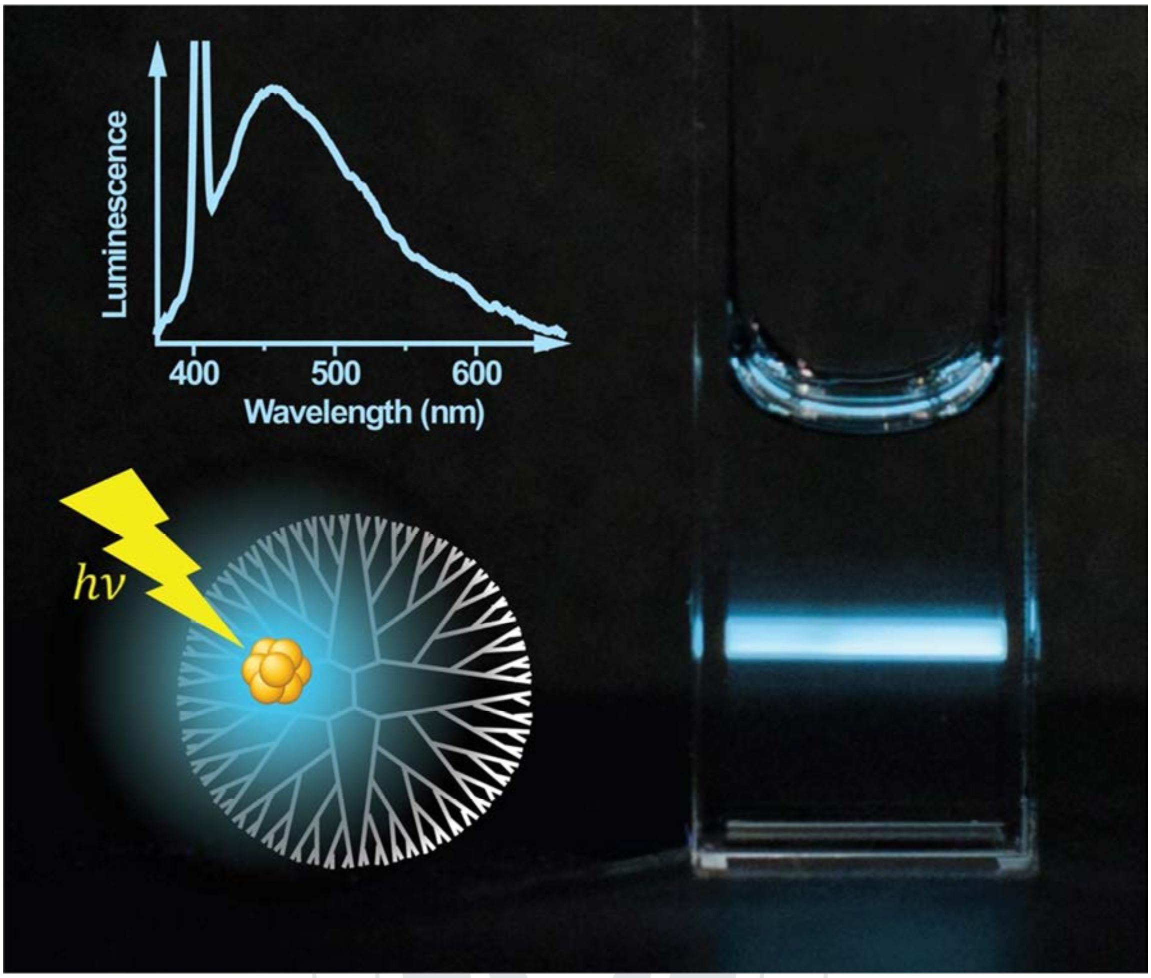
발표종류: 구두발표, 발표일시: 금 11:35, 좌장: 신익수

Blue Luminescence of Dendrimer-Encapsulated Gold Nanoclusters

김준명 김주훈*

경희대학교 화학과

In this study, we reported the blue luminescence of gold nanoclusters encapsulated inside hydroxyl-terminated polyamidoamine (PAMAM) dendrimer (G4-OH). The blue luminescence of the gold nanoclusters was probed by spectroscopic measurements and theoretical calculations. In the steady-state and time-resolved spectroscopic measurements, the luminescence of the gold nanoclusters encapsulated inside G4-OH dendrimer was clearly distinguished from the emission of G4-OH dendrimer. Also, the luminescence of gold nanoclusters was found to be composed of two electronic transitions. In the theoretical calculations, the two electronic transitions were attributed to the different sizes of the gold nanoclusters (Au8 and Au13). Such fluorescent nanoclusters are expected to be useful in a range of analytical applications including cellular imaging, immunoassays, and chemical sensing.


Luminescence
400
500
600
Wavelength (nm)
$h\nu$

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ANAL.O-5**
발표분야: Oral Presentation of Young Analytical Chemists
발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 신익수

Synthesis and Characterization of Highly Fluorescent Metal Nanoclusters

표경림 이동일*

연세대학교 화학과

Thiolate protected gold nanoclusters (AuNCs) have been one of the most studied materials for the past few years owing not only to their high chemical and thermodynamic stability, but also to their interesting size-specific physicochemical properties. There is growing interest in the use of AuNCs in catalysis and electrochemical sensing. However, the application using their luminescent properties is still scarce mainly because of their low quantum yield. In this talk, we present the synthesis and characterization of stable, water soluble and highly luminescent AuNCs which are protected by glutathione(GS) ligands. The key to synthesizing highly luminescent AuNCs, was to reduce gold(III) salt slowly with sodium borohydride in the presence of ligands. To slow down the reducing reaction, the synthesis was carried out in a very dilute alkaline condition. Thus prepared cluster mixture was purified by poly-acrylamide gel electrophoresis (PAGE), which isolated a distinctive red-emitting luminescent cluster. The luminescent cluster was found to be $Au_{22}(GS)_{18}$ by characterizing with electrospray ionization mass spectrometry (ESI-MS) and the luminescence quantum yield was higher than 40%. With its ultrafine size (< 2nm), high quantum yield, and low toxicity, it is expected to be a promising material in diverse fields such as biosensors and bioimaging. Furthermore, the slow reduction strategy has been successfully extended to preparation of stable and luminescent silver nanoclusters.

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장소: 광주 김대중컨벤션센터

발표코드: **ANAL.O-6**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 12:25, 좌장: 신익수

The applicability of minimized bioreceptors in localized surface plasmon resonance (LSPR) sensor for analysis of biomolecules

변주영 김민곤[1,*]

광주과학기술원(GIST) 물리화학부/화학과 [1]광주과학기술원(GIST) 화학과

Binding of an analyte on the surface of a nanoparticle typically promotes a change in the local refractive index, which gives rise to a shift in the wavelength of the localized surface plasmon resonance (LSPR) absorption band. The magnitude of the LSPR wavelength change is dependent on both the location of the analyte relative to the surface of the nanoparticle and the degree of alteration of the refractive index. In particulars, the sensitivities of LSPR measurements are dependent on the location of analytes relative to the surface of nanoparticles. Most immunosensor systems utilize antibody (ca. 15 nm) as capture receptor. Limit exists on the size of the receptor-analyte binding pair in order to insure that the binding of the analyte takes place sufficiently close to the surface of the nanoparticle. Consequently, the sensitivity of the plasmonic immunosensor systems should be enhanced by minimizing the size of antigen binding molecules. In this study described, we have employed small size of receptor as the basis for designing sensitive approach for the detection of the biomolecules. The sensor utilizes the full-length antibody, single chain variable fragment (scFv) and aptamer (single strand DNA) as receptor to bind biomolecules. The scFv and aptamer utilized in this system are small size molecules that bind the target with a high affinity and specificity. As a result of the use of small size receptor and the fact that it causes the distance between analytes and surface of nanoparticle to become shorter, the refractive index associated with the local dielectric environment near the surface of nanoparticle significant changes and results in a peak shift of the LSPR band. Therefore, the minimized receptor conjugated nanoparticles showed much higher sensitivity than that using full-length antibody as capture receptor. To our knowledge, the sensitivity of plasmonic LSPR sensor could enhance through adjusting of receptor size.

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발표코드: **BIO.O-1**
발표분야: Oral Presentation of Young Biochemists
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이상호

Structural basis for regulation of tumor suppressor protein p53 with CBP/p300 and MDM2 interaction

이철원

전남대학교 화학과

The activity and stability of the tumor suppressor p53 are regulated by interactions with key cellular proteins such as MDM2 and CBP/p300. The transactivation domain (TAD) of p53 contains two subdomains (AD1 and AD2) and interacts directly with the N-terminal domain of MDM2 and with several domains of CBP/p300. Using NMR spectroscopy and other biophysical methodologies, we have dissected the binding interactions between the TAD of p53, the TAZ1, TAZ2, KIX, and nuclear receptor coactivator binding domain (NCBD) of CBP, and the p53-binding domain of HDM2 (the human homolog of MDM2). The p53 TAD can bind simultaneously to HDM2 (through AD1) and to any one of the CBP domains (through AD2) to form a ternary complex. The NMR structure of the full-length p53 TAD in complex with NCBD of CBP indicate that the p53 TAD and NCBD are intrinsically disordered and fold synergistically upon binding, which provides the first insights into simultaneous binding of the AD1 and AD2 motifs to a target protein. The transcriptional activity of p53 is regulated by a cascade of posttranslational modifications. We investigated the role of single site and multiple site phosphorylation of the p53 TAD in mediating its interaction with CBP and with HDM2. Phosphorylation at Thr18 functions as an on/off switch to regulate binding to the N-terminal domain of HDM2. In contrast, binding to CBP is modulated by the extent of p53 phosphorylation; addition of successive phosphoryl groups enhances the affinity for the TAZ1, TAZ2, and KIX domains of CBP in an additive manner. Activation of p53-dependent transcriptional pathways requires that p53 compete with numerous cellular transcription factors for binding to limiting amounts of CBP/p300. Multisite phosphorylation represents a mechanism for a graded p53 response, with each successive phosphorylation event resulting in increasingly efficient recruitment of CBP/p300 to p53-regulated transcriptional programs, in the face of competition from cellular transcription factors. Multisite phosphorylation thus acts as a rheostat to enhance binding to

CBP/p300 and provides a plausible mechanistic explanation for the gradually increasing p53 response observed following prolonged or severe genotoxic stress.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **BIO.O-2**

발표분야: Oral Presentation of Young Biochemists

발표종류: 구두발표, 발표일시: 금 10:25, 좌장: 이상호

Functional and structural consequences of metalloenzymes

이승재

전북대학교 화학과

Soluble methane monooxygenase (sMMO) in methanotropic bacteria converts methane to methanol. The mechanistic elucidation of this enzyme is a critical factor for its application in the fields of bioenergy and bioremediation. The sMMO consists of a hydroxylase (MMOH, 251 kDa), a regulatory (MMOB, 15.9 kDa), and a reductase (MMOR, 38.6 kDa) component. MMOB is essential for catalytic activity in the MMOH which houses the diiron active sites. The detailed mechanism, unfortunately, has remained ambiguous due to the lack of atomic-level information. We recently reported the crystal structure of the MMOH-MMOB complex and this makes clear how methane is converted to methanol in the sMMO system. Two MMOB units bind to MMOH and cause crucial conformational changes. The MMOH-MMOB complex provides an elegant model of how a large enzyme complex precisely controls its chemistry. This presentation will explain how four substrates including methane, oxygen, electrons, and protons are controlled by MMOB.

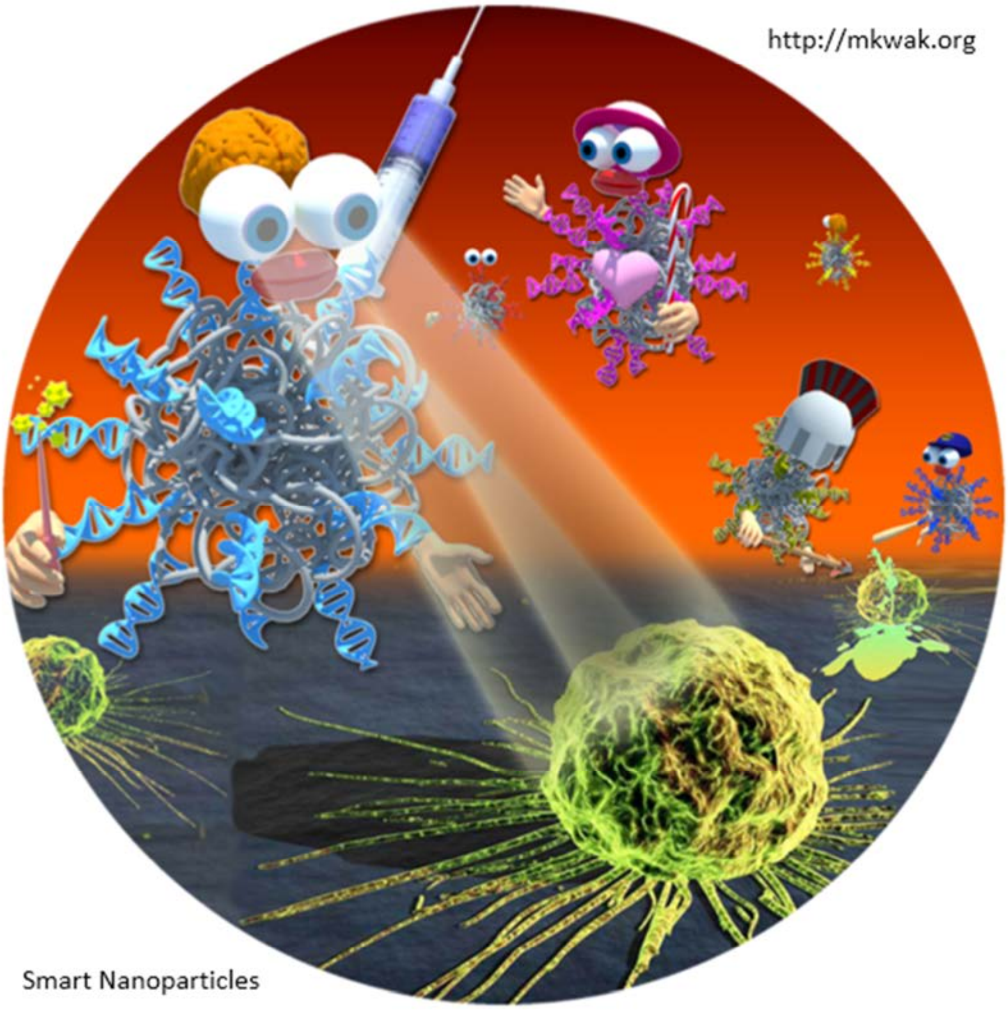
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **BIO.O-3**
발표분야: Oral Presentation of Young Biochemists
발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 이상호

DNA Hybrids and Nanostructures for Applications in Biomedicine

곽민석

부경대학교 화학과

DNA has been extensively studied in the context of self-assembled nanostructures. Due to the specificity of DNA hybridization and programmability of the DNA codes, it is possible to create intricate and beautiful DNA structures on the nanoscale. This talk will mostly focus on a related class of materials, DNA amphiphiles that have synthetic hydrophobic segments covalently connected to oligonucleotides. These materials exhibit both the self-recognition properties of DNA and the aggregation behavior of amphiphilic molecules. Among such self-assembled aggregates micelles are templating the formation of virus-like particles and at the same time allow to develop a general loading scheme for equipping interior of virus capsids with various payloads. Secondly, using analogous nanoparticles, in vivo ophthalmic delivery onto cornea of animal and human tissues has proved the potency of the DNA amphiphiles for advanced therapeutics. Lastly, precisely defined DNA nanostructures, so called DNA origamis, will be briefly introduced as a novel delivery system.


http://mkwak.org
Smart Nanoparticles

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **BIO.O-4**
발표분야: Oral Presentation of Young Biochemists
발표종류: 구두발표, 발표일시: 금 11:35, 좌장: 이상호

Exploring Outer & Inner Life with Nanoantennae : Plasmonic Nanosensors for Bio/Chemical Analyses

최인희

서울시립대학교 생명과학과

Recent progress in plasmon-based sensors has greatly overcome the limitations of conventional optical sensors, in terms of sensitivity, tunability, photostability, and in vivo applicability, by employing nano-structured plasmonic materials (i.e., single metallic nano-particle and well-fabricated nanostructured metal substrate). In this presentation, notable approaches for new types of plasmonic nanosensor platforms and their potential applications to biological and chemical detection would be introduced. Our recent achievements including excellent plasmonic nanoprobes, nanoassembly-based plasmonic signal amplification, novel nanobiophotonic interfaces and their integration into microfluidic platforms provide new opportunities toward ultrasensitive biological and chemical analyses and point-of-care biomedical devices. In this respect, the plasmonic nanosensors have a bright future and would contribute to innovative biomedical and environmental breakthrough.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **BIO.O-5**
발표분야: Oral Presentation of Young Biochemists
발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 이상호

Genetic Incorporation of Unnatural Amino Acids and Its Applications

이현수

서강대학교 화학과

Proteins are involved in virtually all of the complex processes of life, from photosynthesis to signal transduction and the immune response. Given the essential roles of proteins in life, understanding the structure and function of proteins is extremely important. Due to the limited functionality of standard amino acids in natural proteins, tremendous efforts have been made to introduce unnatural amino acids (UAAs) into proteins to study protein structure and function.Recently, a method to encode unnatural amino acids with diverse chemical and biological properties genetically in bacteria, yeast and mammalian cells was developed. Over 70 unnatural amino acids have been genetically incorporated into proteins with high fidelity and efficiency using a unique codon and corresponding tRNA:aminoacyl?tRNA synthetase pair. This method has been providing a powerful tool for exploring protein structure and function in vitro and in vivo, and for generating proteins with new or enhanced properties. In this seminar, development of a simple method for protein conjugation by copper-free click reaction and genetic incorporation of unnatural amino acids biosynthesized from α-keto acids by an aminotransferase will be discussed.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **BIO.O-6**

발표분야: Oral Presentation of Young Biochemists

발표종류: 구두발표, 발표일시: 금 12:25, 좌장: 이상호

N-Terminal Acetylation and the N-End Rule Pathway

황철상

포항공과대학교(POSTECH) 생명과학과

One fundamental question in the ubiquitin-proteasome system is what features trigger the ubiquitylation of a target substrate and its subsequent proteasomal degradation. In other words, what is a protein degradation signal? The first protein degradation signal to be identified is N-terminal degradation signals, termed N-degrons. Detailed analysis of these N-degrons gave rise to the N-end rule which enables the N-terminal residue of a protein to dictate its stability. The N-end rule pathway comprises two branches: the Ac/N-end rule pathway and the Arg/N-end rule pathway. The Ac/N-end rule pathway targets proteins for degradation through their Nα-terminally acetylated residues. In contrast, the Arg/N-end rule pathway mediates degradation of proteins with unacetylated N-terminal residues. Here, I will present our recent discoveries about the crosstalk of two branches of the N-end rule pathway.

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발표코드: **ORGN.O-1**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김민

Privileged Substructure-Based Diversity-Oriented Synthesis Pathway for Diverse Pyrimidine-Embedded Polyheterocycles

김희준 박승범*

서울대학교 화학부

Facile fabrication of a structurally diverse small-molecule library plays a crucial role in drug discovery and chemical biology. In particular, the unbiased collection of small molecules has become an inevitable resource because it can provide a unique opportunity for the identification of novel chemical entities from phenotype-based screening, which is the leading approach for the development of first-in-class drugs. Diversity-oriented synthesis (DOS) plays an indispensable role to access the unexplored molecular frameworks with maximum structural and stereo-chemical diversity. Along with this endeavor, we proposed a privileged substructure-based DOS (pDOS) for the efficient generation of distinct polyheterocyclic core skeletons embedded with privileged substructures. Pyrimidine has been extensively explored in synthetic and medicinal chemistry owing to its unique mimicking of nucleosides and hydrogen bonding ability with nucleic acids in biological systems. We developed a new pDOS strategy with pyrimidine as the privileged substructure. Five core skeletons were synthesized by silver- or iodine-mediated cascade cyclization with various amines under different reaction conditions. The resulting discrete scaffolds consist of unique pyrimidine-embedded polyheterocycles fused with distinct sizes and orientation. This pDOS strategy allows the fabrication of unique polyheterocycles along with a wide spatial coverage around pyrimidine as the privileged substructure that ensures high potential for molecular interactions with biopolymers in a selective and specific manner.

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발표코드: **ORGN.O-2**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 김민

Biomimetic Organocatalytic Reactions Promoted by Chiral Hydrogen-Bonding Donors

배한용 송충의*

성균관대학교 화학과

Nature uses water as sole reaction medium for enzymatic catalysis. The hydrophobic hydration effect lies at the heart of countless valuable biological as well as chemical phenomena that scientists devoted considerable effort to exploiting it for catalytic reactions over the past decades. Moreover, especially in the biosynthesis of polyketide, Nature freely takes malonic acid half thioester (MAHTs) enolate precursors to accomplish decarboxylative iterative asymmetric C-C bond formation reaction. Inspired by Nature's operations, we are interested in developing bimomietic organocatalytic reactions promoted by chiral hydrogen-bonding donor catalysts. Very recently, we successfully reported water accelerated catalytic enantioselective Michael addition via hydrophobic hydration,[1] catalytic asymmetric decarboxylative Michael addition[2] and aldol reaction[3] using MAHTs as efficient enolate precursors. In this context, my presentation will discuss the design, scope and mechanism of biomimetic organocatalytc reactions as well as practical routes to preparation of bioactive molecules.[1] H. Y. Bae, S. Some, J. S. Oh, Y. S. Lee, C. E Song* : *Chem. Commun.* 2011, 47, 9621.[2] H. Y. Bae, S. Some, J. H. Lee, J. Kim, M. J. Song, S. Lee,* Y. J. Zhang,* C. E. Song* *Adv. Synth. Catal.* 2011, 353, 3196.[3] H. Y. Bae, J. H. Sim, J. Lee, B. List,* C. E. Song* *Angew. Chem. Int. Ed.* 2013, 52, 12143.

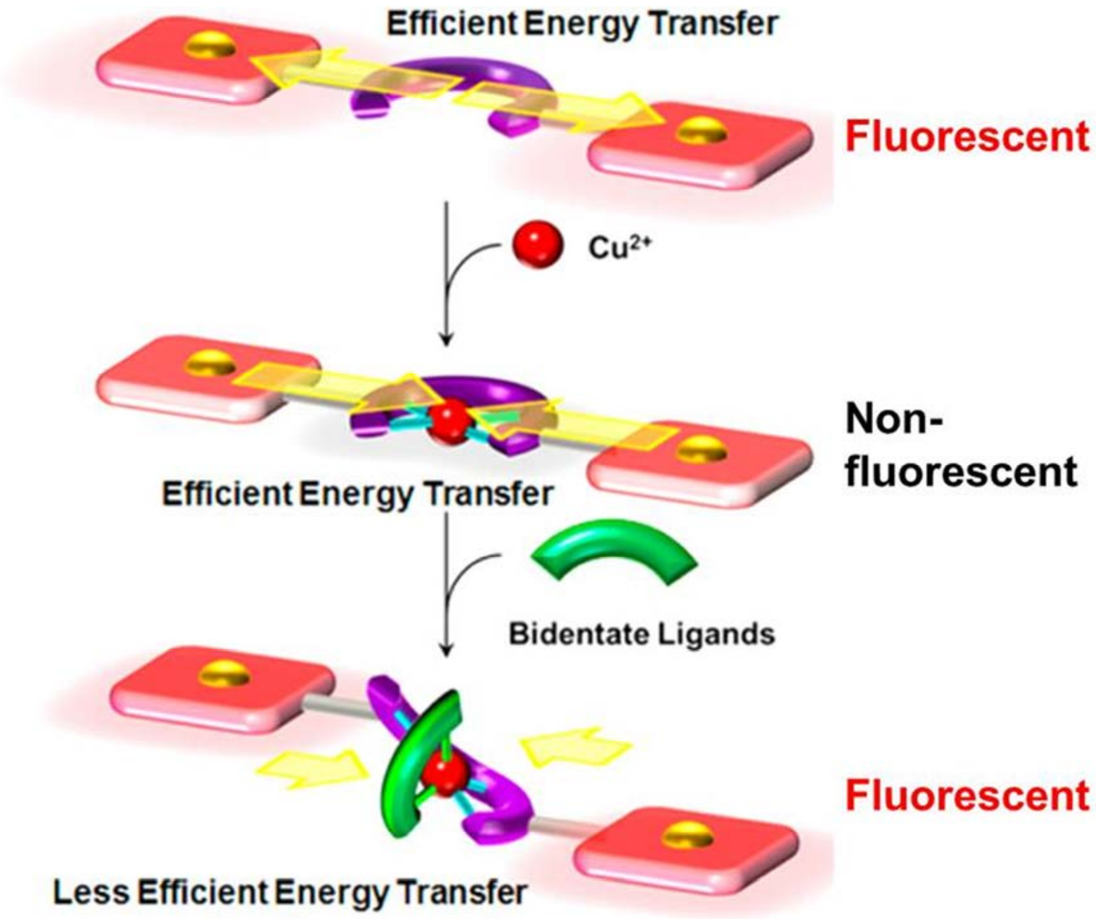
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.O-3**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 김민

Energy Transfer Switching of Porphyrin-based Molecular Tweezer

윤홍식 장우동*

연세대학교 화학과

A bisindole-bridged-porphyrin tweezer (1) exhibited unique switching in forward and backward photo-induced energy transfer by specific guest bindings. Among various metal ions, the addition of Cu^{2+} only caused a change in electronic absorption and fluorescence quenching of 1. MALDI-TOF-MS and FT-IR analyses indicated the formation of stable coordination complex between 1 and Cu^{2+} (1-Cu(II)). Without Cu^{2+} coordination, the excitation energy flows from biindole bridge (BB) to porphyrin (P_{Zn}), where the energy transfer efficiency was estimated to be 99%. In contrast, the direction of energy flow in 1 was completely reversed by the coordination of Cu^{2+}. The difference in fluorescence quantum yield between 1 and 1-Cu(II) indicates that more than 95% of excitation energy of P_{Zn} flows into Cu(II)-coordinated BB. The energy transfer efficiency was further controlled by bidentate ligand coordination onto 1-Cu(II). When pyrophosphate ion was added to 1-Cu(II), the recovery of fluorescence emission from P_{Zn} was observed. The quantum mechanical calculations indicated that the Cu(II)-coordinated BB has square planar geometry, which can be distorted to form octahedral geometry due to the coordination of bidentate ligands.


Efficient Energy Transfer
Fluorescent
Cu²⁺
Non-fluorescent
Efficient Energy Transfer
Bidentate Ligands
Fluorescent
Less Efficient Energy Transfer

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.O-4**

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 김민

Phosphaannulation of Aryl and Benzyl Phosphonic Acids with Unactivated Alkenes through Palladium-Catalyzed C-H Activation/Oxidative Cyclization Reaction

전우형 이필호*

강원대학교 화학과

An efficient phosphaannulation via Pd(II)-catalyzed C-H activation/oxidative cyclization by 6-*endo* mode is reported for the synthesis of 3-substituted phosphaisocoumarins from the reaction of aryl phosphonic acids with unactivated alkenes under aerobic conditions. Also, α,α-disubstituted benzyl phosphonic acids were phosphaannulated with unactivated alkenes, producing phosphaisochromanones having (*Z*)-alkylidenyl groups via *anti*-phosphoryoxypalladation by 6-*exo* mode.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.O-5**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 김민

Palladium-Catalyzed Cross-Coupling Reactions with Aryl Chlorides using New Phosphorus Ligands

김소한 김민* 김영조*

충북대학교 화학과

The palladium?catalyzed arylation is one of a relatively emerging field within the cross?coupling area and organic transformations. Although aryl chlorides are less expensive and more abundant than other aryl halides, they are much less reactive. Thus, a valuable arylation reaction for carbon?carbon or carbon?nitrogen bond formation by palladium?catalyzed cross?coupling of aryl chlorides is much less developed than others. The examples of palladium/phosphorus catalytic system as catalysts for the arylation reaction of aryl chlorides have been reported in the literature. However, the arylation reaction has been studied with relatively large quantities of palladium loading or under harsh conditions in the following study. We reported new phosphorus complexes and their efficacies as catalysts for the arylation of a broad range of aryl chlorides under mild reaction conditions.

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발표코드: **ORGN.O-6**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 김민

Unexpected Chemical Transformations of Aldehydes via Metal-Free Aerobic Oxidation in the Presence of Cyanide : Trimerization of Aldehydes and Aerobic Oxidative Esterification of Aldehydes with Alcohols

김유진 천철홍*

고려대학교 화학과

A new, unusual trimerization of aldehydes in the presence of cyanide via metal-free aerobic oxidation was developed. Various aromatic aldehydes were applicable to this protocol to afford the corresponding trimeric products in good to excellent yields. Mechanistic studies suggested that trimers of aldehydes would be formed via the cyanide-catalyzed benzoin reaction, followed by aerobic oxidative esterification between the resulting benzoin products and aldehydes in the presence of cyanide. Furthermore, this cyanide-mediated aerobic oxidation of aldehydes was extended to metal-free aerobic oxidative esterification of aldehydes in the presence of alcohols. Various types of aromatic aldehydes, including electron-rich ones, as well as sterically congested secondary alcohols were amenable to this protocol. In addition, this method could be applied to the preparation of thioesters with thiols.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.O-7**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 김민

Total synthesis of Fimsbactin B

이희수 김학중*

고려대학교 화학과

Iron is an essential element for the survival of all forms of life, in which it functions as a cofactor for enzymes involved in key metabolic processes. However, due to the low aqueous solubility of Fe(III), all organisms possess dedicated systems to actively assimilate the iron from the aerobic environment. Siderophores are small molecule, high affinity Fe(III)-chelators produced and utilized by most bacteria for that purpose to actively scavenge Fe(III) from the environment. Here we have embarked on establishing the synthetic route for preparation of fimsbactins, a set of recently identified siderophores produced by Acinetobacter baumanii.

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발표코드: **ORGN.O-8**
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:45, 좌장: 김민

Catalytic Asymmetric Hydroamination and Hydroalkoxylation of Alkoxyallene : Mechanism and Application

임원택 이영호*

포항공과대학교(POSTECH) 화학과

Recently, we reported the asymmetric synthesis of *N,O*-acetals[1] and *O,O*-acetals[2] via Pd-catalyzed hydroamination and hydroalkoxylation of alkoxyallene. Herein, we will describe the first example of metal-catalyzed asymmetric intermolecular hydroalkoxylation of alkoxyallene with aliphatic alcohols which were generally known as the inactive nucleophile. Mechanism and application in the synthesis of bioactive natural product will also be discussed.

References

1.(a) Kim, H.; Rhee, Y. H. *J. Am. Chem. Soc.* 2012, *134*, 4011. (b) Kim, H.; Lim, W.; Im, D.; Kim, D.;Rhee, Y. H. *Angew. Chem., Int. Ed.* 2012, *51*, 12055.
2.Lim, W.; Kim. J.; Rhee, Y. H. *J. Am. Chem. Soc.*, 2014, submitted.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **MAT.O-1**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 박종남

One-pot solvothermal synthesis of heteroatom (S or N)-doped graphene for energy storage and conversion

권파 박원철[*]

서울대학교 융합과학기술대학원 나노융합학과

In this work, we successfully synthesized sulfur-doped graphene and nitrogen-doped graphenes by using a solvothermal method with dimethyl sulfoxide and dimethylformamide as precursors, which are common laboratory reagents. These heteroatom-doped graphene materials exhibited high surface areas and high contents of heteroatoms. Furthermore, the lithium-ion storage properties and oxygen reduction reaction catalytic activity of these materials were also investigated. The success of this approach might facilitate the development of other advanced graphene-based materials with relative simplicity, scalability, and cost effectiveness for use in various potential applications. We expect that our synthetic approach will be developed to produce doped carbon materials with other elements (e.g., B, P, and F) which can expand potential application fields.

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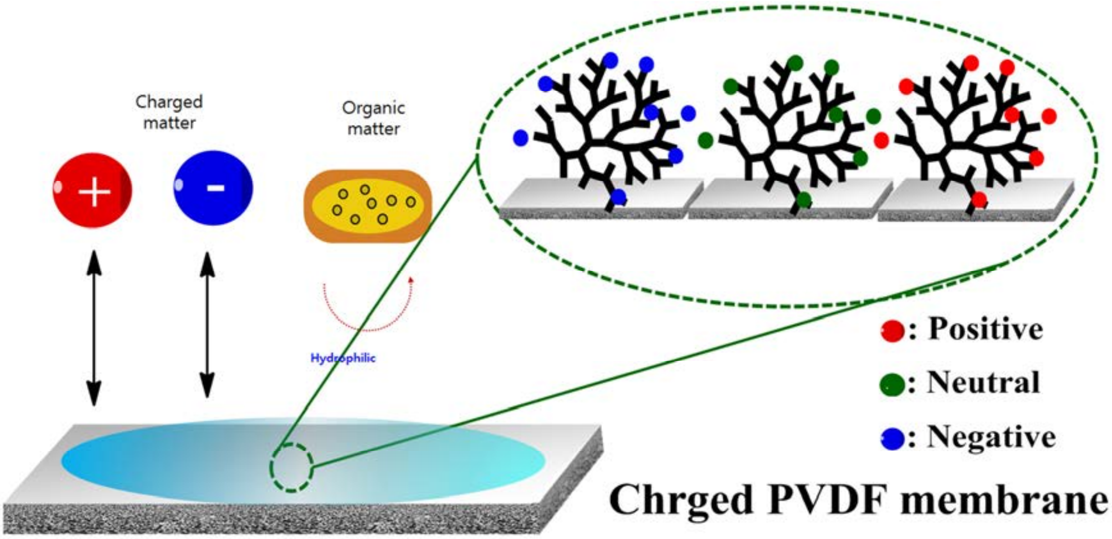
장소: 광주 김대중컨벤션센터
발표코드: **MAT.O-2**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:12, 좌장: 박종남

Surface Charged PVDF Membrane via Assembly of Charged Hyperbranched Polyglycerol (HPG) for Suppression of Membrane Fouling

김예지* 곽승엽*

서울대학교 재료공학부

Ultra/micro (UF/MF) filtration membrane can effectively purified contaminated water by remove of small pollutants such as colloidal particles, microorganisms and etc. However, membrane often lose performance due to fouling which is defined as accumulation of undesired materials on surface of membrane to deteriorate membrane performance and lifetime. It has been well known that the fouling is caused by electrostatic forces and the hydrophobic interaction between particulate and hydrophobic membrane surface. In this study, we develop polyvinylidene fluoride (PVDF) UF/MF membrane with fouling resistance by surface modification with charged hyperbranched polyglycerol (HPG). First, we prepared three types of charged HPG, i.e. neutral, positive, negative charges, by end-group modification. Next, commercialized PVDF membrane treated with plasma irradiation to introduce functional groups. Finally, the charged HPGs were assembly to the modified membrane using a cross-linking agent. Assessment for anti-fouling property was conducted by charged proteins (bovine serum albumin and lysozyme) contained water. These results indicated that electrostatic repulsive force of charged membrane surface and identical charged contaminants decreased foulants adsorption on membrane surface. Thus, membrane surface modification with charged HPG makes eco-friendly membrane as application to various waste water applications.


Charged matter
+
-
Organic matter
Hydrophilic
●: Positive
●: Neutral
●: Negative
Chrged PVDF membrane

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **MAT.O-3**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:24, 좌장: 박종남

Intrinsic Relationship between Enhanced Oxygen Reduction Reaction Activity and Nanoscale Work Function of Doped Carbons

천재영 주상훈[1,*]

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) 에너지화학공학부

Nanostructured carbon materials doped with a variety of heteroatoms have shown promising electrocatalytic activity in the oxygen reduction reaction (ORR). However, understanding of the working principles that underpin the superior ORR activity observed with doped nanocarbons is still limited to predictions based on theoretical calculations. We demonstrate, for the first time, that the enhanced ORR activity in doped nanocarbons can be correlated with the variation in their nanoscale work function. A series of doped ordered mesoporous carbons (OMCs) were prepared using N, S, and O as dopants; the triple-doped, N,S,O-OMC displayed superior ORR activity and four-electron selectivity compared to the dual-doped (N,O-OMC and S,O-OMC) and the monodoped (O-OMC) OMCs. Significantly, the work functions of these heteroatom-doped OMCs, measured by Kelvin probe force microscopy, display a strong correlation with the activity and reaction kinetics for the ORR. This unprecedented experimental insight can be used to provide an explanation for the enhanced ORR activity of heteroatom-doped carbon materials.

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발표코드: **MAT.O-4**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:36, 좌장: 박종남

Interface Controlled Synthesis of Heterodimeric Silver-Carbon Nanoparticles Derived from Polysaccharides

최유리 김병수*

울산과학기술대학교(UNIST) 친환경에너지공학부

Hybrid nanoparticles composed of multiple components can offer unique opportunities for understanding the nanoscale mechanism and advanced material applications. Here, we report the synthesis of heterodimeric silver-carbon dot nanoparticles (Ag-CD NPs) where Ag NP is grown on the surface of CDs derived from polysaccharide such as chitosan and alginate through the photoelectron transfer reaction between CD and Ag^+ ions. The nanoscale interface between the Ag NPs and the CDs is highly tunable depending on the precursor of CDs and the amount of additives, resulting in fine modification of photoluminescence of the CDs as well as the related surface plasmon resonance of the Ag NPs. This result demonstrates the critical role of interface between the hybrid nanoparticles in governing the electrical and optical properties of respective nanoparticles.

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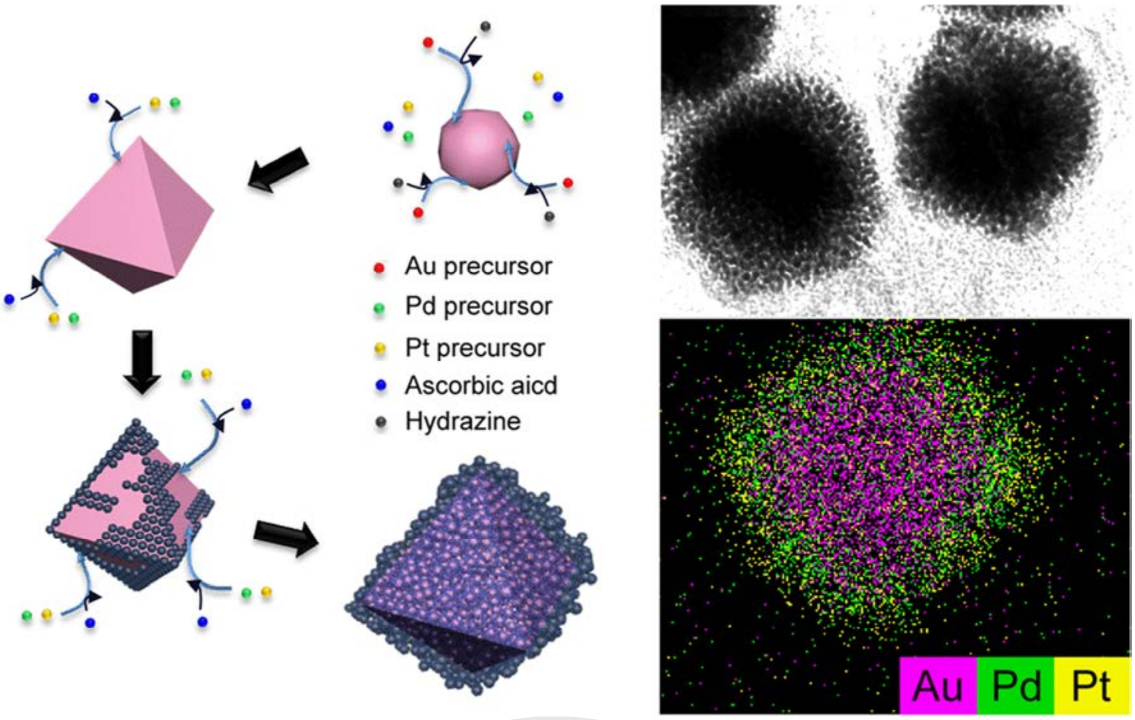
발표코드: **MAT.O-5**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:48, 좌장: 박종남

One-Pot Synthesis of Trimetallic Au@PdPt Core-Shell Nanoparticles with High Catalytic Performance

강신욱 한상우*

한국과학기술원(KAIST) 화학과

The development of an efficient synthesis method to produce multi-metallic nanoparticles (NPs) with a desirable structure is strongly required to clarify the structure-composition-property relationship of NPs and to investigate their possible applications. However, the controlled synthesis of NPs consisting of multiple ($n \geq 3$) noble metal components has been relatively unexplored in comparison to bimetallic NPs. In the present work, we have demonstrated a facile one-pot aqueous approach for the controlled synthesis of trimetallic Au@PdPt core-shell NPs with a well-defined octahedral Au core and a highly-crystalline dendritic Pd-Pt alloy shell (Au_{oct}@PdPt NPs). The simultaneous reduction of multiple metal precursors with dual reducing agents, namely, ascorbic acid and hydrazine, gave a fine control over the nucleation and growth kinetics of NPs, resulting in the formation of noble Au_{oct}@PdPt NPs. The prepared NPs showed excellent catalytic performance for methanol electrooxidation, which can be attributed to their optimized binding strength toward adsorbate molecules due to the improved charge transfer between core and shell of the NPs. The present strategy can offer a convenient and valuable way to fabricate multi-component nanostructures with desired structures and functions.


Au precursor
Pd precursor
Pt precursor
Ascorbic aicd
Hydrazine
Au
Pd
Pt

일시: 2014년 10월 15~17일(수~금) 3일간
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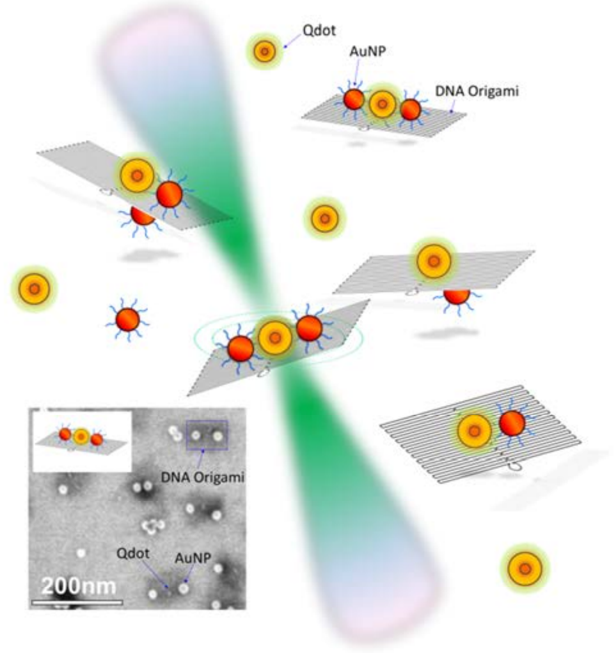
발표코드: **MAT.O-6**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 박종남

DNA Origami Constructs for Controlling Optical Behaviors of Nanoparticles

고승현

기초과학연구원 나노물질및 화학반응 연구단

The ability to organize nanostructures of disparate types and materials ? such as metal nanoparticles and semiconductor quantum dots ? is challenging but essential for the creation of novel materials and devices. Metal nanoparticles (NPs) have interesting individual plasmonic properties and can be organized to exhibit useful collective responses. Quantum dots (Qdots) provide a powerful means to optically access the nanoscale. Bringing the two together in a well-controlled manner can create structures with interesting properties such as fluorescence enhancement/quenching and high efficiency F?rster resonance energy transfer.Here we report a novel, flexible approach to fluorescence lifetime engineering of CdSe/ZnS (core/shell) Qdots by controlling their coupling to adjacent gold nanoparticles (AuNPs) at geometrically different locations on the DNA origami. To examine these constructs in their native state in solution, we use a 3-D, real-time, single-particle tracking system. We determine the influence of AuNPs on Qdot fluorescence lifetime by systematically varying the location, number, and size of AuNPs as well as interparticle distance and spectral overlap between AuNP and Qdot. The DNA origami serves as a programmable nano-pegboard for heterogeneous integration of Qdots and AuNPs wherein complex geometries are created by using modified staple strands on the DNA origami to capture specific nanoparticles. In this work, we manipulate and control the average photon count rate and lifetime of Qdots by varying the geometrical configuration of Qdot-AuNP conjugates on DNA origami and observe good agreement between theory and measurement. In addition, we will introduce our current efforts to integrate carbon dot and metal nanoparticle using DNA based assemblies.


Qdot
AuNP
DNA Origami
DNA Origami
Qdot
AuNP
200nm

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **MAT.O-7**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 11:12, 좌장: 박종남

Density-varied vertical silicon nanowire arrays for cell manipulation

강동희 윤명한*

광주과학기술원(GIST) 신소재공학부

Recently, vertical nanostructures were fabricated using several inorganic materials such as silicon, InAs, ZnO and GaP for cell manipulations in biotechnology. Among them, vertical silicon nanowire arrays (vSiNWs) is one of the most intensively studied platforms for intracellular drug delivery, cell capture, and cell function recording due to their biocompatibility and established surface chemistry. Herein, we developed a modified method of metal assisted chemical etching (MACE) for ultra-low density vertical silicon nanowire arrays (vSiNWs) in addition to the fine control over nanowire diameter, height, and pattern. Furthermore, we examined the detachment efficiency of cells deposited on vSiNWs by varying nanowire density and proved that the density of vSiNWs is one of the most important geometric parameters for cell manipulation on top.

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발표코드: **MAT.O-8**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 11:24, 좌장: 박종남

Random copolymer-directed synthesis of crystalline mesoporous oxides with uniform mesopores

조창범 유룡[1,*]

기초과학연구원 나노물질 및 화학반응 연구단 [1]기초과학연구원 나노물질및화학반응연구단

Mesoporous materials have attracted significant attention in numerous applications such as catalysis, gas sensing, optics, energy storage/conversion and photovoltaics. Currently, one of the most widely employed method for synthesizing mesoporous materials is the use of surfactant micelles and block copolymer assemblies as the structure-directing agents (SDAs). Here, we present a new synthetic route to mesoporous materials using amorphous random copolymers as the SDAs. The copolymers are randomly functionalized with side groups that can strongly bind to inorganic precursors. In this synthesis, tight binding of the side groups with an inorganic precursor leads to the formation of a mesostructured polymer-inorganic composite gel. The tight bonding is strong enough to maintain during crystallization process. As the crystal started the growth, polymer backbones are proposed to gather around the surfaces of the inorganic crystals, giving rise to a huge steric hindrance between the backbones. Therefore, crystal growth is restricted to a thickness of a few-nanometers. We demonstrate this method for a variety of mesoporous inorganic materials such as zeolite nanosponges, their aluminophosphate analogues, sub-nanometer thick TiO_2 nanosheets, and nanosponges of TiO_2, SnO_2 and ZrO_2.

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장소: 광주 김대중컨벤션센터

발표코드: **MAT.O-9**

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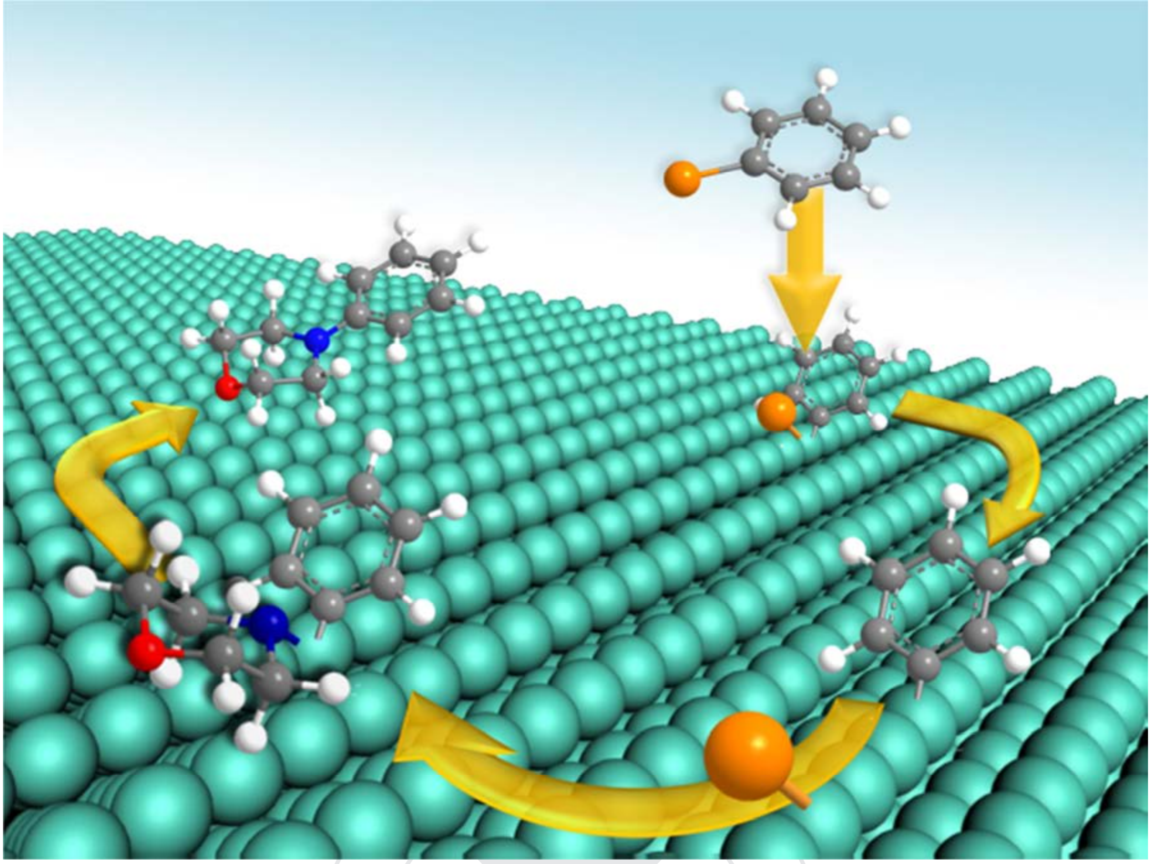
발표종류: 구두발표, 발표일시: 금 11:36, 좌장: 박종남

Facet-dependent enhanced catalytic activity of Pd nanocrystals

김민준 한상우*

한국과학기술원(KAIST) 화학과

The systematic study on heterogeneous Buchwald-Hartwig amination using shape-controlled Pd nanocrystals (NCs) with distinctly different surface facets was investigated. Shape-controlled Pd NCs, which includes octahedral, cubic, and rhombic dodecahedral Pd NCs, were prepared with the equal surfactant and reductant to exclude the adsorbent effect1 during catalytic reaction when the shape-controlled Pd NCs were utilized. We found that the catalytic activity of the Pd NCs strongly depends on their facets, and rhombic dodecahedral Pd NCs enclosed exclusively by {110} facets are the most desirable catalyst among the various types of Pd catalysts including Pd/C and homogeneous Pd catalysts. From density functional theory calculations, the origin of the facet-dependence and a plausible reaction pathway of heterogeneous Buchwald-Hartwig amination could be proposed.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **MAT.O-10**

발표분야: Current Trends in Materials Chemistry

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Spatially controllable method in hydrothermal growth of ZnO nanowires using liquid masking layers

장훈수 손보경 고흥조*

광주과학기술원(GIST) 신소재공학과

This study demonstrates a simple and controllable method in hydrothermal growth to generate spatially well-defined multi-length-scale ZnO nanowires on curvilinear substrates. Compared to the case of using a solid lid that is widely used, introducing immiscible liquid masking layers (LMLs) above and beneath an aqueous nutrient solution offers diverse advantages. LMLs preserve the volatile reactants and solvent in the nutrient solution and thereby stabilize pH during the entire growth process, which plays an important role to generate desired shapes of ZnO nanowires. The conformal wettability of LMLs offers easy access of additional equipment such as linear/rotation motion stages. Selective growth in a growth zone that is defined by LMLs in dynamic/static modes enables controllable growth of gradual, terraced, and spiral ZnO nanowire arrays. As an application, we developed cylindrical photodetectors with a configuration of Cr/ZnO seed/ZnO nanowires/poly(3-hexylthiophene-2,5-diyl)/poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate).

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발표코드: **MAT.O-11**

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발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 박종남

Fabrication of Tungsten Disulfide / Reduced Graphene Oxide Composites for High Efficient Thermoelectric Devices

김수현 이현정*

국민대학교 신소재공학부

Thermoelectric performance is determined by figure of merit, ZT. Achievements of high electrical conductivity, high Seebeck coefficient and low thermal conductivity are important for high performance thermoelectric devices. Tungsten disulfide (WS_2) has been interested as thermoelectric materials because it has high Seebeck coefficient(α) as 375-1000(μV/K). However, it has low ZT values due to its low electrical conductivity (10^{-1}-10^{0}S/m). On the other hand, carbon based materials usually have high electrical conductivity. Specifically, thermally reduced graphene oxide (rGO) used in this study showed high electrical conductivity of $2.0x10^{4}$(S/m) and large charge carrier mobility (15,000 cm^2/Vs). In this respect, we expect that rGO provides an effective conductive path for transfer of charge carriers in WS_2/rGO composites and their thermoelectric property increases. In addition, restacked WS_2(R-WS_2) has been reported with decrease of thermal conductivity because their disordered structures by restacking induce an effective phonon scattering. Therefore, in this study, we fabricated composites of WS_2/rGO as a function of weight percent of rGO in order to obtain optimized ZT values and we compared their properties with those of R-WS_2/rGO composite.

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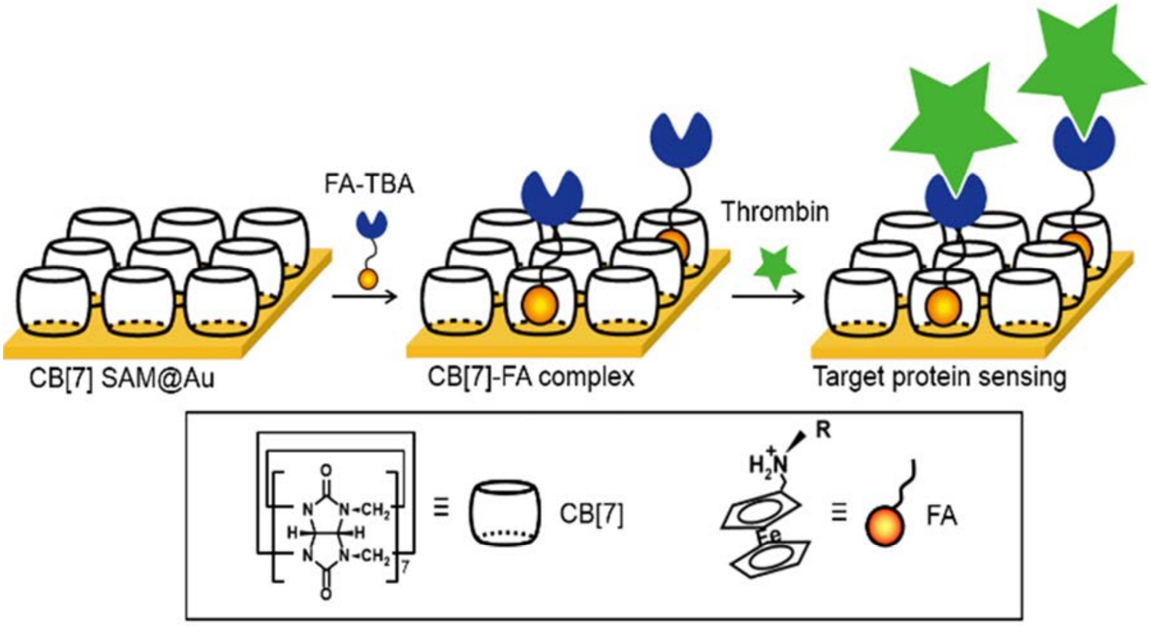
발표코드: **MAT.O-12**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 12:12, 좌장: 박종남

A Simple and Modular Aptasensor Platform Utilizing Cucurbit[7]uril and Ferrocene Derivative As an Ultrastable Supramolecular Linker

박경민 공보경[1] 김기문[1,*]

기초과학연구원 복잡계자기조립연구단 [1]포항공과대학교(POSTECH) 화학과

Aptasensors have been investigated for efficient detection of biomolecules utilizing aptamers as selective biorecognition components. One of major concerns in the development of aptasensors to date is the influence of immobilization of aptamers on surfaces. Here we demonstrate the use of an ultrastable artificial binding pair system, ferrocenemethylammonium (FA)-cucurbit[7]uril (CB[7]) (K ~10^{12} M^{-1}), as an efficient and versatile supramolecular linker to immobilize FA-conjugated aptamers on self-assembled monolayer (SAM) of CB[7] for surface plasmon resonance (SPR) studies. The unique features of this linker system include 1) an easy preparation, 2) resistance to harsh conditions, 3) versatility for various aptamers, and 4) long term durability due to the uses of stable synthetic molecules. This FA-CB[7] linker-based aptasensor may provide efficient sensing of various biomolecules including proteins, and thus widen the practical applications of aptasensors.


FA-TBA
Thrombin
CB[7] SAM@Au
CB[7]-FA complex
Target protein sensing
CB[7]
FA
R
Fe

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **MAT.O-13**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 12:24, 좌장: 박종남

Nanocarrier-Functionalized Magnetite as Nanosorbents for Removal of Heavy Metal Ions in Water

이지환 곽승엽*

서울대학교 재료공학부

Heavy metals are defined as transition metals or metalloids with a density higher than 5.0 gcm^{-3}. Especially, some of heavy metals (e.g., As, Pb, Cu, etc.) are highly toxic even at a low level. It is well known that toxic heavy metals become serious problem threatening human health and ecosystem integrity. Simple and effective methods are presented here to prepare multi-functional adsorbents by introduction of hyperbranched poly(amidoamine) (PAMAM) and positively-modified branched polyethylenimine (p-PEI) onto magnetite (PM-MG and p-MG) for the removal of heavy metal ions in contaminated water. PAMAM and p-PEI are capable of adsorbing the heavy metal cations and anions respectively. The properties of PM-MG and p-MG were characterized via FT-IR, XPS, WXRD, FE-SEM, TEM. Their magnetic properties were also evaluated by VSM. The adsorption capacities of PM-MG and p-MG for Cu(II) and As(V) were measured by ICP-AES. Especially, PM-MG and p-MG have a characteristic of super-paramagnetism resulting in facile removal from water under a relatively low external magnetic field. Therefore, these results suggest that PM-MG and p-MG have a great potential for efficiently separable and reusable adsorbent with high efficiency for removal of heavy metal ions in contaminated water.

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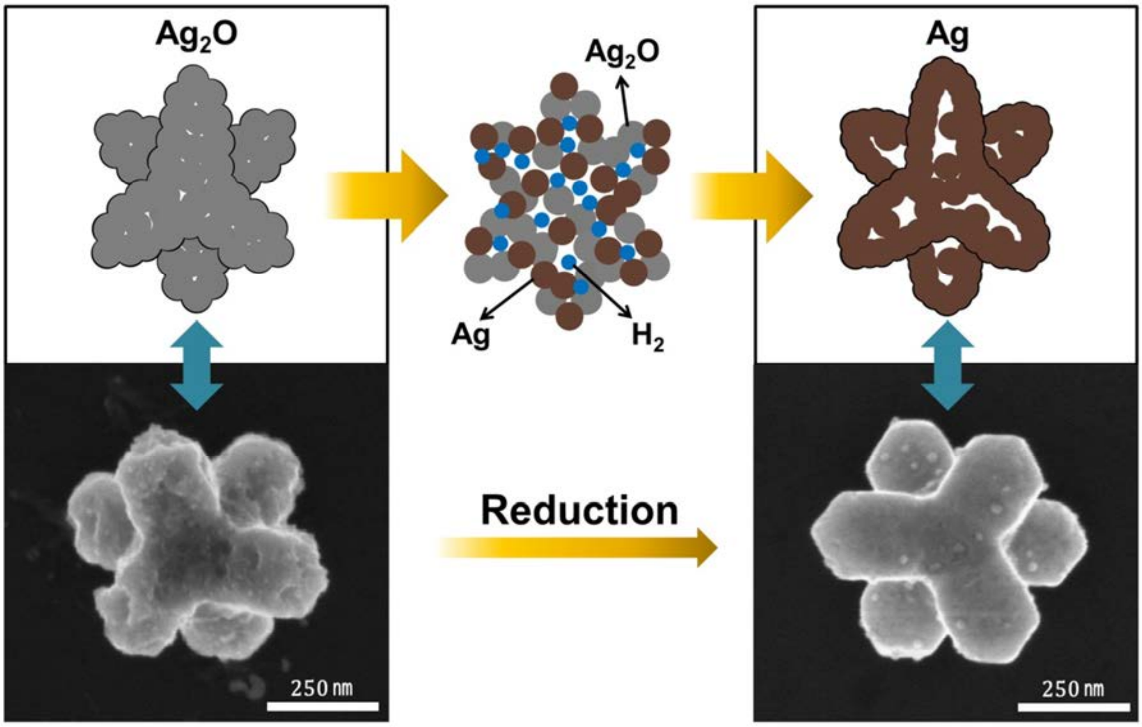
발표코드: **MAT.O-14**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 12:36, 좌장: 박종남

The Synthesis of Hollow Silver Hexapods using Silver Oxide Hexapods as Templates

조지희 임종국*

조선대학교 화학과

For the synthesis of a variety of nanoparticles, many different methods have been developed. One of powerful method to make nanoparticles is template-based approach. Since the size or shape of nanoparticles is confined by such templates, more diverse nanoparticles can be obtained by the template-based method. In this paper, we firstly synthesize Ag_2O hexapods using a new method, and use them as templates for the synthesis of hollow Ag hexapods. The synthesized Ag_2O hexapods are reduced into Ag in the vicinity of surfaces, and Ag_2O hexapods are finally transformed into hollow Ag hexapods. We will show the experimental evidences for this unprecedented shape-keeping reduction of semiconductors into metals with plausible mechanism.


Ag_2O
Ag_2O
Ag
Ag
H_2
Reduction
250 nm
250 nm

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **MAT.O-15**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 12:48, 좌장: 박종남

Stimuli-Responsive Fluorescent Azobenzene Nanofibers

한민아* **조성준[1]** **Yasuo Norikane[2]** **Masaki Shimizu[3]** **Akinori Kimura[3]** **Tomokazu Tamagawa[3]** **Takahiro Seki**

Nagoya University [1]전남대학교 응용화학공학부 [2]National Institute of Advanced Industrial Science and Technology (AIST) [3]Kyoto Institute of Technology

The creation of diverse nano/microstructures and their functions depends not only on the nature of their molecular components but also on the spatial arrangement of the functional groups. For instance, C3-symmetrical molecules show a propensity to be effectively packed into one-dimensional (1D) cylindrical tubules, fibers, or helices through non-covalent interactions such as pi-pi stacking, hydrogen bonding and/or van der Waals interactions. The 1D structures have received much attention due to their potential for molecular alignment, conductivity, mass transporting, and optoelectronic materials.In this study, we designed a trigonal azobenzene-based chromophore to create fluorescent one-dimensional (1D) structures with high crystallinity. Our experimental results indicate that a conformational transformation from a distorted to a partially planar form during assembly would allow the chromophore to effectively assemble into a crystalline fiber in an inclined fashion. The formation of the crystalline fibers is thus accompanied by a significant red shift in absorption bands and an increase in fluorescence efficiency. The enhanced fluorescence can be readily switched off by weakening the degree of crystallinity. Moreover, even in a solvent-free polymer matrix in which azobenzene-based chromophores are well dispersed, the chromophores are distinguished from the polymer matrix by their strong ability to assemble into cylindrical aggregates and by the resulting color and fluorescence characteristics.References 1.M. Han and M. Hara, J. Am. Chem. Soc. 127, 10951 (2005).2.Y. Hong, J. Lam, B. Z. Tang, Chem. Soc. Rev. 40, 5361 (2011). 3.B. An, J. Gierschner, S. Y. Park, Acc. Chem. Res. 45, 544 (2012).

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **POLY.P-1**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Chromonic nanofiber embedding self-assembled discotic Sunset-Yellow dyes

강동규 임푸른[1] 윤원진 최유진[2] 김지태 정광운[3,*]

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

Chromonic nanofibers with the self-assembled Sunset-Yellow(SSY) nanocolumns were fabricated by electrospinning method. Molecular packing structures and optical behaviors of the anisotropically aligned H-SSY/PVP nanofiber mats were investigated by the combined various techniques such as 2D wide angle X-ray diffraction(WAXD), polarized optical microscopy(POM) and scanning electron microscopy(SEM). When the H-SSY/PVP nanofiber mats were annealed above T_g of PVP, H-SSY nanocolumns further self-organized to form crystals. This means that the electrospun nanofiber below the Tg of PVP was in a metastable state.This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education (2013R1A1A2007238), Global Ph.D Fellowship Program (2013H1A2A1033907), and BK21 PLUS Program, Korea.

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장소: 광주 김대중컨벤션센터

발표코드: **POLY.P-2**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermal, Mechanical, and Morphological Properties of Poly(ester amide) Elastomers

오성진 우정오 박종은 손경선*

충남대학교 화학과

A family of synthetic poly(ester amide)s composed of polyols, a diaminoalcohol, and a diacid were developed. The resulting elastomers were comparatively investigated in terms of thermal and mechanical properties, swelling behaviors, and morphologies. The material properties of these polymers could be tuned by adjusting the nature of the polyol and the stoichiometry of the reactants.

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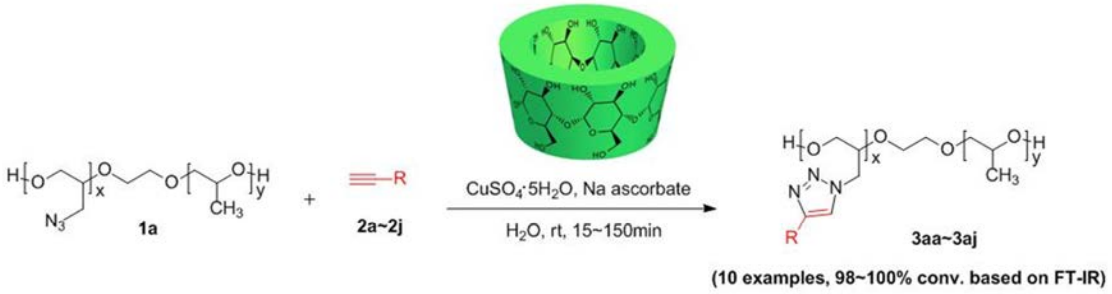
발표코드: **POLY.P-3**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Triazole-containing Copolymers in Water catalyzed by Cyclodextrin

신정아 임영권[1,*]

국방과학연구소 4본부 2부 [1]국방과학연구소 4-2

Cyclodextrin (CDs) are cyclic oligosaccharides with a hydrophilic hydroxyl group on their outer surface and a hydrophobic cavity in the center. CDs are capable of forming inclusion complexes with many chemicals including polymers by taking it up into the cavity. These inclusion complexes have been shown to improve solubility of poorly water soluble chemicals. In general, water is the ideal solvent which is eco-friendly, non-toxic, cheap and abundant. Thus, CuAAC reactions in water without organic solvent are valuable. However, while click reactions of organic substrates using water only as solvent have been well known, the cases of polymer are still rare. We found that cycloaddition rate of glycidyl azido polymer (GAP) with alkynes was accelerated under CDs in the water. And in the presence of catalytic amount of CD, we could obtain various triazole-containing copolymers from cycloaddition of GAP with terminal alkynes in water in 98~100% conversion yields.



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

Universal water-soluble cyclodextrin polymer-carbon nanomaterials with supramolecular recognition

ZHANGWANG 박원철*

서울대학교 융합과학기술대학원 나노융합학과

Functionalization of carbon nanomaterials (including fullerenes, single-walled carbon nanotubes, multi-walled carbon nanotubes (MWCNTs), and graphene sheets) dispersed in water with macromolecules was achieved by a one-step strategy using β-cyclodextrin polymer (CDP). These nanomaterials showed high solubility and stability in water because of the noncovalent interaction between carbon nanomaterials and CDP. The conjugates (PATP-CDP-MWCNTs) were ideal templates for the highly efficient assembly of noble metal nanoparticles (Au and Pt) with dramatically different properties. Methanol oxidation of Pt-decorated PATP-CDP-MWCNTs in CV analyses indicated its potential application in direct methanol fuel cells, facilitating the feasibility of metal-decorated CDP-carbon nanomaterials in real technological applications. This universal method of producing carbon nanomaterials functionalized with macromolecules is beneficial for investigating the structure-performance relationship of carbon nanomaterials for designing compounds with specialized functions.

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

Thermogelling system for VEGF delivery to hind limb ischemic mouse model

고두영 정병문*

이화여자대학교 화학나노과학과

Ischemic vascular disease of the circulatory system and the heart cause death or loss of limb. It is caused by an insufficient supply of oxygen and nutrients to the tissues, leading to cellular apoptosis and tissue degeneration. There are many reports about VEGF (vascular endothelial growth factor) treated in ischemic model. However, this drug have problem such as denaturation, short half-life; require the osmotic pressure equipment for the sustained release of the drug. So, new drug delivery systems, such as hydrogel have been studied. We investigated a thermosensitive hydrogel system that possible to sustained drug release and to overcome these limitations in current delivery. mPEG-PAF (5wt.%) aqueous solution seems to sol-gel transition at 25oC. According to the in vitro drug release profile of VEGF using thermogel, VEGF is continuously released over 7days. In addition, make the hind limb ischemia BALB/c mice model for in vivo experiments. In vivo study was divided by 4 groups such as PBS, thermogel, VEGF, and co-treatment (thermogel with VEGF). As a result, co-treatment (thermogel with VEGF) system shows fast recovery and angiogenesis compared to thermogel or VEGF only system after 14days. ROI value showed the co-treatment group (52±18%) significant neovascularization compare to thermogel (31±6%) or VEGF (27±9%) alone.

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발표코드: **POLY.P-6**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Poly(glycidyl triazole-co-glycidyl amino tetrazole)

정지혜 **배세원[1] 임영권***

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부

Tetrazoles are nitrogen-rich compounds which have high heat of formation. So they have been used as promising candidates for explosive and gas generator. To obtain high energy density material(HEDM), we designed polymer containing both azide and tetrazole pendants. So poly(glycidyl triazole-co-glycidyl amino tetrazole)(PGAAT) are synthesized by two step reactions. The structures of PGAAT are confirmed by IR, ^{1}H and ^{13}C NMR spectral analyses. Thermal properties of the PGAAT are evaluated using differential scanning calorimetry(DSC).

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발표코드: **POLY.P-7**
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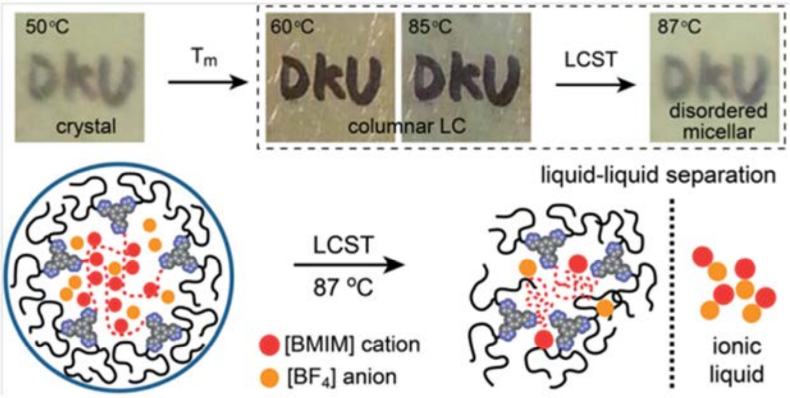
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembling and LCST properties of Dendron-coil-dendron Block copolymer/ionic liquid electrolytes

노민주 조병기*

단국대학교 화학과

Nanostructured molecular systems have played an important role as platform materials for the development of high performance electro-active materials. Structurally distinct BCPs based on dendritic or miktoarm polymers have been known to show different assembling properties from linear BCPs due to their asymmetric chain architecture. Ionic liquids (ILs) consisting of large and asymmetric ionic species are unique solvents with some merits, including non-volatility, non-flammability, high electrochemical stability, and good ionic conductivity. And imidazole salt derivatives have mainly been used for the IL component, and they were selectively swollen in ionophilic blocks such as PEO, PMMA, and PSS. We prepared several electrolytes by mixing a dendron-coil-dendron BCP and molecularly different ILs, and examined their phase, conductivity and LCST behavior.


50°C
crystal
T$_m$
60°C
85°C
columnar LC
LCST
87°C
disordered micellar
liquid-liquid separation
LCST
87 °C
[BMIM] cation
[BF$_4$] anion
ionic liquid

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발표코드: **POLY.P-8**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Poly(glycidyl azide-co-glycidyl tetrazolone)

정지혜 신정아[1] 임영권[*]

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부

Glycidyl azide polymer(GAP) has been used for energetic binders. GAP has good properties such as low T_g, low viscosity, high density, high positive heat of formation, and good compatibility with eco-friendly oxidizers. Tetrazolone is thermally stable nitrogen-rich compounds. And it also has very low sensitivity. To make insensitive energetic binder, we designed poly(glycidyl azide-co-glycidyl tetrazolone)(PGATN), polyether containing azide and tetrazolone pendants. Moreover it is expected that oxygen in tetrazolone may improve oxygen balance of PGATN. The structures of PGATN are confirmed by IR, ^{1}H NMR, ^{13}C NMR spectral analyses. Thermal properties of the PGATN are evaluated using differential scanning calorimetry(DSC).

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발표코드: **POLY.P-9**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorinated graphene oxide/Nafion composite membrane for VRB applications

유호연 조창기*

한양대학교 유기나노공학과

In this study, sulfonated graphene oxide (sGO) was prepared from GO, then the product was reacted with phenyl isocyanate to prepare isocyante modified sGO (isGO) in order to increase some hydrophobicity for a better miscibility with Nafion. Also fluorinated GO (FGO) was prepared from GO and HF in order to prepare a GO derivative which is expected to have a better miscibility with fluorocarbon containing Nafion polymer. The GO derivatives were characterized by FTIR and X-ray photoelectron spectroscopy. Composite membranes of Nafion with GO, isGO, and FGO were prepared, and their adaptability as membranes for vanadium redox battery (VRB) was investigated in terms of proton conductivity, water uptake, and methanol permeability. For all these membranes pristine Nafion membrane was used as a reference.

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발표코드: **POLY.P-10**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

TPD-based Donor-Acceptor Alternating Conjugated Copolymers containing Thiophene and Selenophene-based Monomers for Electronic Applications

이대희 박지은 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

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

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

Comparison of synthetic methods of fully alicyclic polyimides

유환철 정찬문*

연세대학교 화학과

Fully alicyclic polyimides (APIs) are promising because of their high optical transparency, high solubility and low dielectric constant. In order for the polyimides to have the desirable properties, they need to have high molecular weight. However, in the preparation of polyimides based on alicyclic diamines, high molecular weight polyimides can't be obtained. This is attributable to the formation of carboxylic acid salt that is due to high basicity of alicyclic amines. In this study, we have compared four synthetic methods of fully APIs, normal 2-step, N-silylation, in-situ silylation and synthesis using m-cresol. Structures of the APIs were confirmed by 1H NMR and FT-IR spectra. Viscosity of the APIs was obtained to compare their molecular weight. Solubility of the APIs was tested in various solvents and thermal property of the APIs was investigated by DSC and TGA.

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

가교폴리에틸렌(cross-linked polyethylene,XLPE)의 열열화 정도에 따른 결정화도 변화 연구

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조선대학교 첨단소재부품공학과 [1]조선대학교 응용화학소재공학과

가교폴리에틸렌(Cross-linked Polyethylene, XLPE)은 초고압 전선 등에 많이 사용하는 절연재로써 저밀도 폴리에틸렌(Low Density Polyethylene, LDPE)을 hydrogen peroxide 로 가교시켜 나온 PE 중의 하나이다. 사용 중에 열, 전기, 산소에 의해 열화되는 현상이 나타나는데, 그 중에서 열에 의한 노화에서 나타나는 현상을 연구하기 위하여 80℃, 대기압에서 18 개월(XLPE18)과 36 개월(XLPE36) 열열화시킨 것을 각각 준비하였다. 질소 분위기 하에서의 TGA 측정으로부터 얻은 열분해 온도는 XLPE18 보다 XLPE36 의 온도가 더 높았다. 이는 열열화가 진행될수록 열분해 온도가 높아진다는 것으로 볼 수 있다. 시간이 지날수록 공기 중의 산소와 결합하여 발생한 새로운 산화물이 시료 안에 많아질 수 있으므로 완전 분해되기까지 시간이 지연되어 열분해 온도가 높아진 것으로 해석하였다. 또한 DSC 와 X-ray 로부터 결정화도를 측정하여 보았는데 각각 XLPE18 이 XLPE36 보다 결정화도가 높게 나왔다. 이를 통해 노화가 진행될수록 결정화도가 낮아짐을 알 수 있었다. FT-IR 로부터는 XRD 와 DSC 결과와 유사한 결정화도의 감소와 더불어 위에서 언급했던 산화성 화합물들의 정체가 무엇인지를 결정할 수 있었다.

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

Synthesis of partial aliphatic polyimides containing anthracene moiety for polyimide application

유환철 이재희[1] 정찬문[*]

연세대학교 화학과 [1]연세대학교 고분자화학연구실

Recently, polyimides are applied to novel devices such as gate dielectric layers in organic field-effect transistors or insulation layers in organic light emitting diodes. However, fabrication of these devices requires much less than 300 °C curing temperature to obtain the satisfactory results. There are several approaches to solve the problem including the introduction of soluble polyimide such as fully aliphatic polyimides or partial aliphatic polyimides. However introduction aliphatic monomers have such problems like low thermal and mechanical stability and chemical resistance. The object of this study is to develop soluble partial aliphatic polyimide precursor and to supplement the precursor by which introduction of cross-linkable site into main chain. We have synthesized of partial aliphatic polyimides containing anthracene moiety than performed cross-linking reaction with bismaleimides in solution state.The cross-linking between polyimides and bismaleimides was confirmed by 1H-NMR and the thermal and mechanical stability were confimed by TGA and DSC.

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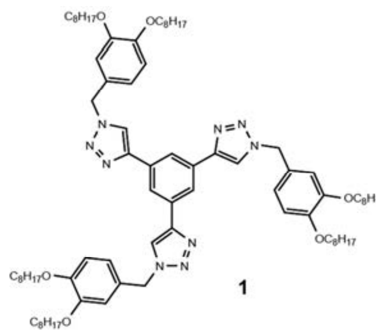
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the conformational effect on C_3-symmetric liquid crystals showing smectic, helical and columnar assemblies

박소영 조병기*

단국대학교 화학과

We studied the self-assembling properties C_3-symmetric liquid crystals (LCs) with triazole-based aromatic cores. In order to examine the conformational effect on the self-assembling behavior, the aromatic structures were somewhat differently designed as below figure. First,1 with the benzylic unit exhibits an unusual smectic E-like organization in the LC state. Based on the conformational consideration, the smectic assembly is attributed to the formation of an endo-type Y-conformer of asymmetric triazolyl and benzylic groups that cannot be accessed in other C_3-symmetric molecules exclusively showing columnar assemblies. The Y-conformers form a two-dimensional oblique lattice in the local aromatic layers of the ordered smectic phase. In addition, the Y-shaped conformer in the smectic phases can changes into a circular shape by the 1 : 1 hydrogen-bonding interaction with a gallic acid derivative, which leads to a hexagonal columnar LC phase. On the other hand, 2 and 3 employed a fully conjugated aromatic core instead of benzylic unit. In contrast to the former example, these mesogens have propeller-like structure due to limited conformations. Depending on degree of space filling of the dendritic wings, the aromatic cores adopt either flat or propeller-like conformer to fulfill the columnar cross-section effectively. Specific helical arrangement from tilted dendritic wings dealt in terms of conformational argument. Furthermore, the propeller-like mesogen in the helical columnar phase changes into a coplanar shape upon heating above the Tg and loses the long-range helical order due to longitudinal fluctuation of the dendiritic wings. Upon further heaing, the column loses the intracolumar order with increasing the conformational motions. The triazole-based LCs design concept prove the engineering of diverse molecular assemblings including the smectic, helical columnar, ordered and disordered columnar structures.



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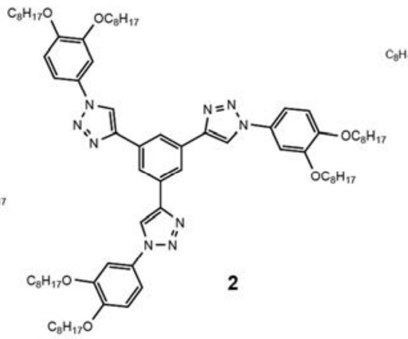

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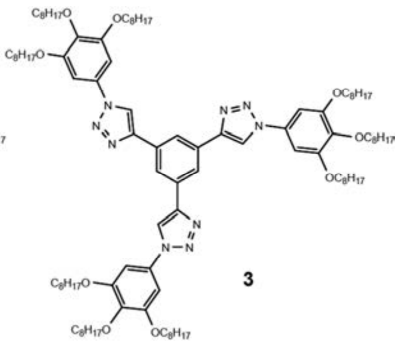

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일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **POLY.P-15**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Tonsil derived mesenchymal stem cell differentiation in alpha-cyclodexrin conjugated hydrogels

정보경 정병문*

이화여자대학교 화학나노과학과

Cyclodextrins are used in pharmaceutical applications for numerous purposes, including improve the bioavailability of drugs. We are reporting reverse thermal gelling poly(ethylene glycol)-poly(L-alanine) (PEG-L-PA) aqueous solution for 3D culture of human tonsil-derived mesenchymal stem cells(TMSC). Polymers were synthesized by ring-opening polymerization, and were characterized by 1H-NMR, GPC, and rheometer. Cyclodextrin conjugated hydrogels were prepared from the inclusion complex of PEG-L-PA, and α-cyclodextrin (α-CD). The TMSC were encapsulated in the polymer aqueous solution and cultured for 3 weeks. In 2D system, TMSC treated α-CD for 3 weeks. We investigated cell proliferation and cell viability by CCK-8 assay and Live/Dead. The gene and protein expression levels in the cells were estimated by real time quantitative PCR, and immunofluorescence. The results of this study shows that α-CD impact on TMSC proliferation and differentiation in 3D environments.

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발표코드: **POLY.P-16**

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Water-enabled Self-healing Nanocomposite based on Poly(ethylene oxide) Prepared by γ-ray Irrdaiation

이호익 유정주 손대원*

한양대학교 화학과

In this study, we describe new stagey for healable materials based on poly(ethylene oxide) (PEO) nanocomposite using chain diffusion by water molecules. As a healing material, organic/inorganic nanocomposite composed with PEO and halloysite is prepared by simple 60Co r-ray irradiation method. This material has the ability repair itself following damage due to segment mobility by addition of water. Two broken species are attached each other by physical approach having water molecules, the fractured surfaces become intermixed through chain diffusion and tangled. It is prepared without any cross-linker and initiator allowing it to retain the characteristic of intact PEO. We found that PEO film irradiated with γ-ray in such manner can be induced by water to heal itself at upon air-drying at room without the need for any external stimulus or healing agent. PEO nanocomposite was cut into two pieces using scissors and the two halves taken from each original nanocomposite were put together. Two ends were placed together and a drop of water was applied on the surface of the sliced end regions. This resulted in the diffusion of PEO polymer chains from one-half of the strip to the other, which then became entangled during the air-dry process. To confirm the healing mechanism, small angle X-ray scattering (SAXS) experiment was conducted.

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Preparation and characterization of Hyaluronic Acid-Silica nanoparticle for drug delivery system of anticancer drug

이정욱 이호익 고재형[1] 손대원*

한양대학교 화학과 [1]한양대학교 고분자 물리화학 연구실

Hyaluronic acid (HA) has currently several therapeutic applications. HA has the relevant advantage of biocompatible, biodegradability, and specific targeting on cancer cell. In the last ten years, it has also been successfully investigated in the field of drug delivery, in the form of HA-anticancer drug conjugates. Conventional method of HA- anticancer drug delivery system is used by HA-spacer-drug conjugate system. But in this method, the binding of HA-spacer-drug can be acted as a limitation in terms of loading quantity. The loading quantity of anticancer drug in HA-spacer-drug system is limited as a factor that how many conjugates of HA-spacer-drug are made. To overcome this limitation, this research focused on another way to get high loading quantity by combining silica particle with HA; core-shell particle. The particles were characterized for the structure, morphology and modification through SEM, FT-IR, and NMR.

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Donor-Acceptor Alternating Conjugated Terpolymers for Organic Photovoltaic Cells

김애선 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Solution processed bulk-heterojunction (BHJ) solar cells have been intensely studied owing to promising advantages for cost-effective manufacturing and applicability to flexible large-scale devices. Recently, donor-acceptor (D-A) type conjugated molecules and polymers displayed promising characteristics in OPVs. In this study, we synthesized diketopyrrolopyrrole (DPP)-based alternating conjugated terpolymers bearing different donating units such as pyrene and thienyl unit. These donor units induced fine-tuning of energy level between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) owing to variation of conjugation length, which is useful to develop high-performance polymer solar cells (PSCs). Thermal analysis, electrochemical analysis and absorption spectroscopy were employed to investigate their material properties. Eventually, based on the study on charge transport properties, we demonstrated the feasibility in polymer solar cell applications.

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

Controlling the Photocatalytic Activity of ZnO/Au Systems Mediated by Thermoresponsive Polymers

윤민지 이지은 김동하*

이화여자대학교 화학나노과학과

Noble metals such as gold and silver are recognized for their unique surface plasmon resonance (SPR) properties resulting from the interaction with light. It has been investigated that the SPR improve the efficiency of photocatalytic activity and the effect is extremely sensitive to the distance between the constituent elements, which is exploited in Plasmon ruler. Thus, noble metal nanostructure coupled with responsive polymer can be used to probe unique plasmonic ? mediated photocatalytic properties associated with swelling-shrinking transitions in polymer chains triggered by specific external stimuli. Poly(N-isopropylacrylamide) (PNIPAM) undergoes a reversible, phase transition at a lower critical solution (LCST) of about 32 ℃ in pure water from a swollen state to a shrunken state upon increasing the temperature due to dissociation of the hydrophobic interaction between NIPAM segments and water.In this work, PNIPAM brushes were anchored on the Au film by atom transfer radical polymerization and ZnO nanoparticles were immobilized on PNIPAM for controlled photocatalytic activity. We demonstrate that the photocatalytic activity was influenced by various features such as the synthesis conditions, grafting density and molecular weight of PNIPAM involved in the ZnO-PNIPAM-Au film. According to the change in temperature with respect to the l, the distance between Au films and ZnO nanoparticles changes, resulting in plasmonic-coupling-controlled photophysical properties. Finally, we observe different plasmonic effects in terms of the degradation of organic pollutants.

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Effective chemical healing of nano-carbon materials via intra-dehydrogenative coupling

최용문 고문주*

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Nano-carbon materials are expected as next-generation materials for its electronic, thermal, mechanical, and optical properties. However, these unique properties are extremely influenced by small structural defect sites. In this study, we report an effective defect healing method of nano-carbon materials via intra-molecular cross-dehydrogenative coupling (ICDC) reaction. Actually, the Raman intensity ratio of the G band to the D band, I_G/I_D ratio, of reduced graphene oxide (R-GO) was increased from 0.77 to 1.64, and the electrical conductivity of R-GO was improved to 14 times higher than that of as-prepared R-GO. Furthermore, after the ICDC reaction, both the electrical conductivity and tensile strength of CNT yarn improved to 3.5 x 10^3 S/cm and 420 MPa, which is 180% and 200% higher than that of neat CNT yarn.

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Synthesis of Microcellular Polypyrrole in a Unidirectional Freeze-dried Polystyrene Template and the Conversion to Microcellular Carbon

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The facile fabrication of polypyrrole (PPy) foams via vapor phase polymerization using microcellular polystyrene, prepared by unidirectional freeze-drying, as a template was demonstrated. Remarkably, the PPy foams maintained the porous morphology of the template, which exhibited a bamboo-like honeycomb channel structure. In addition, the PPy foams were carbonized at 800 °C with iodine doping and the carbon products showed similar morphologies to that of the precursor. The carbon foams were characterized by Raman spectroscopy and XRD analysis and were confirmed to be amorphous carbon with a nitrogen content of about 7%.

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Synthesis and Characterization of Modified Poly(4-vinylphenol) with Thermally Curable 4-Trifluorovinyl Moiety for Gate Insulator in Thin Film Transistor

양훈주 안택*

경성대학교 화학과

To date, poly(4-vinylphenol) (PVP) (especially in the cross-linked form) is the most promising gate dielectric materials in organic electrics in the sense of realizing complex circuits on rigid and flexible substrates. However, crosslinked PVP using poly(melamine-co-formaldehyde) methylated as a cross-linking agent was known forming a “Bakelite” structure. This means that the hydroxyl group of PVP still remains after crosslinking reaction. Such hydroxyl groups can absorb moisture and could be an origin of severe hysteresis in TFT operation. Here, we modified PVP structure with thermally curable 4-trifluorovinyl moiety. Thin film properties of novel thermally crosslinked PVP (TFVOB-PVP) were systematically investigated such as chemical structures, surface roughness, surface energy, and capacitance, etc. Pentacene thin film transistor with TFVOB-PVP as a gate insulator showed a field effect mobility as 0.14 cm^2/Vs with almost no hysteresis behavior.

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

양훈주 안택*

경성대학교 화학과

Conjugated polymers have emerged as viable electronic materials for numerous applications. So far, the majority of work on conjugated polymers has been focused on linear one-dimensional polymers. Although a few of two-dimensional conjugated polymers, such as hyperbranched conjugated polymer have been reported to exhibit comparable charge transferring and processing properties to their linear counterparts, two-dimensional conjugated polymeric light-emitting materials have been less discussed in the literature. Here, we report the synthesis and light-emitting properties of fluorene containing hyperbranched conjugated poly(para-phenylene vinylene) derivatives through A2 and B3 type monomer. A synthesized fluorene containing hyperbranched polymer showed pure blue emission as film state at 462 nm in photoluminescence (PL) measurement and was found to showing almost no excimer emission peak even the polymer film was annealed at 80 °C.

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Novel materials including nanoparticles for tinted hydrogel ophthalmic lens

노정원 김득현 성아영*

세한대학교 안경광학과

The physical and optical characteristics for copolymers produced by adding the 2,4-difluoroaniline, titanium dioxide and Ag nanoparticle were compared with the basic hydrogel contact lens materials. The high functional ophthalmic lens was manufactured by cast mould method and the copolymerized ophthalmic lenses were stored in a 0.9% NaCl normal saline for 24 hrs. After polymerization, the physical properties such as refractive index, water content, contact angle and spectral transmittance of produced ophthalmic lenses were measured. The results showed that the average value of refractive index increased and the water content decreased as the ratio of additive increased. And also, the physical characteristics of the copolymerized showed the water content of 37.55~38.33%. The measurement of the optical transmittance of the copolymerized polymer with addition 2,4-difluoroaniline, titanium dioxide and Ag nanoparticle showed that the transmittance for visible ray, UV-B and UV-A is 73.0~82.2%, 7.4~23.8% and 26.4~47.0%, respectively. The produced ophthalmic polymer is expected to be used usefully as a material for UV-block ophthalmic hydrogel lense.

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Constructing Peptoid-Polymer Conjugates Via ROMP

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Proteins and peptides have received considerable attention due to variousfunctionsof enzyme, antibody, transporter, and structural scaffold. However, natural proteins have several issues including no resistance to protease in the physiological condition. Peptoids, oligomers of N-substituedglycines, in which the side chain is attached to the backbone amide nitrogen instead of the α-carbon, havemany advantages such as proteolysisresistance, minimal immunogenicity, structural stability, and chemical diversitymainly due tothe lack ofchirality and hydrogen bonding donors. In this work, we introduce the peptoid-polymer conjugate by connecting peptoid and polymer using ring opening metathesis polymerization (ROMP). We expect that this new molecular architecture will serve as a promisingstructural material for many interesting applications in the future.Thus, synthetic polymers conjugated with protein system can be considered to solve the proteolysis in vivo and control the molecular structure precisely. Peptide-polymer conjugated system, however, has still problems which are lack of oral activity, rapid metabolism and low stability at harsh environment. For these reasons, it is important to use the peptoid.

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Constructing Bio-Electronics Interfaces Based on Highly Conductive Conjugated Polymers

백고은 윤명한[1,*]

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Conjugated polymers (CPs) have been intensively studied due to electrical conductivity, optical transparency, mechanical flexibility, and economical synthesis. Recently, their superb biocompatibility and electrochemical properties attracted many researchers in the field of biotechnology. However, the relatively poor conductivity compared to metallic materials has hindered their application to implantable bio-electronics interfaces for electrical stimulation and sensors. In this study, we constructed the cellular interfaces using highly conductive CP electrodes based on crystallinity-controlled PEDOT:PSS via sulfuric acid treatment. With this transparent and conductive interface, cell viability, morphology, and migration were examined for the future bio-electronics application. We expect that the highly conductive PEDOT:PSS electrode will serve as a useful platform for studying the fundamental mechanism of tissue regeneration and wound healing induced by electrical stimulation.

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DPP-Based Small Molecule의 OPVs : side chain의 각기 다른 위치에 대한 계산결과

고은지 김동욱*

경기대학교 화학과

organic solar cell 의 효율은 side chain 의 갯수나 위치, 입체이성질체에 의존한다.우리는 위치의 영향을 알아보기 위해 back bone 인 DPP 에 cyano 기를 ortho, meta, para 위치에 붙이고 이들의 HOMO,LUMO 값과 IP,EA 값 등을 계산하였다. 또한, 다른 방향으로 만든 dimer 들의 계산을 통해 packing 했을 때 어떤 영향을 끼치는 지에 대해서도 알아본다.

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Surface Interaction of Graphene Oxide Monolayers with Polymers

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We investigated the interaction of graphene oxide (GO) sheets with polymer chains by using three different techniques; dewetting dynamics, diffusion dynamics of polymers and self-assembled structure measurement of block copolymer on the surface of GO monolayers. For dewetting dynamics study, closely-packed graphene oxide monolayer was deposited at the interface between polystyrene (PS) and deuterated poly(methyl methacrylate) (dPMMA) layers by empolying Langmuir-Schaefer (LS) technique. We found that the dewetting hole growth was significantly suppressed by the GO monolayer due to the GO-PMMA interaction which was characterized by dynamic contact angle measurement using atomic force microscopy (AFM). Neutron reflectivity results show that this GO monolayer can also reduce the diffusion dynamics of dPMMA/PMMA layer interface near the GO surface. By using block copolymer (dPS-b-PMMA), we obtained its perpendicular orientation on graphene oxide sheets to the substrate, indicative of the neutral amphiphilic surface property of graphene oxide sheets, which can eventually facilitate stabilization of thin film polymer bilayers against dewetting.

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Evaluation and fabrication of tissue engineering scaffold using the porous micro-particles's sintering method

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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. Additionally, curcumin as a model hydrophobic drug was loaded in the porous microparticles using nanogel, which were prepared for the porous scaffolds . The release rate of curcumin from the nanogel-incoporated scaffold was slower than that from the control scaffold. Moreover, nanogel-incoporated scaffold showed different release profile of curcumin. Thus, nanogel-incorporated scaffold seems to be a promising method to control the drug release profile from the scaffold for tissue engineering.

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A diketopyrrolopyrrole-containing hole transporting conjugated polymer (PDPPDBTE) for use in stable perovskite solar cell

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

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Fast-drying comparison of cellulose fabrics using three hydrophobic agents

김태경

한국화학연구원 그린화학연구단 환경자원센터

In recent years there has been an increase in the range of fast-drying textile based products available, especially the health sector and the sports wear industry. This article reports on the fast-drying finish of cellulose fabrics with three hydrophobic agents using a simple finishing process. Active ingredients of the treated fabrics included poly tetrafluoroethylene, silicone softener and hydrocarbon-based finishes. Fibres claiming fast-drying properties such as cotton and bamboo were also tested. The three finishes were assessed through weight gain while the properties conferred to the fabrics were determined in terms of water contact angle, moisture adsorption and drying time. FTIR-ATR spectra of each finished fabrics showed typical peaks of C-F, Si-O and aliphatic groups. The treated fabrics with poly tetrafluoroethylene exhibited as the high contact angles with water (>127°) even at low add-on (1 %) which enables water drops to roll off the surface easily and dried up to twice as fast as untreated fabrics. The treated fabrics also retain moisture transmissibility that is as good as that of the untreated cotton fabrics. They also show robust washing fastness with the chemical cross-linking process. .

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Multiple proton peaks in ^{1}H MAS NMR spectra of Nafion: Insight into proton transfer mechanism in fuel cells

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The proton transport mechanism in hydrated Nafion, the most widely utilized membrane in a polymer electrolyte membrane fuel cell (PEMFC), has been extensively investigated for decades to enhance the efficiency and stability of fuel cells. Despite the extensive nuclear magnetic resonance (NMR) studies of hydrated Nafion, ^{1}H magic-angle spinning (MAS) NMR spectroscopy has had difficulties in resolving the multiple proton sites in Nafion because the proton exchange between protons of water molecules and sulfonic acid groups reduces the spectral resolution. In this work, Nafion swollen in deuterated water was employed to enhance the resolution of the ^{1}H NMR spectra. Three types of proton peaks were resolved: 1) bulk water on the surface of membrane at ~ 4.9 ppm, 2) water in the middle of hydrophilic channels in Nafion at ~ 5.6 ppm, and 3) protons near sulfonic groups of Nafion at ~ 6.8 ppm. These three types of protons in Nation show different behavior in ^{1}H MAS and pulsed field gradient (PFG) NMR experiments. At higher magic-angle spinning speeds, the peak positions slightly shifted to high field and the peak widths also increased. These phenomena were more significant for surface and channel water than sulfonic acid groups. The ^{1}H PFG NMR results also showed lower diffusion coefficients for sulfonic acid groups than surface and channel water. These results suggest that the water and sulfonic acid groups play different roles in proton transport mechanism. Further ^{1}H NMR experiments are currently underway to investigate different dynamic behavior of water and proton in Nafion at various hydration stages with an expectation to provide insight into the proton transport mechanism in Nafion.

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Asymmetric supercapacitors based on conducting polymer nanostructures and carbon nanohybrids

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Asymmetric cell configuration has offered unique opportunities for achieving enhanced performance in supercapacitors. Hierarchically structured conducting polymer nanomaterials was coupled with graphene/carbon nanofiber hybrids to construct asymmetric supercapacitor cells. A commercialized capacitor cell was used to examine the capacitive behavior of the materials. Cyclic voltammetry analysis and charge/discharge test were conducted under various conditions. Considering the main device characteristics such as capacitance, cycling stability, and coulombic efficiency, asymmetric cell with the conducting polymer nanomaterials at the positive electrode and the carbon nanohybrids at the negative electrode showed the best performance in an acidic electrolyte.

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Conjugated polymer membranes for the selective detection of Hg(II) ion in flow systems

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There is no doubt that detecting heavy metal ion in solution is of importance. Herein, we describe the electrochemical detection of Hg(II) ion using conjugated polymer-coated cellulose membrane in flow systems. A home-made electrochemical sensing device with a counter electrode and a reference electrode was fabricated to measure real-time sensor responses in flow systems. Under different applied potentials, the conjugated polymer membrane gave rapid, selective, and quantitative responses to Hg(II) ion. Importantly, principal component analysis technique was employed to screen the unique response profile of the membrane to only Hg(II) ion from many response signals. It is believed that our findings will offer possibility of fabricating a cheap and efficient mercury sensor.

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Self-Healing Coating Healed with Viscoelastic Substance

송영규 정찬문*

연세대학교 화학과

In this work, a capsule-type self-healing protective coating has been developed using vegetable oils as healing agent. Healing-agent-loaded microcapsules are embedded in a coating matrix to obtain a self-healing protective coating. Upon damage-induced cracking, the microcapsules are ruptured by the propagating crack fronts, resulting in release of the healing agent into the crack by capillary action. A healing reaction occurs by atmospheric oxygen, generating a viscoelastic substance. The self-healing coating was evaluated as protective coating for steel, and it was demonstrated that our system has good self-healing capability.

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Synthesis and Electrophosphorescence of Iridium(III) Complex Containing 4-Methylquinoline-Based Ligand

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Orange phosphorescent Ir(III) complex, $(MPQ)_2Ir(acac)$ based on 4-methylquinoline ligand as the main ligand and acetylacetone (acac) as the ancillary ligand, was synthesized for application in orange phosphorescent organic light-emitting diodes (PhOLEDs). The device structure of PhOLEDs was ITO (50 nm)/PEDOT:PSS (40 nm)/TAPC (20 nm)/mCP (10 nm)/TCTA:TPBi:dopant (x%)/TSPO1 (35 nm)/LiF (1 nm)/Al (200 nm). In these devices, the dopant were Ir(III) complex, the doping ratio of TCTA to TPBi was 1:1, and the doping ratios of the red dopant (x%) were 5%, 10%, and 15%. The device employing $(MPQ)_2Ir(acac)$ as the dopant exhibited EL emission peak at 589 nm with a broad band width of 81 nm.

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Synthesis and Characterization of High Refractive Index Organic/Inorganic Hybrid Polymer

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전북대학교 고분자나노공학과

OLED 는 전압이 가해지면 스스로 발광하는 유기발광재료를 이용하여 화면을 표시하는 장치이다. OLED 는 넓은 광시야각, 선명한 화질, 빠른 응답속도를 지니지만 유기 발광층으로 인해 수명이 짧다는 점, 굴절률이 차이가 나는 층 사이의 전반사로 인해 광효율이 낮은 단점이 있다.본 연구에서는 유기 발광층에서 발광된 빛이 ITO 와 glass 기판 사이에서 높은 굴절률 차이에 의해서 발생된 전반사로 인해 기판 혹은 ITO 전극으로 waveguiding 되는 현상을 줄이고자 높은 굴절률을 가지는 organic/inorganic 하이브리드 폴리머 기판을 사용하여 OLED 의 광 추출 특성을 향상시키고자 한다. 따라서 유기물인 폴리이미드를 기반으로 하여 굴절률을 향상시킬 수 있는 무기물인 BaTiO3 nanoparticle 을 넣어 높은 굴절률을 가지는 하이브리드 기판을 제작하였고, 또한 이를 기존 glass 기판을 사용했을 때 보다 높은 효율을 가지는 OLED 를 구현하고자 한다.본 연구에 사용하는 BaTiO3 nanoparticle 은 FT-IR, HR-TEM, XRD 를 이용해 합성됨을 확인하였고, BaTiO3 nanoparticle 의 함량에 따라 glass 기판에 코팅한 필름의 굴절률은 prism coupler, ellipsometer 를 이용해 측정하였다.

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Conducting polymer/graphene nanocomposites for electrochemical capacitor application

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There has been enormous effort to make functional materials for fabricating supercapacitors with excellent energy and power densities. Polyaniline/graphene nanocomposites were readily prepared through a simple physical method. The microstructure of the nanocomposites were observed using scanning and transmission electron microscopies. The nanocomposites were further characterized by four-probe conductivity and ultraviolet-visible spectroscopy. In-depth scientific insight into the electrochemical properties of the nanocomposites was given by cyclic voltammetry and galvanostatic charge/discharge test. As a result, the nanocomposites showed good discharge capacitance values and cycling stability in an acidic electrolyte.

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Effect of Associated Structures of Sodium Diphenylamide Initiator on Anionic Polymerization of Isocyanates

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The stiff helical backbone and self-assembly nature of polyisocyanates have been verified to be great merits for the potential applicability to chiroptical switches, drug vehicles, micropatterning, and photonic crystals. The primary work to take advantage of desired properties of polyisocyanates is to achieve the controlled molecular weight (MW) and narrow polydispersity. We found anionic polymerization using sodium diphenylamide (NaDPA) initiator fulfills this prerequisite. The initiation efficiency of NaDPA was constant to 40%. Polymerization behaviors were strongly affected by several types of additives. Most notably, the addition of sodium tetraphenylborate a common ion salt led to increase of initiation efficiency of NaDPA to 50%. Through DFT calculation, we estimated NaDPA is stabilized by its possible association into dimer and trimer in the polymerization condition. The associated structures of NaDPA are expected to strongly affect the initiation mechanism.

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Flow Behaviors of Smart Nanofluids Containing Silica Nanoparticles Grafted with Interactive Zwitterionic Polymer Brushes

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Recently, there are growing interests in fabrication of “smart nanofluids”, since they can change the flow property in complex fluid systems. This study introduces novel nanofluid systems containing 20 nm-sized silica nanoparticles grafted with interactive zwitterionic polymer brushes. Basically we chemically graft poly (2-methacryloyloxyethyl phosphorylcholine) on the surface of silica nanoparticles with changing the chemistry of polymer brushes. Then, we investigate how the nanoparticles behave at the interfaces, such as oil-water interface and oil-rock interface. We also study the interaction of hydrophobically-modified silica nanoparticles with viscosity enhancing polymers, which enables development of an advanced nanofluid system having strong tolerance to salts and pH. The results obtained in this study highlight that the incorporation of interactive zwitterionic polymer layers on the surface of nanoparticles is indeed useful for regulation of flow behaviors of nanofluids.

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Touch Sensors Based on Liquid Crystal-Integrated-Organic Field-Effect Transistors

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경북대학교 화학공학과

Organic electronics, which is based on organic semiconducting materials, have been extensively studied because of their potential for creating new applications after conventional silicon electronics. The benefit of organic electronics is primarily ascribed to realization of soft and flexible devices as well as utilization of low-temperature process leading to low-cost fabrications. However, it is quite tedious to chase conventional devices with inorganic semiconducting materials. Recently, we invented new concept devices by combining liquid crystals (LCs) and organic field-effect transistors (OFETs) for ultrasensitive tactile sensors. In addition to the previous invention, this presentation will demonstrate another new device and will discuss its potential for touch sensors.

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Effects of nanoclay on CTE value and optical property of polyethersulfone/clay nanocomposite

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성균관대학교 화학공학과

In the study, nanoclay, three different montmorillonites (MMT) were selected according to the kinds of intercalated molecule: Na-MMT, MMT 6A modified with 2M2HT (dimethyl dehydrogenated tallowquaternary ammonium) and MMT 30B modified with MT2EtOH (methyl tallow bis-2-hydroxyethyl quaternary ammonium). Nanocomposites of Polyethersulfone (PES) and MMT were prepared by solution casting. The intercalation and exfoliation of MMT in PES matrix was characterized by small angle X-ray scattering and scanning electron microscopy. The thermal, optical, and mechanical properties of the nanocomposite were characterized by thermo mechanical analysis, UV-vis spectrometer and universal testing machine, respectively. PES film having MMT 30B exhibits high transmittance (83 %) and low CTE value (42 ppm/oC). MMT modified with long alkyl chain can be exfoliated easily and dispersed well in PES matrix. PES film can maintain high transmittance and be reduced the CTE value.

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Nanoporous Thin Films from Fully Alicyclic Polyimides

이웅희

연세대학교 화학과

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

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Molecular sieving of liquid mixtures through ultrathin covalent organic networks

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Nanometer-thick covalent molecular networks were synthesized on the molecular level by pore-limited molecular layer deposition (MLD) process. The deposition phenomena were different when the MLD was conducted on the nanoporous substrates such as AAO membrane unlike flat substrates. The deposition of molecular networks was restricted by the pore structures. The ultrathin covalent organic nets were then deposited on the surface of the membrane as a skin layer. Alternating deposition of multi-functional, polyhedral molecules gives nanometer thick films of three-dimensionally cross-linked organic molecular networks. Varying the number of deposition cycles enables to control the pore size of the molecular networks membrane precisely on the molecular level. Molecular sieving performance confirmed by filtration of various aqueous solutions containing organic solutes. Molecular nets membrane is a promising strategy to overcome the limitations of the conventional separation system using membranes.
This research was supported by Global Frontier Program through the Global Frontier Hybrid Interface Materials(GFHIM) of the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT & Future Planning (2013M3A6B1078869).

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Influence of different bifurcation point of branched side chain on the Hole Mobility of Polymer Thin-Film Transistors

박지은 신지철 이대희 조민주 최동훈*

고려대학교 화학과

Systematically moving the alkyl-chain branching position away from the polymer backbone afforded two new Isoindigo-dithienylethylene (PIIDDTE) polymers. The new design strategy of the position of the alkyl-chain branching point have advantages which are reducing the steric hindrance between bulky side chain and polymer backbone and the intermolecular π-π stacking distance. In this work, we designed and synthesized highly π-extended D-A conjugated polymers (PIIDDTE_S3 and PIIDDTE_S6) by introducing 4-decyl-1-hexadecyl (S3) and 7-decyl-1-nonadecyl (S6) having three and six linear spacers between the polymer backbone and the side-chain branching points. We found that by increasing the size of spaces of side chain from S3 to S6 π-π distance decreased and film morphology was enhanced. After thermal annealing at 230 °C, PIIDDTE_S6 containing TFT exhibited very high mobility of 4.34 cm^2/Vs, which is much higher than that of PIIDDTE_S3 (2.26 cm^2/Vs).

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Extremely stable nanoemulsions fabricated by interfacial assembly of amphiphilic block copolymers at oil-water interfaces

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Recently, there have been intense interests in fabrication of stable nanoemulsions by incorporation of amphiphilic block copolymers. These block copolymers have abilities not only to reduce the interfacial tension at the oil-water interface, but also to form a mechanically flexible but tough polymer film at the interface. These unique behaviors make them truly useful as polymeric surfactants. The objective of this study is to demonstrate that extremely stable nanoemulsions can be produced by effective assembly of amphiphilic block copolymers during phase inversion from a water-in-oil emulsion to an oil-in-water emulsion. The phase inversion emulsification process is established by characterizing the emulsion phase properties as well as by confirming remarkably improved emulsion stability. We also conduct the feasibility tests for a variety of oils, including natural oils, hydrocarbon oils, and synthetic oils. Finally, we show experimentally that the nanoemulsions fabricated in this study remarkably improve transdermal delivery, which would explore practical applications in dermatology and cosmetics. Acknowledgement: This study was supported by a grant of the Korea Healthcare Technology R&D Project, Ministry of Health & Welfare, Republic of Korea (Grant No.: A103017)

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Synthesis and Characterization of Thieno[3,4-*b*]thiophene(TT)-based Donor-Acceptor Alternating Copolymers

최수나 박지은 신지철 조민주 최동훈*

고려대학교 화학과

Recently, Donor-acceptor (D-A) alternating conjugated copolymers are the most promising and attractive materials for electronic and optoelectronic applications. As a acceptor moiety, thieno[3,4-*b*]thiophene (TT) unit enhances the backbone planarity and promotes the delocalized electron distribution along a polymer backbone. Also, anthracene (ANT) unit in polymer structures affects the chain-packing and alignment behavior as a donor. In this study, we demonstrate synthesis and characteristics of TT-ANT-based conjugated polymers. The effect of anchoring position of TT unit from the 2,6- to the 9,10-position in the anthracene ring was investigated on the semiconducting property. In addition, we investigated their physical properties by thermal analysis, cyclic voltammetry and absorption spectroscopy. Eventually, we successfully fabricated field-effect transistor devices to study their charge transport properties.

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Formation of Alginate-Polydopamine Core-Shell Microcapsules: Prevention of Cell Leakage and Cytoprotection

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In the microbial microencapsulation, the uncontrolled exposure of the encapsulated microbes to the outside has been problematic, because any cell leakage causes the detrimental outcomes, such as immune rejection, capsule instability, and uncontrolled microbial growth. The swelling of the ionotropic hydrogels (e.g., alginate) encapsulating microbes leads to the diffusion-based cell leakage, and the microbial growth in capsules is another factor to cell leakage. In this work, these two pathways of cell leakage were prevented effectively by coating the alginate beads with mechanically durable polydopamine under cytocompatible conditions. The polydopamine shell also prevented the cell leakage from enzymatic digestion of the alginate core and effectively protected the cells inside from UV-C irradiation.

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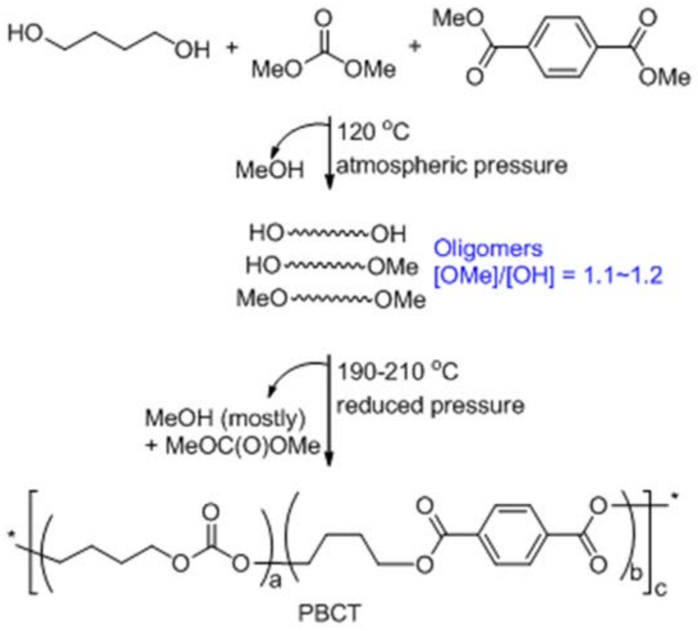
Polymerization of High-Molecular-Weight Poly(1,4-butylene carbonate-co-terephthalate) and its thermal properties

박성연 이분열*

아주대학교 분자과학기술학과

The condensation copolymerizations of 1,4-butanediol (BD), dimethyl carbonate (DMC), and dimethyl terephthalate (DMT) were conducted by a two-step procedure using sodium alkoxide (0.1?0.2 mol%) as a catalyst with a variation of [DMT]/[BD] feed ratio. In the first step, oligomers bearing almost equal numbers of hydroxyl and methoxycarbonyl end-groups were generated, which were polycondensed mostly by the elimination of methanol at 190??210 °C under a reduced pressure. By this procedure, high-molecular-weight poly(1,4-butylene carbonate-co-terephthalate)s (PBCTs) were easily prepared with Mw 60000??200 000 in a reasonably short reaction time, totaling 8.5 h, and even in a large scale (110 g polymer/batch) using 250 mL glass reactor. The PBCTs prepared at high [DMT]/[BD] feed ratio 0.38??0.50 were a semi-crystalline polymer with a fast crystallization rate showing the melting temperature in the range 112?146 °C, which was adjustable by the [DMT]/[BD] feed ratio. These thermal properties are comparable to those of the commercialized compostable polyesters such as PLA, PHA, PBAT, and PBSA.


HO
OH
+
MeO
OMe
O
+
MeO
O
O
OMe
120 °C
atmospheric pressure
MeOH
HO~~~~OH
HO~~~~OMe
MeO~~~~OMe
Oligomers
[OMe]/[OH] = 1.1~1.2
190-210 °C
reduced pressure
MeOH (mostly)
+ MeOC(O)OMe
a
b
c
PBCT

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Cellulose와 poly (pyrrole) 복합체를 상대전극으로 응용하기 위한 성능 연구

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염료 감응 태양전지에서 상대전극은 외부회로를 통하여 주입된 전자를 전해질에 전달하여 산화 종을 환원시키는 과정에 관여한다. 이때 상대전극의 전기화학적 촉매 활성도, 표면적, 전도도는 염료 감응 태양전지의 성능에 영향을 준다. 가장 보편적으로 상대전극에 사용되고 있는 물질은 백금으로 투명하고 전도도가 높아 전극으로서 좋은 성능을 나타내는 반면 가격이 비싸고 전해질과 장기적으로 접촉하면 표면이 부식되는 문제점을 나타낸다. 이러한 단점을 보완하기 위해 백금 대체 물질 개발이 활발히 이루어 지고 있다. 본 연구는 백금 대체 물질로 전도성 고분자 poly (pyrrole) (ppy)을 선택하였고 ppy 의 전기화학적 물성과 기계적인 물성을 증대 시키기 위해 TEMPO-oxidized celloulose/ppy 복합체를 제조하고 특성을 연구하였다. 먼저 투명 전도성 유리 기판에 cellulose 를 코팅한 뒤에 산화제인 $FeCl_3$ 를 침투시키고 vapor polymerization 을 통해 상대전극을 제작하였다. 복합체의 morphology 를 확인하기 위해 SEM 이미지를 확인하였고 전도도를 측정해 보았다. 또한 HCl, SDS (sodium decylsulfonate)와 같은 도펀트의 유무에 따른 전도도 변화를 확인하고 염료 감응 태양전지를 제작하여 상대전극으로서 응용 가능성을 논의해 보고자 한다.

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셀룰로오스와 카라기난을 이용한 복합막 제조 및 특성 연구

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천연 셀룰로오스와 전도성 고분자 카라기난을 이용하여 이온 전도성을 가지는 복합막을 제조하였다. 실험에 사용한 kappa-카라기난은 단위체 당 하나의 설폰기를 가지고 있으며, 이 설폰기는 막을 구성하고 있는 고분자 사슬 사이로의 이온 이동 경로로써 막에 도입하였다. 또한 셀룰로오스로 복합막의 기계적 강도와 열적 안정성을 보완하였다. 다양한 조성의 셀룰로오스와 카라기난 혼합 용액을 용매 치환법을 이용하여 복합막으로 제조하였다. Thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), electrochemical impedance spectroscopy (EIS)를 이용하여 열적 안정성, 막의 형태, 이온 전도도 등 복합막의 특성을 분석하였다.

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Ionic gel : application to the membrane

황용하 원종옥*

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이온성 액체를 이용한 분리막은 이산화탄소와 올레핀과 같은 특정 기체에 대해 높은 가스 선택성을 가지고 있다. 특히 이온성 액체는 이산화탄소에 대해 높은 용해도와 높은 흡수력, 매우 낮은 증기압으로 분리하기 때문에 기체를 분리하는데 효과적이라 할 수 있다. 1-butyl-3-metylimidazolium tricyanomethnide(BMIM TCM), 1-ethyl-3-metylimidazolium tricyanomethnide(EMIM TCM)과 같은 이온성 액체의 장점을 활용하여 이산화탄소를 분리하는 연구가 진행중이다. 하지만 이산화탄소를 분리하기 위해서는 높은 압력이 막에 가해져야 하기 때문에 capillary force 에 의해 막 내구성에 문제가 생길 수 있다. 이러한 문제를 해결하기 위해 tri-block copolymer 인 Poly(styrene-block-ethylene oxide-block-styrene)(SEOS)를 이용하여 이온성 액체를 다공성 막 내에서 gelation 시킨다. 기존에 사용한 BMIM TCM, EMIM TCM 과 양이온을 바꾼 1-butyl-1-methylpyrrolidinium tricyanomethanide(BMPyrr TCM)과 1-butyl-4-methylpyridinium tricyanomethanide(BMPY TCM) 4 가지 이온성 액체를 gel 로 만듦으로써 기존 이온성 액체만으로 측정한 기체 투과도와 비교하여 gelation 하였을 때 막의 안정성을 확인해 보았다.

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MOF와 matrix 사이의 상호작용을 증가시킨 기체 분리막의 특성 연구

김지영 원종옥*

세종대학교 화학과

Metal Organic Frameworks(MOFs)는 그 기공의 크기를 조절 할 수 있고, 용매를 제거하여도 안정하며, 기공에 수소와 이산화탄소를 저장할 수 있다는 장점 때문에, 기체 정제나 기체 분리에 응용되고 있다. 기존의 MOF 를 이용한 대부분의 기체 분리막은 matrix 와 MOF 를 물리적으로 분산시켜 제조한 분리막으로써 matrix 와 MOF 사이의 직접적인 상호작용은 없었다. 따라서, 본 연구는 matrix 에 존재하는 카르복시기를 MOF 의 합성 단계에 이용하여 matrix 와 MOF 사이에 직접적인 상호작용이 존재하는 분리막을 제조하였다. matrix 로 사용한 고분자는 가격 경쟁성이 있고 생분해성이 있으며 자연에서 가장 풍부한 고분자인 셀룰로오스를 이용하였다. 셀룰로오스에 카르복시기를 도입하게 위하여 수용액 상에서 sodium hypochlorite, sodium bromide, 그리고 2,2,6,6-tetramethylpiperidine-1-oxyl(TEMPO) 라디칼을 첨가하여 산화시켜, TEMPO-oxidized cellulose nanofiber(TOCN)로 이용하였고, TOCN 에 존재하는 카르복실기를 바탕으로 Cu^{2+}를 이용한 MOF 을 합성하여 기체 분리에 선택성이 있는 MOFs-TOCN 분리막을 제조하였다. 분리 막의 기체 선택성은 soap bubble meter 를 통해 확인하고 분리막의 형태는 SEM 이미지로 확인하였다.

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바나듐 레독스 흐름전지의 Nafion 막의 두께에 따른 특성 연구

방호선 원종옥*

세종대학교 화학과

바나듐 레독스 흐름전지(Vanadium redox flow battery, VRB)는 대용량 전력저장 시스템의 하나로 전해질 용액의 오염이 발생되지 않는 장점과 충.방전 이 자유로워 연구가 많이 진행되고 있다. 이온 교환막은 VRB 의 핵심 물질중 하나이며, 이온 교환막의 특성으로 높은 양성자 전도도, 낮은 이온투과성, 그리고 우수한 화학적 안정성과 기계적 강도가 요구된다. 실험에서는 Nafion 117 과 Nafion 112 막을 비교하여 두께의 따른 성능을 확인하였다. 막의 성능은 VRB single cell test 기를 사용하여 충,방전 실험을 진행하였고, 흡수도와 열적 안정성 테스트로 막의 특성을 확인하였고, (Electro impedence spectrosocopy, EIS)를 통해 프로톤 전도도를 확인 하였다.

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Robust Protein Films Fabricated via Nanoimprint Lithography

정은희 **Bradley Duncan[1] Vincent M. Rotello[1,*]**

강릉원주대학교 화학신소재학과 [1]University of Massachusetts Amherst, USA

Protein films provide an inherently biocompatible and sustainable platform for the generation of functional materials. Maintaining film stability under aqueous conditions is crucial for successful implementation in biological applications. However, current protein based films are limited to using specific structural proteins or require the addition of harmful additives such as crosslinking agents. We describe a generalized nanoimprint lithography (NIL) based method for the fabrication of stable, patterned protein films. The NIL process involves the physical deformation of a thin film deposited on a substrate using a rigid mold precisely controlling the temperature and pressure applied. Parametric variation of processing conditions revealed that films have tunable biodegradability, are stable to cell culture conditions, and promote selective cellular adhesion. Furthermore, by imprinting with patterned molds, the films directed cell growth along nanoscale features. This generalized method is amenable to a wide variety of proteins and expands the toolkit to create patterned, functional materials from the previously underused library of available proteins.

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Increase of Efficiency in a Multilayer Bulkhetrojunction Solar Cell by using Water Soluble Polymers

남궁한솔 박동규*

경성대학교 화학과

We have fabricated a bulkheterojunction solar cell (BHJ-SC) from the conventional active polymer blend, P3HT:PCBM, by constructing a polymer multilayer structure with novel electron transporting while the one without WSP layer shows a PCE of 2.0 %. water-soluble polymer (WSP), poly(fluorene-co-benzothiadiaziole), on the top of the polymer active layer. The UV-Vis spectra of water soluble polymer are found to be 498 nm (2.49 eV). The device with WSP layer shows a power conversion efficiency (PCE) of 2.7 % in concentration of 0.0125 % while the device without WSP layer shows a PCE of 2.0 %. And It shows that the improvement in J_{sc} then the device without WSP layer.

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SI-ARGET ATRP of 2-aminoethyl methacrylate hydrochloride on solid substrates

이봉수 최인성*

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Recently, the direct synthesis without protection process via Activators ReGenerated by Electron Transfer (ARGET ATRP) of 2-aminoethyl methacrylate hydrochloride (AEMA) has been successfully performed in aqueous media near room temperature notwithstanding the catalyst poisoning induced by complex between the primary amine groups of the monomers and Cu-based catalysts.[1] The side primary amine groups of pAEMA films grown by ARGET ATRP have been utilized in postpolymerization reactions, such as Michael addition or ring-opening of epoxy groups, as well as nanogel formation for gene/drug delivery carriers. But the surface-initiated polymerization (SIP) of AEMA on any surface has not been reported until now. For the first time, we perform surface-initiated ARGET ATRP (SI-ARGET ATRP) of AEMA on solid substrates at room temperature. The polymeric films grown by SI-ARGET ATRP are characterized by FT-IR, ellipsometry, XPS, and contact angle goniometry.References [1] J. E. J. Coelho *et al. Macromolecules* 47, 4615-4621 (2014).

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Acid sensor based on Chitosan-graft-Polyaniline copolymer film

이상용 최동철 손용근*

성균관대학교 화학과

Polyaniline(PANI) is a conjugated polymer which shows good electrical conductivity through acid/base doping process. Thus PANI can used acid or base sensor. But PANI has known to be poor in solvent solubility. So that it is very difficult to make independent PANI film. Therefore, we tried to use chitosan(CS), to make CS-g-PANI copolymer. Because CS can povide good mechanical and solubility properties. We identified formation of copolymer by a preferable X-ray diffraction (XRD), Scanning Electron Microscope (SEM), FT-IR. Resistance of copolymer is observed using a home made 4-point probe. We have fabricated copolymer to improve mechanical properties and processibility. The copolymer can be easily used for film-forming. As a substrate a piece of PET film on which 2-lines of Ag paste were coated was used. We drop acid solution on sensor surface, then the resistance change of the copolymer was observed. As a result, resistance has decrease up to 1/500 than the value obtained before proton dopping. In conclusion, CS-g-PANI copolymer could be applied in the fabrication of acid sensor.This work was supported by the Component and Material Technology Development Program (No.10046641, Development of Electronic Ink and Coating Material for Leak Monitoring of the Hazardous Chemicals) funded by the Ministry of Trade, industry & Energy (MOTIE, Korea)

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Synthesis and Characterization of New Benzothiadiazole Derivative as a Electron Acceptor Unit forOrganic Photovoltaic cells

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부산대학교 화학과 [1]부산대학교

We synthesized two fused pentacyclic donor-acceptor structures where the two different outer electron rich thiophene (DTPBT) and electron poor benzene (ICTh) moieties are covalently fastened with the central electron-deficient benzothiadiazole core by two nitrogen bridges. These new electron-acceptor DTPBT and ICTh building blocks were copolymerized with fluorene as the electron donor part via Suzuki coupling polymerization to afford two new alternating copolymers PFDTPBT, PFICTh, respectively. The average molecular weights of the synthesized polymers were determined by GPC. The number-average molecular weight of PFDTPBT and PFICTh were 19,000 (PDI= 2.5) and 20,000 (PDI= 4.0), respectively. The optical bandgap energies of the polymers were measured from their absorption onsets to be 2.15 and 2.55 eV depending on the polymer structure. The HOMO energy levels of the polymers were determined by measuring the oxidation onsets of the polymer films by cyclic voltammetry. The measured HOMO energy levels of PFDTPBT and PFICTh were -5.10 and -5.57 eV, respectively. When the polymers were blended with $PC_{71}BM$ as active layer for bulk-heterojunction photovoltaic devices, power conversion efficiency were 2.08 % and 0.34 %, respectively, under AM 1.5 G (100 mW/cm²) conditions.

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Hetero Aromatic Compounds : Synthesis, Characterization and Properties

김영범 김인태* 김영선

광운대학교 화학과

Thiophene based linear π-conjugated oligomers have their potential applications for active materials in organic electronic and photonic devices. We synthesized three novel compounds of Thiophene based materials containing hetero aromatic compounds with unique electronic and opitical properties. The structure of the resulting compounds were characterized by ^{1}H NMR, ^{13}C NMR, and FT-IR. The optical properties of the oligomer can be checked in the UV-vis absorption, Photoluminescence (PL). The compounds will be applied to emitting material in LED.

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Influence of Ionic Liquids on the Physical Properties of Polyaniline and Application in Dye-Sensitized Solar Cell

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In this study, we investigated the interaction studies between the ionic liquids (ILs) of ammonium and imidazolium families and polyaniline (PANI). In order to increase PANI utility, we have studied the interactions between the PANI and ILs using various techniques such as UV-Vis spectroscopy, FT-IR spectroscopy, Cyclic Voltammograms (CV). Further, we have studied the conductivity, morphology and roughness of the PANI-IL mixture. The morphology and roughness of the mixture were investigated using scanning electron microscopy (SEM) and atomic force microscopy (AFM). We observed that ammonium ILs such as diethylammonium dihydrogen phosphate (DEAP), triethylammonium hydrogen phosphate (TEAP) and tributylmethylammonium methyl sulfate (TBMS), from ammonium family and 1-methylimidazolium chloride ([Mim]Cl), and 1-butyl-3-methylimidazolium chloride ([Bmim]Cl) from imidazolium family have potential to interact with the polymer. Further, we have shown the utilization of PANI-ILs additive as electrolyte for dye-sensitized solar cell and also observed that aprotic ILs have more efficiency than protic ILs. This study provides the combined effect of polymer and ILs that may generate many theoretical and experimental opportunities.

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Synthesis, characterization and properties of a new conjugated polymer

장원 김인태* 차주현

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A new conjugated polymer is successfully synthesized by stille's reaction. The new polymer has good solubility in organic solvent such as THF, chloroform and chlorobenzene. The new polymer was characterized by ^{1}H NMR, FT-IR. The properties of the polymer were measured by GPC, UV-spectrometer, cyclovoltammetry and thermogravimetric analysis. The λ_{max} of the polymer shows at about 650 nm in chloroform. It will be applied to active layer in polymer solar cell

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Molecular interactions between newly synthesized azo-benzene polymers and four Ionic liquids and their photo-active properties

박정호 김인태* 김준헌 조태종

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In this work, we have studied the synthesis of a new holographic polymer and their diffraction efficiency. We have obtained photo-induced Surface Relief Grating (SRG) formation and a holographic image on the polymer films. The diffraction efficiency is observed to less than 1%. In order to increase their diffraction efficiency, we have mixed with Ionic liquids. We have explored the interaction properties and diffraction efficiency of four ionic liquids (ILs) such as DEAP, TBH, MIM-Cl and TMEOS with our newly synthesyzed polymers. The resulting mixture showed a little increase of the diffraction efficiency with reduced recording time as compared with only polymers. These results were successfully characterized by general organic spectroscopic methods (^{1}H and ^{13}C NMR, FT-IR, UV-vis, DSC and GPC), and the SRG formation were measured by Atomic Force Microscopy (AFM) image. These behaviors are a consequence of the difference in the surface morphology of the four sets of Ionic liquid. As a result, we conclued the difference of the diffraction efficiencies and molecular interactions between azo-benzene polymers and four kinds of the Ionic liquids is due to their difference in structure properties.

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Fluorous Solvent-Soluble Imaging Materials containing Anthracene Moieties

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Manufacture of organic electronic devices has been drifted toward solution processing of active materials. To realize this, several issues need to be overcome in particular patterning matter. Conventionally, organic electronics is fabricated by photolithographic techniques and organic solvents are used as coating solvent, developer and stripper. However, when this technique is applied to organic based devices, organic solvents in the process may permeate into organic components beneath photoresist film. Furthermore, debris following decomposition reaction by UV irradiation to photoresist and photo acid generator can be potential threat causing deterioration of materials' performance. In order to resolve these problems, we designed a highly fluorinated photoresist polymer [copolymerization of 6-(anthracene-9-yl)hexyl methacrylate (AHMA) and semi-perfluorodecyl methacrylate (FDMA)] taking advantage of orthogonal patterning. Through merits of orthogonal process that minimizes chemical interaction between fluorous solvents and organic devices and photo-dimerization without photo acid generater, we examined photolithography on organic electronic devices. Synthesis of P(AHMA-FDMA) by random radical polymerization and Lithographic evaluation were reported. Finally, P(FDMA-AHMA) and fluorous solvents were applied to the photolithographic patterning of OLED pixels.

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Large DNA Block Copolymers Engineered by Restriction and Ligation Enzymes

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Nucleic acids enzymes are precise and efficient tools to engineer DNAs and RNAs. Herein we report a method for large DNA architectures containing polymer block(s). On one hand, we prepared DNA diblock copolymers (DBCs) consisting of oligonucleotides and polymer segments (i.e. PEG, PPO, PNIPAM). On the other hand, with restriction enzymes we engineered DNA segments, in different lengths, derived from a plasmid DNA. Then T4 ligase helped us paste the DBC segments to small, medium and large DNA segments, respectively. We achieved a 3 M Da large architecture of DBC through the enzyme-based engineering. This method may pave the way to build programmable biomaterials.

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Preparation of Fabric-Hydrogel Composite Membranes for Microalgae Mass Culture

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New type of semi permeable hydrogel membranes was prepared by adding fabric to 2-hydroxyethyl methacrylate(HEMA) hydrogels physically. To developing marine microalgae as the bio fuel energy source, we needed new semi permeable membrane that have high ion permeability and many good mechanical property. Although existing semi-permeable membranes made of cellulosic materials have been introduced to energy industry for culturing microalgae mass, they have limited ion permeability and are not proper in the respect of economic. To overcome these drawbacks, we have proposed a new concept of “fabric-hydrogel composite membranes”. By controlling ratio of the materials, we could get a better high ion permeability and transparency. Also this fabric-hydrogel membranes had the frame composed of cotton fabric which is combining hydrogel network inside, it’s possible to get excellent mechanical properties. As a result, fabric-hydrogel composite membranes were developed and we confirm that membranes function as important parts of the photobioreactor

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Development of highly fluorinated high k dielectric hybrid material for solution processable dielectric layer

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현재 다양한 전자소자의 발전에 따라 그에 대한 대면적화, 유연화가 활발하게 연구되고 있다. 소자의 대면적화와 유연화를 위해서 OTFT(Organic Thin-film transistor)와 같은 유기전자소자의 개발이 이루어지고 있으며 소자를 제작하는 방법으로는 비교적 간단하면서 저온에서 진행할 수 있는 solution process 가 유리한 방법 중 하나로 뽑히고 있다. 이에 따라 OTFT 에 사용되는 절연층(dielectric layer)에 대해서도 용액공정을 적용하기 위한 다양한 연구가 시도되고 있다. 그 예로 높은 유전상수를 갖는 HfO_2, ZrO_2, $BaTiO_3$, $Ba_{1-x}Sr_xTiO_3$ 등과 같은 무기산화물을 TOPO 나 Oleic acid 와 같은 유기리간드와 결합하여 나노입자화한 연구가 진행되었다. 하지만 위와 같은 유무기 hydrid dielectric materials 는 유기용제를 근간으로 하기 때문에 유기소자에 적용할 경우, 상하부 유기물질과 용매간섭을 일으키는 문제가 있다. 이러한 문제는 제작된 유기소자의 성능의 저하를 가져오게 된다. 이와 같은 문제는 유기물질과는 화학적 상용성이 없는 불소계 용제를 이용하여 해결할 수 있다. 따라서 우리는 본 연구에서 유기리간드가 아닌 고불소계 리간드를 이용하여 불소계용제에 녹을 수 있는 고불소계 유전물질을 합성하였다. 고불소계 물질과 높은 유전상수를 갖는 무기산화물 중 수 nm 크기의 $BaTiO_3$ 를 사용하였다. Decanoic acid 에 의해 안정화된 Barium titanate 를 합성한 후, 리간드 치환을 통해 입자 표면에 Highly fluorinated ligands 를 도입하였다. 이렇게 불소계 리간드가 도입된 입자는 불소계 용매에서 우수하게 분산이 되었고, spin coating 으로 소자를 제작한 결과 우수한 유전상수를 보였다.

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[발표취소] A Novel Xanthate is designed for Photoinitiated RAFT Polymerization of Vinyl Acetate with dual Character (as Initiator and Chain transfer agent)

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발 표 취 소

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Molecular level ordered poly(2-vinylpyridine) and its metallic behaviors

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Chemical crosslinking is considered to be a random reaction that creates an irregular structure (Figure 1 , Case I). For a controlledcrosslinking reaction at the molecular level by self-assembly, herein we selected an amorphous polymer with reactive functional groups and a bi-functional cross-linker (Figure 1 , Case II). Molecular-level self recognition and organization during the chemical reaction of poly(2-vinylpyridine) (P2VP) with 1,4-dibromobutane effect on the tacticity of P2VP, leading to the sub-nanometer level ordering of pyridine moieties in the polymer chain. This long range hexagonal organization switches P2VP from an amorphous to a 3D metallic polymer. The morphologies were studied with a high voltage electron microscope (HVEM) and X-ray diffraction (XRD). Also, the optical analysis was performed by Raman spectroscopy, UV-Vis-NIR spectrophotometer. Moreover, the electrical properties of 3D metallic polymer were analyzed by optical reflectance and I-V characteristics.

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CNT Transistor through Solution Process: from Selection of Semiconducting Species to Self-Assembly onto Substrate

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This presentation deals with utilization of DNA block copolymers (DBCs) with one of promising nanomaterials, single-walled carbon nanotube (SWNT), for eventual incorporation into practical technologies. So far the use of SWNTs is limited by difficulties in solubilizing and isolating individual species and precisely manipulating the structures while preserving their exceptional properties. Dispersing SWNT with DBC is a potentially scalable solution to these obstacles using DBCs consisting of a single-stranded DNA block covalently connected to a hydrophobic polymer segment. This combination of materials enables each to contribute its full potential - self recognition and sorting semiconducting SWNTs, respectively - to the utilization of SWNTs. It is demonstrated that one such hybrid is capable of the whole gamut of solution-based SWNT technologies, from selective dispersion to non-destructive functionalization to high-yield device fabrication such as field-effect transistors. These powerful applications are mediated by simple programmed DNA self assembly, opening the door to broader multidisciplinary materials research in the field of carbon nanotubes.

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Blended Micelle of Block Copolymer: Stabilization and DNA Functionalization

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DNA diblock copolymers (DNA-*b*-PPO) were utilized to form mixed micelles together with Pluronic™ triblock architectures (PEO-*b*-PPO-*b*-PEO). The formation and characterization of these blended micelles with a DNA/PEO corona and PPO core, which can be loaded with hydrophobic molecules and stabilized by the formation of a semi-interpenetrating network, are described. Furthermore, the corona is conveniently functionalized by hybridization either with dye-modified complementary DNA, with demonstrable distance control, or with DNA-labeled gold nanoparticles. The resulting objects represent excellent candidates for smart drug delivery vehicles with stealth function due to the presence of the PEO chains on the surface.

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Reversible Morphological Transformation between Polymer Nanocapsules and Thin Films through Dynamic Covalent Self-assembly

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포항공과대학교(POSTECH) 화학과 [1]기초과학연구원 복잡계자기조립연구단

In biological systems, morphological transformations of nano/microstructures in response to environmental stimuli are integral to many of the processes necessary for life, including allosteric conformational changes of enzymes, pseudopodium formation during chemotaxis, and the formation and fusion of various vesicles during a variety of cell growth and signalling events. Synthetic nanostructures that can similarly undergo morphological transitions in response to physical and chemical stimuli have attracted a great deal of attention particularly for the development of “smart” functional materials. We developed a facile method for synthesizing polymer nanocapsules and thin films using multiple in-plane stitching of monomers via the formation of reversible disulfide linkages. Due to the reversibility of the disulfide linkages, the nanostructured materials readily change their structures in respond to environmental changes at room temperature. For example, the polymer nanocapsules release loaded cargo molecules in a reducing environment. Moreover, reversible morphological transformations between these structures are achieved by simple solvent exchanges. Our work presents a novel approach for the formation of robust nano/microstructured materials with dynamic response to environmental stimuli.

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Surface-induced transition of the rod-disc and Surface Anchoring Interactions

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We newly designed and synthesized molecule rod-disc liquid crystal (RD12) to characterize and understand of surface-induced phase transition behaviors of RD12 by changing the surface chemistry and the physical interaction Upon varying the LC cells thickness and their surface chemical and physical environment, the RD12 phase transition behaviors were dramatically changed compared with in the bulk. The nematic phase of RD12 in the LC cell with a low cell gap and polyimide rubbed surface could be preserved and the crystallization of RD12 was thoroughly controlled. The tailored molecular alignment and anisotropic physical properties of RD12 can allow us to develop the smart optical and electrical thin films for practical applications in electro-optical devices. This work was mainly supported by the Basic Science Research Program and BK21 PLUS program, Korea.

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Fluorescence switch for nanomolar silver ion detection utilizing dimerization of DNA-Ag nanoclusters

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포항공과대학교(POSTECH) 화학과

A fluorescence switch that consists of DNA-templated silver nanoclusters (DNA-AgNCs) triggered by silver ion (Ag^+) is used to detect Ag^+. The mechanism of the fluorescence switching of DNA-AgNCs is investigated by fluorescence spectroscopy, circular dichroism spectroscopy, DNA hybridization assay and mass spectrometry. Ag^+ induce a dimeric structure of Cyt_{12}-AgNCs by forming a bridge between two Cyt_{12}-AgNCs, where Cyt_{12} is cytosine 12-mer; this change cause the fluorescence of Cyt_{12}-AgNCs to change from red to green. Using this Ag^+-triggered fluorescence switch, we successfully detected Ag^+ at concentrations as low as 10 nM. Furthermore, Ag^+ detection using this fluorescence switch has high selectivity and sensitivity, and short response time, and can be used successfully even in the presence of other metal ions.

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Synthesis of biomembrane-mimic polymers with various phospholipid head groups

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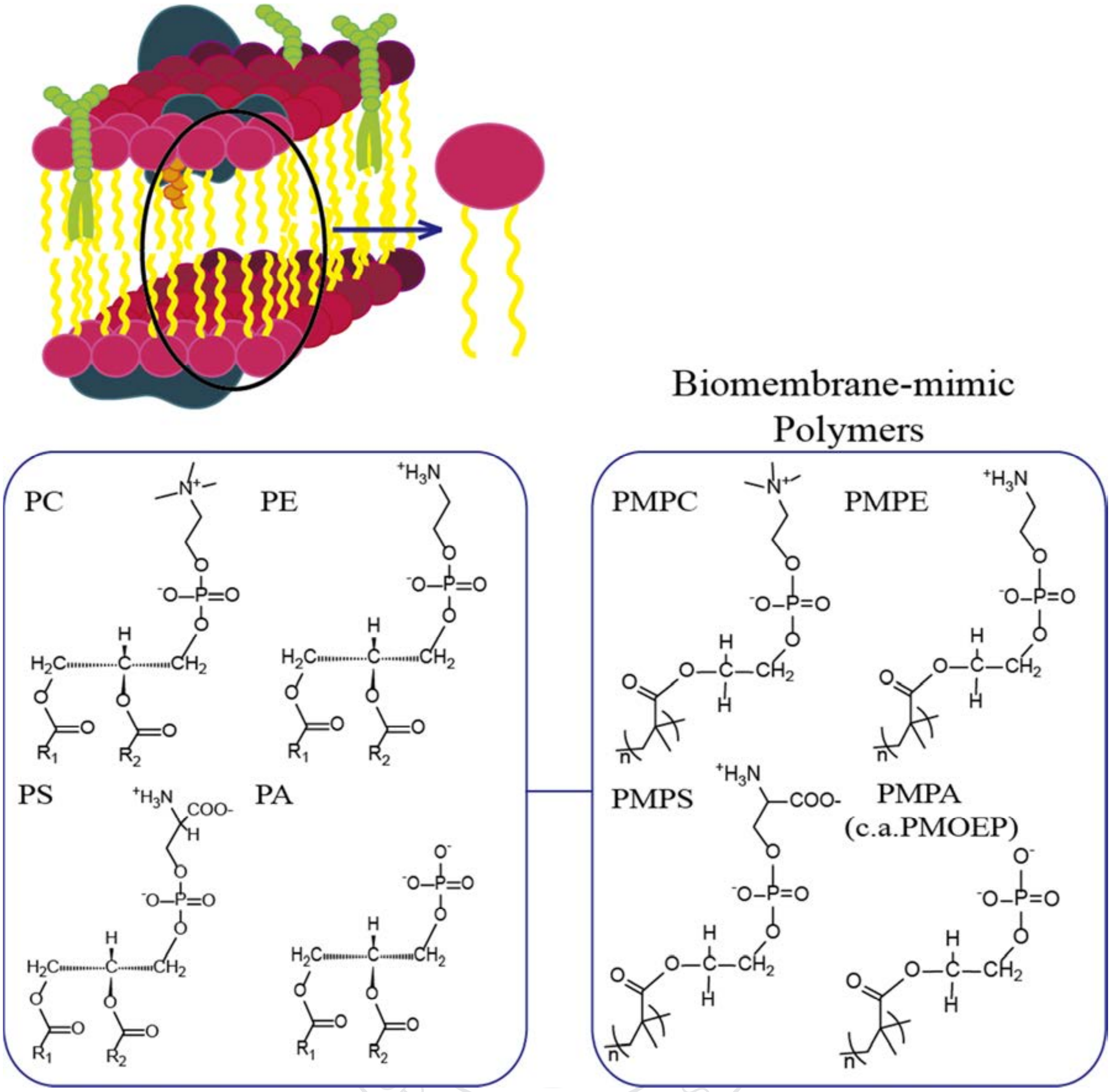
Bio-mimic polymers derived from biological origins are attractive materials for the preparation of biocompatible surfaces. Polymers based on protein or peptide, sugar, and lipid structures have shown great potential in the preparation of biocompatible hydrogels, drug delivery carriers, and tissue scaffolds.Among them, poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC), which mimics the head group of phosphatidylcholine (PC), showed exceptional hemocompatibility, antiprotein adsorption activity, and antithrombotic activity. Lipid bilayers in biomembranes consist of diverse phospholipids, including phosphatidic acid (PA), phosphatidylcholine (PC), phosphatidylethanolamine (PE), and phosphatidylserine (PS) with various compositions according to the cell and tissue type. Inspired by the outstanding biocompatibility of PC-based polymers, we synthesized phospholipid-mimic polymers, poly(2-methacryloyloxyethyl phosphoric acid) (PMPA), poly(2-methacryloyloxyethyl phosphorylethanolamine) (PMPE), and poly(2-methacryloyloxyethyl phosphorylserine) (PMPS), with head groups other than the phosphocholine moieties, PA, PE, and PS head groups, respectively. Each biomembrane-mimic polymer was successfully synthesized by atom transfer radical polymerization (ATRP). The molecular weight distributions of PMPA, PMPE, and PMPS were analyzed by gel permeation chromatography (GPC) in vitro cytotoxicity was also examined by 3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide (MTT) and lactate dehydrogenase (LDH) assay. Considering phospholipid compositions in cell membranes vary between organs, tissues, cells, and even cellular organelles, the biomembrane-mimic polymers based on diverse phospholipid head groups can be a potential platform for the preparation of cell- or tissue-specific surfaces with both biocompatibility and bioactivity, which are difficult to be obtained by only PC-based polymers for biomedical applications.


Biomembrane-mimic Polymers
PC
PE
PS
PA
PMPC
PMPE
PMPS
PMPA (c.a.PMOEP)

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Synthesis and Opto-electrical and Photovoltaic Properties of Pyrrolo[3,4-c] pyrrole-1,3-dione (DPPD)-based Polymers Incorporating 4,8-bis(2-ethylhexyloxy)benzo[1,2-b:4,5-b′]dithiophene unit

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부산대학교 화학과

New electron accepting pyrrolo[3,4-c]pyrrole-1,3(2H,5H)-dione (DPPD) derivatives incorporating different alkyl groups such as heptyl, decyl and dodecyl on DPPD back bone were prepared and copolymerized with electron rich 4,8-bis(2-ethylhexyloxy)benzo[1,2-b:4,5-b′]dithiophene (BDT) derivative to give three new polymers P1?P3. All three polymers displayed similar band gap and energy levels. The estimated band gaps of polymers are 2.11 eV. The highest occupied and lowest unoccupied molecular orbital energy levels of polymers are located around ?5.39 eV and ?3.28 eV, respectively. The single layer polymer solar cell (PSC) fabricated with a simple device structure of ITO/PEDOT:PSS/Polymer:PC70BM/Al offered a overall power conversion efficiency (PCE) of 1.65%, 1.24% and 0.87 %, respectively. While, the PSC device performances was future improved up to 3.45%, 2.60% and 2.04 %, respectively, with the use of processive additive such as 1,8-diiodoocate (DIO, 3 vol%).

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Synthesis and Property of Temperature-Responsive Diblock Copolymers having P3HT

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

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Synthesis of Triarylamine-containing Poly(arylene ether)s by Nucleophilic Aromatic Substitution Reaction

<u>이진희</u> 박창준[1] 서명은[1,*] 김상율[1,*]

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

Poly(arylene ether)s are high performance engineering polymers providing excellent thermal stability and good mechanical properties. Poly(arylene ether) backbone is also a good platform to incorporate functional moieties such as triarylamine useful in electro-optical applications. To this end, we synthesized AB type triarylamine monomers which could be polymerized via nucleophilic aromatic substitution (S_NAr) reaction to form triarylamine-containing poly(arylene ether)s. Introduction of electron-withdrawing groups (EWGs) at the para position of the nitrogen atom in the monomer effectively increased reactivity and enabled tuning electro-optical properties of the polymers by varying EWGs. Synthetic routes for the monomers, characterization of the polymers, and their electro-optical properties will be presented in detail.

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발표코드: **POLY.P-79**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and scale-up process of hyperbranched poly(amidoamine) particles via inverse suspension polymerization

이상화 이슬아 김상율*

한국과학기술원(KAIST) 화학과

Hyperbranched polymers have received much research attention because of their unique properties based on three-dimensional shape. Especially, hyperbranched polyamidoamine(PAMAM) which possess functional amine and amide groups can bind and separate heavy metal ions in aqueous solution. We developed a process to fabricate 50~300μm PAMAM particles by inverse suspension polymerization with N,N'-methylenebisacrylamide and ethylenediamine. In this study, scale-up of the polymerization was attempted to assess the commercial viability of the process. Detailed synthesis and characterization of the particles and their swelling ratio and metal ion absorption behavior will be presented.

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발표코드: **POLY.P-80**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Soluble Aromatic Polyamides Derived from Unsymmetrical Diamine Containing Two Trifluoromethyl Groups

변태준 김상율* 정임식[1]

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Aromatic polyamides(PA) are widely used as a high-performance polymer in advanced technologies due to their outstanding thermal and mechanical characteristics. Nevertheless, PAs have a problem like poor solubility in most organic solvents leading to limitation on their application. To overcome this problem, many research efforts have been made to enhance its solubility by introducing bulky pendant groups or flexible linkage into polymer backbone. Ether linkage is easily considered as a flexible linkage and offers enhanced solubility, color, and melt-processing properties. In addition, incorporation of CF_3 pendant group can also be considered as an effective means to improve the polymer solubility without deteriorating their properties. In this study, we designed unsymmetrical diamine monomer containing ether and CF_3 groups as a linkage and pendant moieties, respectively, and synthesized a series of PAs from the monomer. These synthesis and characterization of the PAs will be presented.

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발표코드: **POLY.P-81**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and development of pH-sensitive Upper Critical Solution Temperature-type Materials in Aqueous Solvent

노민우 이연*

서울대학교 화학부

Upper critical solution temperature (UCST) materials exhibit abruptly poor solubility in aqueous solvent below a certain temperature. Because of their special characteristic of hydrophilic-hydrophobic changes, those materials have been used in the various fields. However, Upper critical solution temperature type materials have been rarely paid attention compared to that of lower critical solution temperature (LCST) type materials. Therefore we introduced the upper critical solution temperature (UCST) properties in branched polyethylenimine (b-PEI) by simple sulfopropylation reaction. We measured the phase transition temperatures of PS-PEI derivatives in distilled water using UV-vis spectrophotometer and drew the phase diagram based on phase transition temperatures. We also checked the effect of pH changes on phase transition temperature. For future applications in the biomedical field, the cytotoxicity of PS-PEI was examined by MTT assay.

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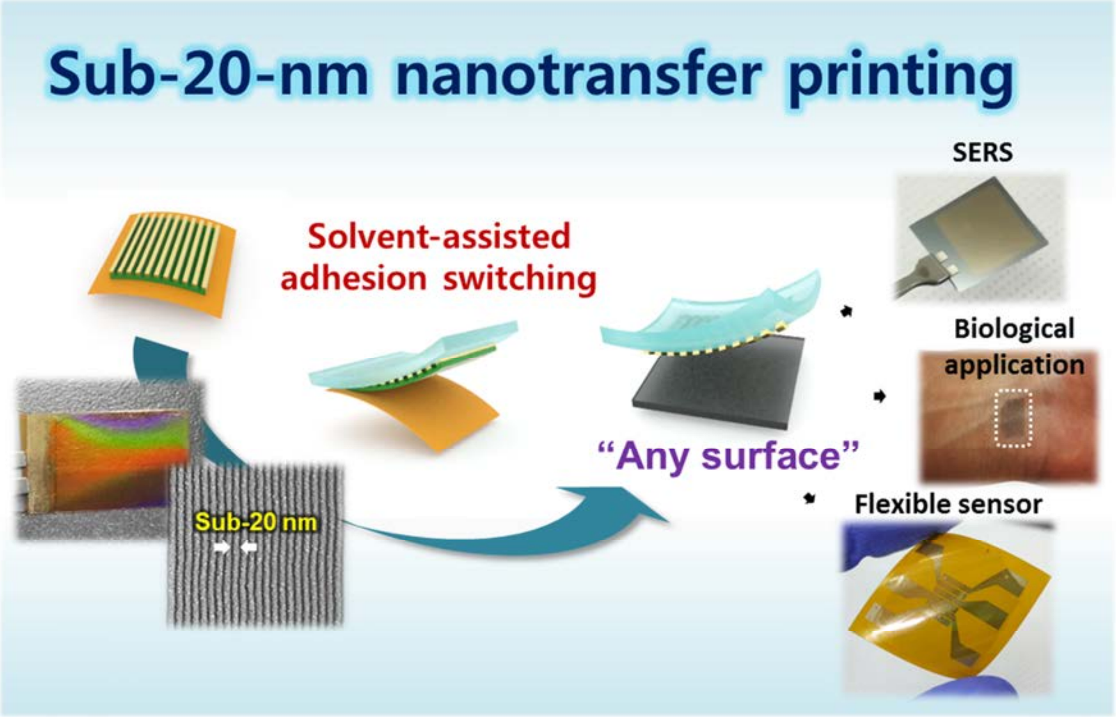
발표코드: **POLY.P-82**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-vapor-assisted nanotransfer printing with sub-10-nm resolution

정재원 허윤형 정연식*

한국과학기술원(KAIST) 신소재공학과

Here, we present a novel nanotransfer printing based on disposable thin-film mold in the help of solvent vapors, and demonstrate sub-10-nm scale nanofabrication on non-conventional surfaces. We conveniently prepared the thin-film mold, which effectively replicates master patterns down to sub-10-nm regime by coating a polymer film on the master substrates, and peeling off the film using common adhesive tape. Through an angled deposition process, various functional nanostructures were easily fabricated on the mold, and they could be transferred to diverse surfaces of receiver substrates through solvent-vapor-induced adhesion control. Our method guarantees sub-10-nm-resolution nanofabrication and remarkably reliable printing, and this method is particularly useful in the fabrication of flexible and printable nanodevices, such as flexible hydrogen sensor as we demonstrated in this work.


Sub-20-nm nanotransfer printing
Solvent-assisted
adhesion switching
"Any surface"
Sub-20 nm
SERS
Biological
application
Flexible sensor

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **IND.P-83**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Dyes Based On the Pyridone and Pyrroline Chromophore and Evaluation of Dye Properties

김헌수 박수열*

한국화학연구원 계면재료공정연구그룹

The synthesis of new donor-acceptor chromophores has been undertaken with examination of their spectroscopic properties. The color of dye could be controlled by choice of suitable donor and acceptor groups. In general, the stonger the donor and/or acceptor, the smaller the energy difference ground and excited states, and the longer the wavelength of absorption. The pyridine and pyrroline acts as active acceptor group due to the powerful acceptor strength by the carbonyl and cyano group. The chromophores was condensed with the donor compounds such as N,N'-dimethylaniline to give dyes. The chromophores is very bathochromic for such a small molecular size and solution are blue in color. Therefore chromophore has been used to synthesise near infrared absorbing dyes.

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발표코드: **IND.P-84**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Liquid phase adsorption of 2,4-dichlorophenoxyacetic acid (2,4-D) with metal-organic framework (MIL-53-Cr)

정범근 정성화*

경북대학교 화학과

A Cr-benzenedicarboxylate (MIL-53, typical metal-organic framework) has been employed for the first time to the adsorptive removal of hazardous 2,4-dichlorophenoxyacetic acid (2,4-D; one of the herbicides) from contaminated water. MIL-53 has a very fast adsorption in one hour and the adsorption capacity of MIL-53 is much higher than that of activated carbon or zeolite (USY). Importantly, the adsorption of 2,4-D over MIL-53 is very favorable especially at low concentrations of 2,4-D. Moreover, the adsorbent can be used several times in adsorptive removal by washing the used adsorbent with a simple solvent. Additionally, zeta potential of the adsorbent and the effect of pH and temperature on the adsorption were also investigated, and a plausible adsorption mechanism could be suggested. Therefore, MOFs such as MIL-53 can be one of adsorbents that could be used in the adsorptive removal of 2,4-D from contaminated water.

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발표분야: 공업화학
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ZSM-5 zeolitic materials synthesized from hexamethylene imine under microwave ageing and application of ZSM-5 in catalytic dehydration of bioalcohols

<u>전종원</u> imteaz ahmed 정성화*

경북대학교 화학과

ZSM-5 zeolite was prepared by using hexamethylene imine (HMI) as a template material. Microwave aging played very crucial role for the crystallization of ZSM-5 from gels. Moreover, adequate reaction conditions (such as Al2O3/SiO2, HMI/SiO2 and H2O/SiO2 ratios, pH, reaction time and so on) for ZSM-5 syntheses are also suggested. The obtained ZSM-5, after ion exchange to the proton form, can be applied in acid-catalyzed reactions because the acidity and surface area of the zeolite are very similar to those of commercial ZSM-5 zeolite. For example, the H-ZSM-5 can be applied in the dehydration of bioalcohols such as ethanol and n-butanol into olefins or aromatics, very similar to a commercial H-ZSM-5 zeolite.

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

Adsorptive denitrogenation of model fossil fuels by Lewis acid loaded metal-organic frameworks

서여송 **imteaz ahmed** 정성화*

경북대학교 화학과

Recently metal-organic frameworks (MOF) are going to be one of the promising adsorbents for their very high surface area and improved functionality. They can be easily modified for specific applications. Here, we report MIL-100(Fe), which was impregnated with a Lewis acidic salt, $AlCl_3$, in order to prepare an acidic adsorbent and it was applied for adsorptive denitrogenation (ADN) of model fuels to investigate the effect of the Lewis acidity of the composite adsorbent. For this, basic adsorbate quinoline (QUI) and a neutral adsorbate indole (IND) were used for deep understanding. A sulfur-containing compound, benzothiophene (BT), was also used along with the two nitrogen-containing compounds (NCCs) in order to investigate the selectivity of the adsorption of the NCCs. It was found that the maximum adsorption capacity of $AlCl_3$/MIL-100(Fe) for QUI was 17% higher than that of the pristine MIL-100(Fe), despite an 8% reduction of the surface area upon loading the MOF with $AlCl_3$. This data show the potential acid-base interaction between acidic Fe_2O_3 and basic QUI. On the other hand, IND as a neutral compound did not show any special interaction with Fe_2O_3 and its adsorption was reduced due to the reduced porosity. And in a combined system of BT, QUI and IND, the adsorption of BT was negligible which confirms the selective adsorption for nitrogen containing compounds. Therefore, it can be concluded that MOFs impregnated with Lewis acidic materials such as $AlCl_3$ can be effectively used for adsorptive removal of basic compounds from fossil fuels especially the NCCs.

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

Graphite oxide/metal-organic framework (MIL-101) composite preparation and its application in adsorptive denitrogenation of model fuels

imteaz ahmed 정성화*

경북대학교 화학과

To improve the functionality of a porous metal-organic framework (MOF), MIL-101 (Cr-benzenedicarboxylate), it was composed with graphite oxide (GO) to obtain GO/MIL-101 composites. Accelerated synthesis was obtained upon adding the GO content to the MOF precursor during the formation of the composite. Additionally, the surface properties also improved in the composite compared with the pristine MOF. The surface area of the composites increased remarkably in the presence of a small amount of GO ($_2$, CH_4, and CO_2 storage) adsorptions and other applications.

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

Influence of Chemical Surface Treatment of Multi-Walled Carbon Nanotubes on Mechanical Interfacial Properties of Basalt/MWCNTs/Epoxy Composites

이성옥 박수진*

인하대학교 화학과

In this work, we studied the influence of chemical surface treatments of multi-walled carbon nanotubes (MWCNTs) on the mechanical interfacial properties of basalt/MWCNTs/composites. The surface properties of the MWCNTs were determined by their acid and base values, Fourier-transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). The mechanical interfacial properties of the composites were assessed by measuring the interlaminar shear stress (ILSS), fracture toughness (K_{IC}).

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

Effect of Chemical Treatment of Basalt Fibers on Fracture Toughness of Basalt Fiber-Reinforced Composites

이성옥 박수진*

인하대학교 화학과

In this work, the effect of chemical treatments of basalt fibers on fracture toughness of basalt fibers/epoxy composites was investigated. The surface properties of the basalt fibers were determined by Fourier transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscope (XPS) analyses. The mechanical interfacial properties of the composites were assessed by interlaminar shear stress (ILSS) and critical stress intensity factor (K_{IC}).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A green process for insoluble sulfur polymerization using electron beam irradiation

박승일 유국현*

동국대학교 화학과

In rubber industry, vulcanization process is certainly needed for using the rubber products. Vulcanization is process that formed crosslinking by sulfur between linear structure of rubber polymer. Insoluble sulfur used vulcanization addictive for preventing blooming effect. Synthesis of Insoluble sulfur is used Thermal polymerization using about 250~300℃ and extraction process is used carbon disulfide for separation between soluble sulfur and insoluble sulfur. But Thermal polymerization process have environmental, economical and safty problem. In this study, we was focus on developing of polymeric sulfur synthesis process using electron beam. The sulfur can be melt by increase temperature or made solution using carbon disulfide. And electron beam is irradiated melting sulfur, sulfur solution and sulfur powder. After irradiation, The high purity polymeric sulfur separated using carbon disulfide. The physicochemical characterizations (XRD and solublity) on obtained insoluble sulfur have been carried out.

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

Effect of Interface Treatments on Pitch-Coated Silicon Composite as the Anode for Lithium-Ion Batteries with Enhanced Performances

김명석 박수진*

인하대학교 화학과

In this work, the effect of interface treatment on pitch coated-layer was formed macroporous that was investigated in electrochemical performance and structural properties of carbonized pitch coated silicon composites. Pitch coated silicon composites were synthesized by mixing of silicon powders and petroleum pitch. And heat treatment as a function of carbonization temperature. The morphologies of composites were observed by scanning electron microscope. And structure of composites was examined using XRD method. The obtained pitch coated silicon composites were assembled as half cell anodes for lithium ion battery which was investigated in their electrochemical properties such as the initial efficiency, the initial discharge capacity and cycle life. From the results, these composites were explained that suitable macroporous size of anode composites interface played an important role in improving initial discharge capacity and cycle life.

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

Effect of Silicon Carbides Coated-Pitch Composites with Improved Thermal Properties and Oxidation Resistance

김명석 박수진*

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In this work, the effect of surface treated-silicon carbide content on the thermal stability, oxidation resistance, and fracture toughness of carbonized pitch coated-silicon carbide composites was investigated. The fracture toughness of the composites was studied using critical stress intensity factor (K1c) measurements. The morphology of the carbonized pitch coated-silicon carbide composites was observed by a scanning electron microscope, and the structure of the composites was examined using X-ray diffraction. In addition, the surface properties of the coated-silicon carbides were determined by Fourier transform infrared spectroscopy. The thermal stability and oxidation resistance of the composites were investigated by thermogravimetric analysis. From the results, it is clear that a suitable amount of silicon carbide played an important role in improving the oxidation resistance, thermal properties, and also fracture toughness of the composites and surface treated composites were improved mechanical properties at suitable amount of surface treated-silicon carbide content.

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발표코드: **IND.P-93**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Desulfurization of fuel by liquid phase adsorption using ionic liquid impregnated metal-organic framework (MOF)

<u>Nazmul Abedin Khan</u> 정성화*

경북대학교 화학과

Liquid phase adsorption of sulfur-containing compounds (SCCs) from fuel was firstly demonstrated by metal-organic framework (MOF) MIL-101 impregnated with ionic liquid species (IL). For that, 1-butyl-3-methylimidazolium chloride (a typical IL) was introduced to one of the widely studied MOFs, MIL-101 (chromium-benzenedicarboxylate) via simple impregnation at ambient condition. A remarkable improvement in the adsorption capacity (~71%) was observed in IL-supported porous MIL-101 compared to the virgin MIL-101 for the adsorption of benzothiophene (BT) from liquid fuel. The improved adsorptive performance could be explained by the acid-base interactions between the acidic ionic liquid and basic BT. Moreover, from this study, it can be suggested that porous MOFs, supported with ionic liquids, may introduce a new class of highly porous adsorbents having the advantage of the imidazolium cationic sites for the efficient adsorption of various compounds.

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발표코드: **IND.P-94**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of Polyethyleneimineon Modified Graphite Oxide for CO2 Capture

신기주 박수진[1,*]

인하대학교 신소재공학부 [1]인하대학교 화학과

AbstractNowadays, the seriousness of global warming was gradually deepens, and because of this major greenhouse gas, carbon dioxide(CO2) emissions are increasing concerns. The CO2 was generated from fossil fuel combustion, but fossil fuels were steady in much need as an essential energy source. So need to contrive technologies to reduce CO2 emission. In this study, modifing the amine groups on the GO surface, modified GO with amine groups for the development of a new CO2 adsorbent. To synthesize amine modified GO surface, polyethyleneimine impregnated of GO surface.GO washed with distilled water and acid treatment. Then make in a neutral aqueous solution, And amine groups were grafted onto the surface of the GO from polyethyleneimine. Consequently GO was impregnated with the polyethyleneimine and investigating CO2 adsorption.

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

Treatment of PCB-laden transformer oil with polyethylene glycols and alkaline hydroxide

유건상* 홍용표

안동대학교 응용화학과

A direct disposal of PCBs (polychlorinated biphenyls) in transformer oil by PEGs (polyethylene glycols) under basic condition has been reported. The transformer oil containing PCBs was treated by the required amounts of PEGs and KOH, along with different reaction times and temperatures. Complete reaction produces aryl polyethylene glycols, the products of nucleophilic aromatic substitution. The relative efficiencies of PCB treatment process were assessed in terms of destruction and removal efficiency (DRE, %). At the experimental conditions of 100 oC and 7 h, 125 oC and 3 h, and 150 oC and 1 h, average DREs of PCBs better than 99.9999% were attained. In studying the chemical reaction of PCBs with PEGs/KOH, it confirmed that the process led to less chlorinated PCBs through a stepwise process with the successive elimination of chlorines. Particularly, the least chlorinated PCBs such as mono- and di-PCBs were not produced in our study. Furthermore, the treated transformer oil can be reused through simple segregating procedures.

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발표코드: **IND.P-96**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Treatment of a highly concentrated PCB-laden transformer oil using counterflow oxidative reaction (COR)

유건상* 최종하

안동대학교 응용화학과

The objective of the present study is to evaluate the efficiency of counterflow oxidative reaction (COR) for direct disposal of a highly concentrated PCBs in transformer oil. The COR technique is based on the limited surface oxidation of carbon through the passage of a flame front in a direction counter to the flow of oxidant. The overall process of COR is completed in a single step, with minimum external energy to initiate a flame. The reaction is exothermic and the energy is derived from oxidation of carbon surface and adsorbed organics in a localized zone, utilizing most of the available oxidant. To assess the performance of COR, the mass loss of carbon and the temperature of a flame in affecting destruction and removal efficiency (DRE) of PCBs were examined. In addition, the surface area, the surface structure, and the adsorptive capacity of regenerated carbons were also studied, by comparing with those of virgin carbon.The results showed that the mass loss of carbon and flame temperature were strongly dependent on the flow rate of oxygen, adsorptive capability of regenerated carbon completely was recovered, as well as destruction and removal efficiency of thermally stable PCBs in transformer oil was achieved with the value of better than 99.9999%.

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Synthesis and characterization of novel surfactants having perfluoroakyl and alkyl groups as a hydrophobe

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Even though a fluorosurfactant has excellent surface activities such as low surface and interfacial tensions, it should be quite interesting a surfactant having two hydrophobes which are perfluoroalkyl and alkyl groups. In this study, fluorinated surfactants having hydrocarbon group as a second hydrophobe were synthesized. Surface tension, interfacial tension and wettability of the synthesized compounds were measured. Surface tensions were below 17 mN/m and interfacial tensions were below 5.5mN/m. The products had much more excellent wettability than commercial fluorinated compounds

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발표코드: **IND.P-98**
발표분야: 공업화학
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High value added production of MFB from industrial waste to available green resources

김선호 김석찬* 유영* 김종천*

국민대학교 화학과

DMT (Dimethyl terephthalate) is well-defined raw material for PET production. In commercial DMT has been synthesized from p-xylene in air oxidation followed by esterification. In this process, partial oxidation of xylene gave rise to major by-products MFB(Methyl 4-formylbenzoate) and MMB (Methyl 4-methylbenzoate). After separation of DMT by distillation under reduced pressure, residues containing DMT, MFB, and MMB with 14%, 80%, and 6%, respectively have been disposed by open burning/detonation. The quantity of PET is getting increased every year, so the quantity of MFB is getting increased, about 70~80% of MFB mixture waste produced, so that we can get a lot of MFB. It is 2,000 MT/year. This kind of incineration has some problems partly because it generates severe nasty smell and lots of CO2, and partly because it costs a lot. And eventually it leads to environmental pollution.Our goal is to get the high value product from useless MFB

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Synthesis and Evaluation of Ecofriendly Nontoxic Cleaning Agents

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국민대학교 화학과

In order to reduce toxicity on the human body, four new cleaning agents (1-4) containing ester and ether functionality have been invented. These synthesized cleaning agents’s physical properties, biodegradability, and LD50 which were conducted by Korea Testing Certification Institute by using standard method showed excellent values. A specimen for cleaning ability was prepared by cutting in 60x40 mm size of stainless steel plate. The surface of the above specimens was applied with four kinds of contaminants, such as cutting oil, anti-rust oil, drawing oil, and lubricating oil. Contaminated specimens were immersed in compounds (1-4) for 1 to 5 minutes to dissolve oil in the cleaning agent. The data indicate that all compounds (1-4) exhibit good cleaning ability toward four contaminants oils. It is also observed that these compounds can be applicable to various industrial cleaning fields as nontoxic and biodegradable cleaning agent because of their excellent biodegradability and LD50 value.

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발표코드: **IND.P-100**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Methane Storage Capacity of Microporous Carbons Derived from Poly(vinylidene fluoride)

최용기 박수진*

인하대학교 화학과

In this study, we have prepared microporous carbons (MCs) using a pyrolysis of polymers for methane storage. The MCs were synthesized by pyrolyzing poly(vinylidene fluoride) without any activation processes. The structural properties were investigated by X-ray diffraction (XRD). The morphological properties were analyzed by scanning electron microscopy (SEM). The textural properties were investigated by N_2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. The methane storage capacity was investigated by a volumetric measurement at 298 K/35 bar.

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발표코드: **IND.P-101**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Heterogeneously catalyzed etherification of glycerol

박서경 이제승* 한태열[1,*]

경희대학교 화학과 [1]경희대학교 에너지청정화학연구실 / 화학과

The catalytic activities of different heterogeneous catalysts were investigated during the etherification reaction of glycerol and the composition of products was evaluated using liquid chromatography. Alkali metal containing zeolite which has strong basicity showed highest catalytic activity among the heterogeneous catalysts used in the experiments. The influences of various reaction variables including the nature of catalyst, the loading amount of catalyst, reaction time, and reaction temperature on the etherification of glycerol were also investigated.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Etherification of glycerol using acetate salts as catalysts

한태열 이제승[*] 박서경[*]

경희대학교 화학과

Recently, glycerol has emerged as a significant worthy bio-resource that can be converted into high valued materials. Diglycerol and triglycerol prepared by the etherification reaction of glycerol have been used as food, cosmetic, and pharmaceutical emulsifiers. Acetate salts used as catalysts showed high catalytic activity with corresponding selectivities of diglycerol and triglycerol. The influences of various reaction variables including the nature of catalyst, the loading amount of catalyst, reaction time, and reaction temperature on the etherification of glycerol were investigated.

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발표코드: **IND.P-103**

발표분야: 공업화학

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Preparation and Characterization of Sucrose-based Porous Carbons for Hydrogen Storage

최용기 박수진*

인하대학교 화학과

In this study, we have prepared porous carbons using a solution of sucrose and sulfuric acid. The chemical activation was performed with various temperatures to enhanced the specific surface area and microporosity. The structural properties were investigated by X-ray diffraction (XRD). The morphological properties were analyzed by scanning electron microscope (SEM). The textural properties were investigated by N_2/77 K adsorption isotherms using Brunauer-Emmett-Teller equation (BET). The hydrogen storage capacity was investigated by a volumetric measurement at 77 K/1 bar.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Methane Storage Capacity of Activated Multi-walled Carbon Nanotubes

최용기 박수진*

인하대학교 화학과

In this study, we prepared activated multi-walled carbon nanoutubes for methane storage. The chemical activation was performed with potassium hydroxide at various temperatures. The structural properties were investigated by X-ray diffraction (XRD). The morphological properties were analyzed by scanning electron microscopy (SEM). The textural properties were investigated by N_2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation. The methane storage capacity was investigated by a volumetric measurement at 298 K/35 bar.

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발표코드: **IND.P-105**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Curing behavior and thermal properties of DGEBA/DDS epoxy resin copolymerized with PES

유한진 박수진*

인하대학교 화학과

In this study, epoxy composites prepared from diglycidylether of bisphenol-A (DGEBA), as the epoxy resin, and polyethersulfone (PES), as the fillers, and 4,4’-diaminodiphenylsulfone (DDS), as the curing agents, to enhance thermal stability and glass transition temperature (Tg). The surface properties were confirmed by X-ray photoelectron spectroscopy (XPS). The surface morphology was examined by scanning electron microscopy (SEM). The structural properties were analyzed by X-ray diffraction (XRD). The thermal properties were investigated by dynamic differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The results showed that thermal stability and glass transition temperature of the epoxy composites were increased with PES amount and dispersion.

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

Phosphorescence of Cyclometalated Iridium Complexes by o-Carborane Substitution

최태섭 손호진[1] 강상욱[1,*] 한원식[2]

고려대학교 세종캠퍼스 신소재화학과 [1]고려대학교 소재화학과 [2]서울여자대학교 화학과

본 연구에서는 대표적인 인광발광재료인 polypyridyl 이리듐 착물에 최근 활발한 연구가 시작된 새로운 광물리적 특성을 보여주는 카보란 (Carborane) 유도체의 도입을 통하여 이리듐(Iridium)-카보란(carborane) 착화합물들이 준비되었다. 화합물의 광물리적, 전기화학적 특성이 및 이론적 계산에 대한 연구를 진행되었으며 카보란 위치에 페닐이 치환된 화합물들이 기준물질로 사용되어 비교되었다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Control of Intramolecular Charge-Transfer Interactions by Incorporating o-Carborane into Dicyanooligothiophene

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A series of o-carborane based dicyanovinyloligothiophenes was prepared as V-shaped A1-D-A2-D-A1 from the developed synthetic protocol with the routes optimized for o-carborane incorporation, where A1 = dicyanovinyl, D = oligothiophene, A2 = o-carborane. Thus, from mono- to sexi-thiophenyl units are divided in half units at the center of o-carborane with the terminal decoration of dicyanovinyl groups as each end-on organic units. Depending on the length between A1 and A2, they showed different intramolecular charge transfer (ICT) properties .

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Rationally Designing Bimetallic Complexes for Light-Driven Redox Catalysis: How to Assign Specific Functions to Each Metal in a Bimetallic Ir(III)-Pt(II) Complex

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고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 신소재화학과

최근 자연계에 존재하는 광합성 안테나 복합체들의 원리를 모방한 인공광합성 연구가 세계적으로 활발히 진행되고 있다. 광에너지를 흡수, 에너지 전달, 그리고 반응점(Reaction Center)에서의 전자전달현상으로 이어지는 자연계 내 촉매반응공정은 실질적인 인공광합성 연구에서 요구되는 다음의 세가지 (1) 집광능력 및 전하분리, (2) 에너지 (엑시톤) 전달, 그리고 (3) 촉매활성점에서의 효과적인 전자이동과 밀접한 연관성을 가지며 광변환 효율을 높이는 결정적인 요인이 된다. 이에 본 연구에서는 효과적인 광변환촉매시스템 개발의 한 방법으로서 집광, 엑시톤전달, 및 촉매 역할들을 한 분자 내에서의 구현되도록 디자인하였다. Polypyridyl 이리듐 (Ir) 착화합물이 집광체로 백금(Pt)착물이 수소발생환원촉매로서 사용되었으며 집광체와 촉매사이의 효과적인 에너지전달을 위하여 2,3-bis(2-pyridyl)pyrazine (dpp) 단위체가 bridge unit 으로 사용되었다. 준비된 다기능 촉매의 광물리적, 전기화학, 그리고 이론계산을 통한 들뜬 전자의 거동 및 촉매작용의 메커니즘 연구가 세밀하게 수행되었으며 수중수소발생 실험을 통한 광촉매 효율이 평가되어졌다.

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

Electronic alteration of bis-triazolyl-silanes to facilitate facile electron injection for deep-blue phosphorescent OLEDs

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고려대학교 소재화학과 [1]서울여자대학교 화학과

A series of four triazol-containing compounds for the type of dimethylbis(4-(4-phenyl-5-(4-(X)phenyl)-4H-1,2,4-triazol-3-yl)phenyl)silane (ST) derivative have been tested as electron-transport material for deep blue phosphorescent OLEDs. A systematic change in the electronic structures is achieved in these compounds by incorporating electron-withdrawing (EW) and -donating (ED) groups (X = -CF_3, -Me, -tBu, and -OMe) at the 4-position of the phenyltriazole group. From their electrochemical properties obtained from cyclic voltammetric measurement, we observed that the LUMO level was significantly affected by different substituents. Overally, all prepared compounds have relatively high triplet energy levels, which is compatible with the energy level of blue phosphorescent emitting layer in blue OLED device. TDDFT calculations were also performed to figure out their frontier orbital distributions and their transition states. Using current-voltage (I-V) and IS measurement of electron only devices (EOD) and OLED, we have obtained values for the Richardson factor, the barrier height, trap density, density of states (DOS) and carrier mobility of ST derivatives and interfaces as device parameters.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon-Carbon Bond Formation in the Electrochemical Reduction of carbon Dioxide Catalyzed by a Iridium Complex

지정민 손호진 강상욱*

고려대학교 소재화학과

화석연료의 사용증가로 생성된 이산화탄소가 야기하는 지구 온난화와 기후변화로인한 자연폐해가 가속화 되면서 전세계적으로 이산화탄소 이용기술의 연구개발에 많은 투자가 이루어지고 있다. 이에 효과적인 이산화탄소환원반응을 위한 방법으로서 많은 연구자들에 의해서 전이금속을 이용한 촉매연구가 활발히 진행되고 있다. 그러나 전이금속을 이용한 CO_2 환원생성물들의 대부분이, 한 개의 Carbon 으로 형성된 C_1 생성물로 고정되며, Two-electron 환원반응의 경우 불균화 반응으로 인해 2 개 이상의 혼합생성물들이 주로 형성되는 한계를 가지고 있다. 본 연구에서 전이금속 화합물들($[(\eta^5\text{-}Me_5C_5)X(bpy)Cl]Cl$; X = Co, Rh, Ir)을 촉매로 사용하여 균일용매 내 electrocatalytic two-electron reduction 을 통한 C2 화합물 ($H_2C_2O_4$)의 선택적인 형성을 확인하였다.

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Rationally optimizing the performance of deep blue phosphorescent materials: A combined computational and experimental study of iridium(III)-based triplet emitters

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The non-radiative decay of the high energy triplet state of a series of Ir(III)-complexes associated with the cleavage of one M-L bond was examined by integrating quantum chemical modeling methods and various experimental techniques. Quantum chemical models suggest that the deep blue phosphorescence originates mainly from a ^{3}MLCT excited state. A chemical pathway for the non-radiative decay of the ^{3}MLCT involving a M-L bond cleavage is explicitly modeled and complete reaction cycles were constructed. Heteroleptic complexes were prepared by employing acetylacetonate (acac), picolinate (pic) and tetrakis-pyrazolyl borate (bor) as ancillary ligands to investigate the stability of the emissive triplet state. A detailed analysis of the computational model and time-resolved luminescence experiments suggest that a combination of electronic effects and the bulkiness of the borate ancillary ligand protect the radiative excited state from non-radiative decay. Finally, developed Ir(III)-complexes were tested as dopants in prototype phosphorescent organic light-emitting diode devices and found to show deep blue electroluminescence with high emission efficiency and color purity.

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Selective Photoreduction of CO_2 by a Re(I) complex stabilized on dye-sensitized TiO_2 with visible light radiation

원동일 곽인혜[1] 손호진[2] 박정희[1] 강상욱[1,*]

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가시광을 이용하여 CO_2 환원을 시키기 위해 TiO_2 반도체에 흡광체로 유기염료(DMOM, Squaraine dye)와 CO_2 환원촉매로 Re(I) complex 를 접합시킨 구조를 제시하였다. 광전환 시스템에서 전자주개(SD)로는 SDN 을 사용하였다. 본 연구에서 가시광 영역인 ≥420 nm 빛을 조사하였을 때, 유기염료가 광자를 흡수하여 들뜬 전자를 TiO_2 의 conduction band 로 넘겨주고 이 전자는 Re(I) complex 로 이동하여 CO_2 가 CO 로 전환되는 메커니즘을 제시하였다. 이때 전자를 건네 준 염료는 SDN 에 의해 전자를 제공받아 재생되는 구조를 이루고 있다. TiO_2 는 3 그룹으로 나뉘어 실험이 진행되었으며 결정형의 [001] facet (S-TiO_2)와 분말형태의 Hombikat UV-10 (H-TiO_2), [001] nanotube (T-TiO_2)를 이용하였으며 S-TiO_2 를 사용하였을 때 가장 높은 광전환 효율을 보였다. 또한 size-controlled Degussa P-25 (D-TiO_2)에 pH 변화 처리를 이용하여 크기를 조절했으며 크기에 따른 광전환 효율을 보았다.

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발표코드: **IND.P-113**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Silicon-based electron-transport materials for highly efficient phosphorescent organic light-emitting diodes

배우리 손호진 강상욱* 한원식[1]

고려대학교 소재화학과 [1]서울여자대학교 화학과

Silicon atoms are used in blue host materials due to their many advantages, such as conjugation blocking for a wide band gap and a tetrahedral geometry for morphology. In this regard, a series of electron-transport materials for deep blue phosphorescent organic light-emitting diode (OLED) were developed employing the tetrahedral structural motif of the silicon atom, $MeSiL_3$, which functioned further to connect triazole, imidazole, triazine, bipyridine, and oxadiazole units in its periphery. Low temperature PL study showed relatively high triplet energy levels for all prepared materials. Furthermore, they have high thermal stability above 100°C. Finally, prepared ETL materials were conducted to the blue phosphorescence OLEDs device and they showed high external quantum efficiency and power efficiency.

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Efficient Light Harvesting and Energy Transfer in Deep-Red Phosphorescent Iridium Dendrimer

장설 손호진 강상욱*

고려대학교 소재화학과

A series of deep-red phosphorescent iridium dendrimers of the type of [Ir(btp)2(pic-PCn)] (Ir-Gn; n = 0, 1, 2 and 3) were prepared in good yield. Harvesting photons on PCn dendrons followed by efficient energy transfer to the iridium center resulted in highly red emissions at around 600 nm by metal-to-ligand charge transfer (3MLCT). The intensity of phosphorescence was gradually enhanced as increasing dendrimer generations. Steady-state and time-resolved spectroscopy were used to investigate the energy transfer mechanism. Based on fluorescence quenching rate-constants of PCn dendrons, the energy transfer efficiencies for Ir-G1, Ir-G2, and Ir-G3 were 99, 98, and 96%, respectively. The energy transfer efficiency for higher generations decreased slightly due to the longer distance between PC dendrons and the core Ir (III) complex which indicated that energy transfer in Ir-Gn is F?rster type energy transfer.

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생산성 향상을 위한 염색 스핀들 장치의 개선 방안

조성우 남대현 정동운*

원광대학교 화학과

기존의 3 분할 방향의 스핀들을 4 분할 형태의 스핀들로 전환하여 유동하는 염색액이 더 강한 압력을 가져 염색원사 사층 내에서도 고르게 염색이 가능할 것으로 예상되고 분량률을 줄일 수 있다. 기존의 스핀들 너트방식에서 원터치방식으로의 개선하여 공정효율증가.

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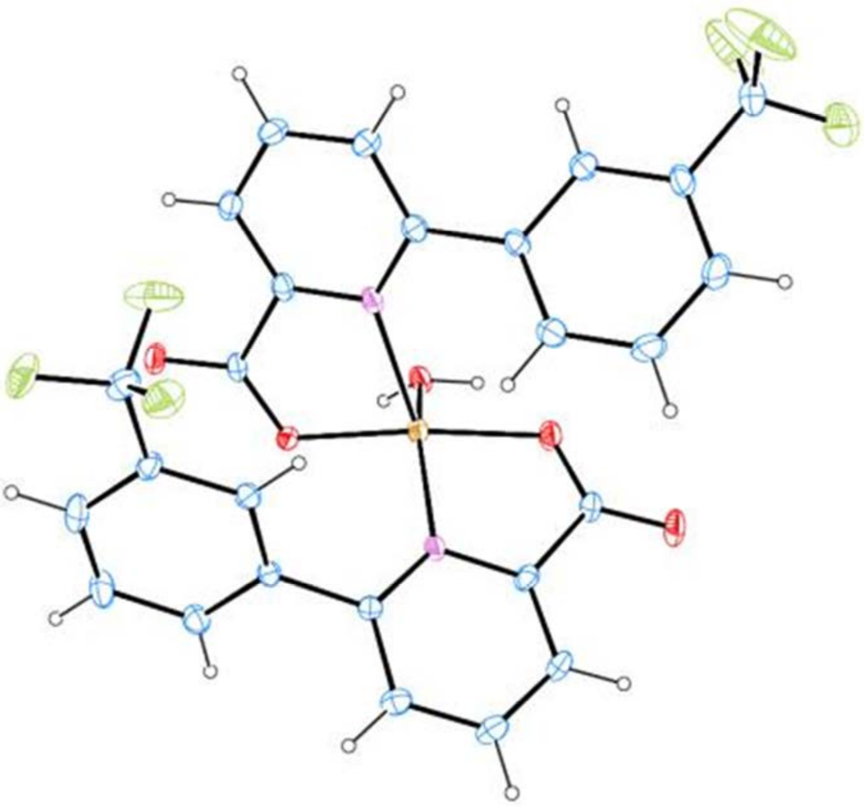
발표종류: 포스터, 발표일시: 수 16:00~19:00

Molecular Structures and Physical Properties of Cu(II) and Tb(III) Complexes with potassium pyridine-2-carboxylate Derivatives

김한얼 강성권[1,*]

충남대학교 화학 생화학부 [1]충남대학교 화학과

Lanthanide trivalent ions are effective for luminescent materials because of their excellent quantum efficiency. Tb atom in the titled complex is eight-coordinated to oxygen atoms of (2,4-dichlorophenyl)pyridine-2-carboxylate [DPC] ligand. The Cu(II) cation is five-coordinated by (trifluoromethyl)phenyl)pyridine-2-carboxylate [TPC] ligand. In the terbium complex, carbonylates of DPC ligand are linked by the two terbium metals and the geometries around metal is square antiprism. In copper complex, the geometries around Cu metal is square pyramid. Tb(III) and Cu(II) complexes have been characterized by UV, IR, PL spectra and X-ray single crystal studies



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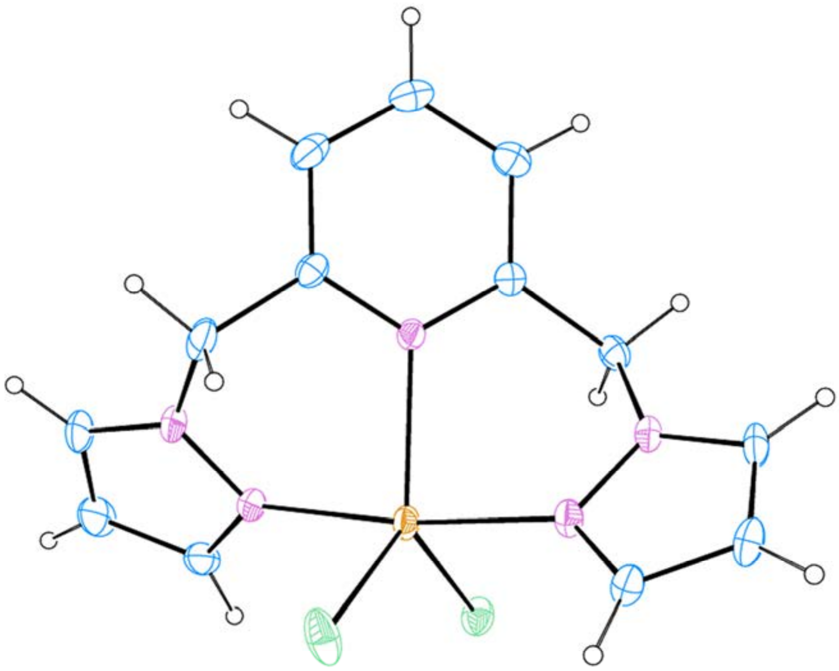
Syntheses and Characterizations of Cu(II) Complexes with 2,6-bis((1H-pyrazol-1-yl)methyl)pyridine

김남훈 강성권*

충남대학교 화학과

The Cu(II) complexes with 2,6-bis((1H-pyrazol-1-yl)methyl)pyridine (PMP) were designed and synthesized. The complexes were investigated by IR, UV-Visible spectroscopy and single crystal X-ray crystallography. The PMP ligand is coordinated to the Cu metal as a tridendate NNN ligand. The three bonding sites are the pyrazole and pyridine nitrogens. X-ray studies show that the Cu(II) metals are five-coordinated two form, trigonal bipyramid and square pyramid, depending on their counter-anion, i.e. Cl^- and NO_3^-



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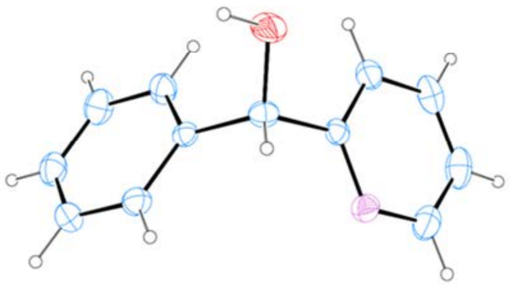
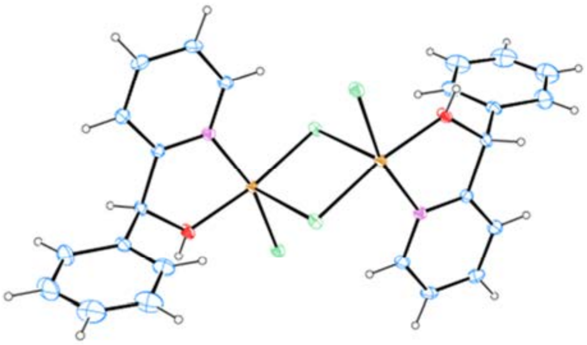
Molecular Structures and Physical Properties of Cu(II) Complexes with PPM Ligands

김한얼 강성권[1,*]

충남대학교 화학 생화학부 [1]충남대학교 화학과

The phenyl-2-pyridinyl methanol (PPM) ligand was made from benzoylpyridine. And the reactions of PPM with CuCl2 were studied to make [Cu2(PPM)2Cl4] complex. These compound have been synthesized and characterized by UV, IR, TGA, and single crystal X-ray diffraction. Geometry around Cu(II) metal is five-coordinated to forrn squre pramid with one oxygen (hydroxy), one nitrogen (pyridine), and three chloride atoms.





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발표분야: 무기화학

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Synthesis of new Pd(II)-NHC (N-Heterocyclic Carbene) Complexes having small organic group and their catalytic activity in Suzuki-Miyaura cross-coupling reactions

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강릉원주대학교 화학과 [1]성균관대학교 화학과

Various σ-allenyl and alkyl Pd(II) Complexes were prepared from the oxidative addition of propargyl halide or dichlorometane to the Pd(0) compounds, Pd(styrene)(PR_3)2] or Pd^0-NHC compound. Treatments of the σ-allenyl complex, trans-[ClPd(CH=C=CH_2)(PR_3)$_2$] with NHC (N-heterocyclic carbene) ligand also caused the ligand substitution to give new σ-allenyl Pd(II) -NHC complexes. Suzuki-Miyaura cross-coupling of aryl halides with aryl boronic acids using the above Pd(II) complexes were examined.

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Synthesis, structures, and chemical properties of novel Pd(II) and Pt(II) complexes containing organic isocyanato group

김용주* 이선계 최근영 박수진[1] 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Several reactions of Pd^0-PMe_3 or Pd^0-PMe_2Ph complexes with two equiv. of R-NCO (R = benzyl, Ph, p-Tolyl, p-ClC_6H_4,P-$MeOC_6H_4$) were examined. Isolated new Pd(II) isocyanato complexes were characterized by spectroscopic and elemental analyses. Aslo, the cyclic trimerization of organic isocyanate was observed. Treatments of new isocyanato Pd(II) complexes with chelated phosphine such as DEPE (1,2-bis(diethylphosphino)ethane) or DMPE (1,2-bis(dimethylphosphino)ethane) readily underwent ligand substitution to afford Pd(II) isocyanates having a chelated phosphine. Detail reaction mechanism will be discussed.

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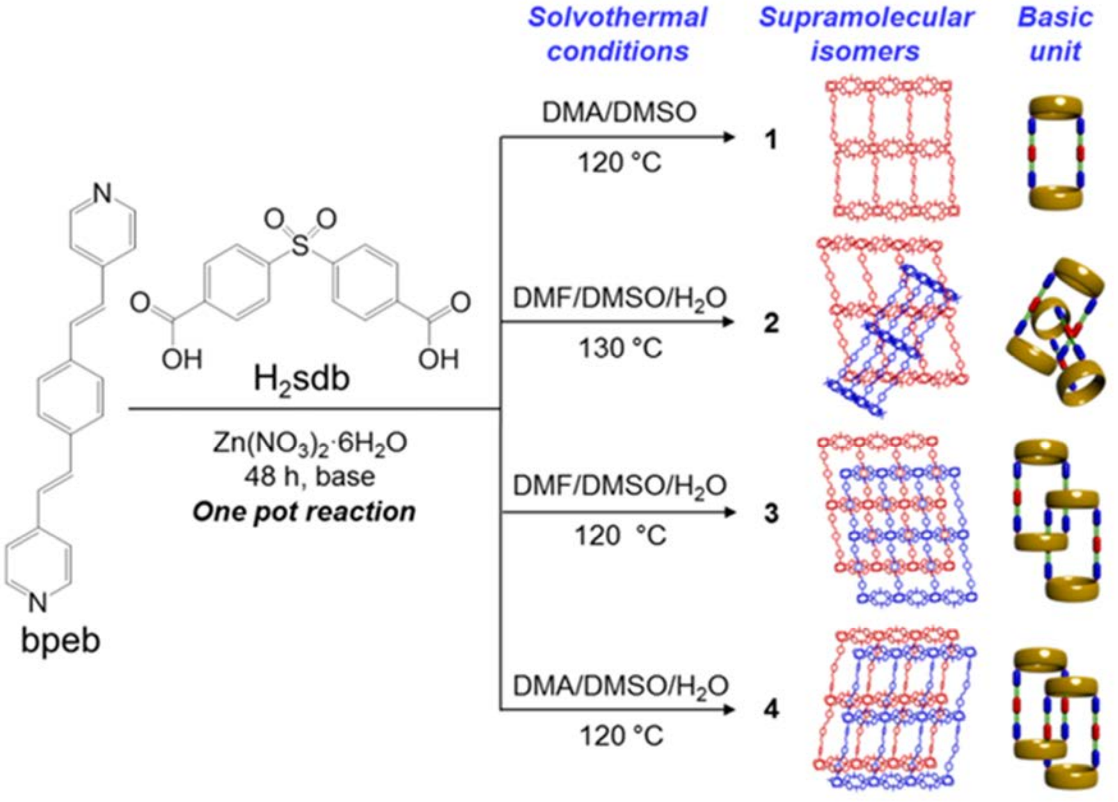
발표종류: 포스터, 발표일시: 수 16:00~19:00

Distortional Supramolecular Isomers of Polyrotaxane Coordination Polymers

박인혁 Raghavender Medishetty[1] 이심성[*] Jagadese J. Vittal[1,*]

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

Distortional isomers are known as bond-stretch isomers differ only in the length of one or more bonds. This distortion has been found to be due to crystallographic disorder in most cases, but shown to exist in Cu(II) due to its plasticity. Here we describe syntheses of four supramolecular isomers of [Zn_2(bpeb)$(sdb)_2$], 1-4, based on 2D CPs from ZnII salt, 1,4-bis[2-(4'-pyirdyl)ethenyl]benzene (bpeb), and 4,4'-sulfonyldibenzoate (sdb) by varying the experimental conditions (*see* below). It is interesting to note that the intentional addition of water produced interpenetrated (2) and polyrotaxane (3 and 4) isomers. The large square formed between two angular space ligand sdb are connected by two [$Zn_2(O_2C\text{-}C)_4$] paddle-wheels to form necklace-like 1D CPs which are further linked by the bpeb ligands through the axial positions of ZnII in the paddle-wheel building unit. The large [$Zn_2(sdb)_2$] square acts as a wheel and the long bpeb spacer from the neighbouring 2D CP acts as an axle in forming two more isomers based on polyrotaxane motif (3 and 4). These two differ by the conformation of the bpeb as well as relative orientations of the axles in the two-fold entanglements. In one entangled structure, the neighbouring C=C bonds are found to be slip-stacked and undergoes single [2+2] cycloaddition reaction under UV light in a single-crystal-to-single-crystal (SCSC) manner. Interestingly, all these compounds exhibit PL. Selective quenching of PL for 4 was observed for 2,4-dinitrophenylhydrazine (2,4-DNPH) compared other nitro analytes and this selectivity has been also shown for the material obtained after [2+2] cycloaddition reaction.


Solvothermal conditions
Supramolecular isomers
Basic unit
bpeb
H₂sdb
Zn(NO₃)₂·6H₂O
48 h, base
One pot reaction
DMA/DMSO
120 °C
1
DMF/DMSO/H₂O
130 °C
2
DMF/DMSO/H₂O
120 °C
3
DMA/DMSO/H₂O
120 °C
4
N
O
S
OH

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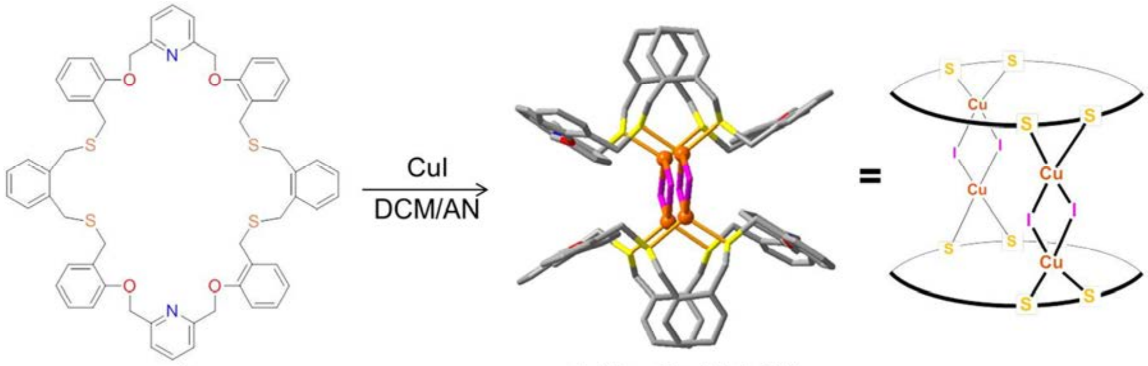
Supramolecular Complexes of 19- and 38-Membered Thiaoxaaza-Macrocycles via 1:1 and 2:2 Cyclizations

강윤지 박인혁 이심성*

경상대학교 화학과

There is a growing interest in a large macrocyclic ligand system that can form binuclear complexes exhibiting electron transport, charge transfer, and allosteric behavior. In this presentation, supramolecular complexation behaviors of a 19-membered NO_2S_2-macrocycle L^1 and a 38-membered $N_2O_4S_4$-macrocycle L^2 (a 2:2 cyclization byproduct) are reported. Four metal complexes (1?4) of L^1 and L^2 with silver(I), cadmium(II), copper(I), or copper(II) were prepared and structurally characterized. When $AgNO_3$ was employed in the reaction with L^1, a typical endocyclic mononuclear complex, $[Ag(L^1)]NO_3$ (1), was obtained. In the cadmium(II) iodide complex of L^1, two mononuclear macrocyclic complex units are doubly linked by two bridging iodide atoms, adopting a double-decker type dimeric complex featuring two separated units of formula $[?_2\text{-}Cd_2I_2)_2(L^1)_2][Cd_2I_6]$ (2). When CuI was reacted with L^1 in the presence of CdI_2, we obtained a mixed metallic complex featuring two separated units of formula $[Cu(L^1)][Cd_2I_6]$ (3). The most fascinating product is a copper(I) iodide complex, $[(?_2\text{-}Cu_2I_2)_2(L^2)_2]$ (4), with the large macrocycle L^2 (*see below*). In 4, two macrocycles are doubly linked by two Cu_2I_2 squares via Cu-S bonds resulting in the formation of a large double decker. In packing, the six aromatic rings directing toward outside the cavity in each complex unit have a star-shape and the intermolecular π-π interactions among the star-shaped supramolecules form a well closely packed structure.



$\mathbf{L}^2$

4, $[(\mu_2\text{-}Cu_2I_2)_2(\mathbf{L}^2)_2]$

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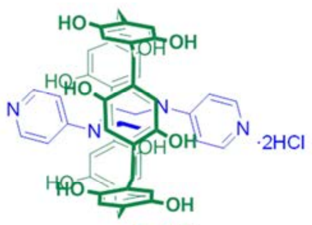
Pseudo-Rotaxanes Constructed From Pillar[5]arene andPolyrotaxane Where String and Bead Are Made from Same Components

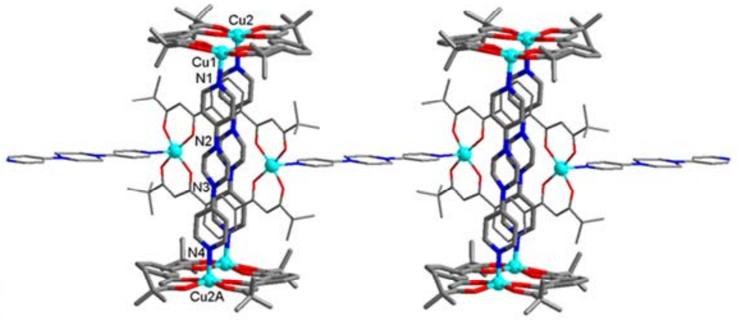
주희영 Jack K. Clegg[1] Leonard F. Lindoy[2,*] 이심성[*]

경상대학교 화학과 [1]School of Chemistry and Molecular Biosciences, The University of Queensland [2]School of Chemistry, The University of Sydney

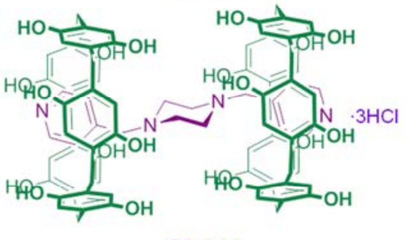
We successfully synthesized new types of two pseudo-rotaxanes, G@H and G'@H_2, and one polyrotaxane, $\{[Cu_2(L)_2(\mu^2\text{-bpypip})_2][Cu_2(L)_2(\mu^2\text{-bpypip})](\text{bpypip})\}_n$ (2), from pillar[5]arene and dicopper(II) bis-ß-diketonato platform $[Cu_2(L)_2(THF)_2]$, respectively. In the construction of the pseudo-rotaxanes, bipyridyl piperazine derivative salts such as bpypip$\cdot$2HCl (G) or bpmpip$\cdot$3HCl (G') serve as guests for the host pillar[5]arene (H). The proposed suprastructures of the pseudo-rotaxanes with 1:1 or 1:2 host-guest complexes are supported by comparative NMR experiments, ESI-mass, NMR titrations, and UV titrations. In the NMR titrations, a good fitting of the data was obtained with the 1:1 for G@H (log K_{11} = 4.7) and 1:2 for G'@H_2 (log K_{11} = 4.5, log K_{12} = 5.8, and log $ß$ = 10.3). While, in the one-pot reaction of the dicopper(II) bis-ß-diketonato platform with bpypip yielded a stairway-type 1D polymer copper(II) complex, $\{[Cu_2(L)_2(\text{bpypip})]\cdot 2THF\}n$ (1), and polyrotaxane-type $\{[Cu_2(L)_2(\mu^2\text{-bpypip})_2][Cu_2(L)_2(\mu^2\text{-bpypip})](\text{bpypip})\}_n$ (2) as a kinetic (1) and a thermodynamic (2) controlled products. As we understand, the product 2 is a first example of polyrotaxane where string and bead are made from same components. Pathways of the formation of the polyrotaxane via '*polymerization (rearrangement)-docking-clipping*' steps are proposed.



G@**H**



1D Polyrotaxane-Type Chain,
$\{[\mathrm{Cu}_2(\mathbf{L})_2(\mu^2\text{-bpypip})_2][\mathrm{Cu}_2(\mathbf{L})_2(\mu^2\text{-bpypip})](\text{bpypip})\}_n$ (**2**)



G'@**H**$_2$

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발표코드: **INOR.P-124**
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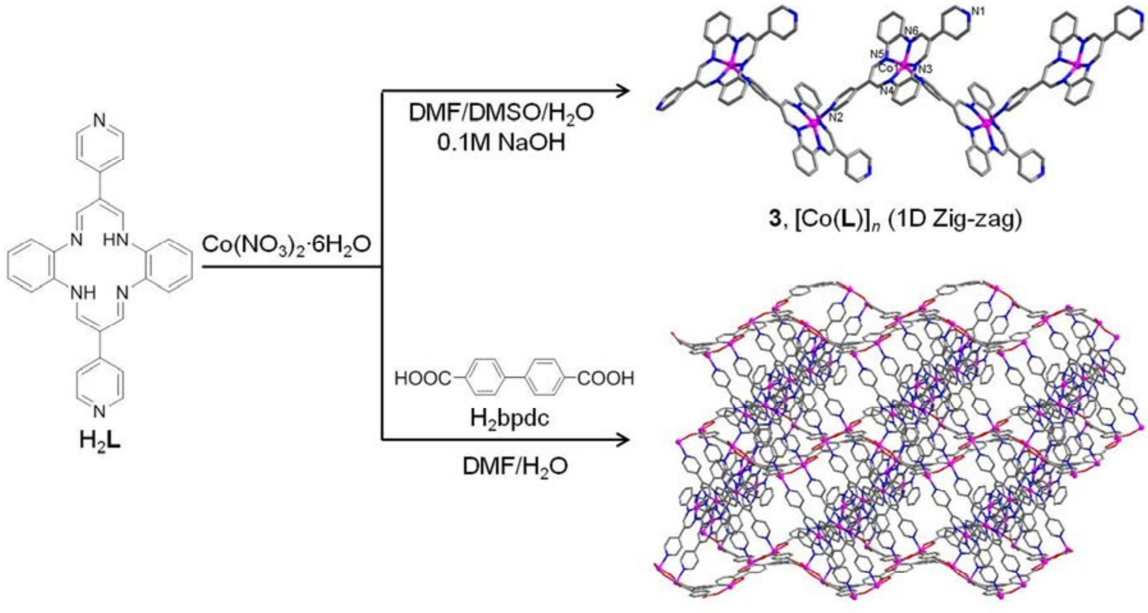
발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of 1-3D MOFs Incorporating Dipyridyl-N_4-Macrocycle as a Pillar Ligand

류현수 Leonard F. Lindoy[1,*] 이심성[*]

경상대학교 화학과 [1]School of Chemistry, The University of Sydney, Sydney , NSW 2006, Australia

Dipyridyldibenzotetraaza[14]annulene (H_2L) has an extended structure of 14-membered dibenzo-cyclen having dipyridyl terminals. Thus, its multiple topic including macrocycle, pyridine base and pillar properties are expected upon complexation.[1] In this work, we synthesized and structurally characterized four complexes of type [Ni(L)][Ni(L)] (1), $\{[Zn(H_2L)(m\text{-bdc})]^{\cdot}DMF^{\cdot}3H_2O\}_n$ (2), $[Co(L)]_n$ (3), and $[Co_4(L)_2(bpdc)_2]_n$ (4), all based on the dipyridyl-derivatized macrocycle, H_2L. In 1, the Ni(II) occupies the macrocyclic cavity, being bound to the N_4-donor of the macrocycle in its doubly deprotonated form. Reaction of H_2L with $Zn(NO_3)_2{}^{\cdot}4H_2O$ and m-H_2bdc afforded a 2D coordination polymer 2, with the L linked by *m*-bdc backbone. In this case, the Zn(II) does not occupy the macrocyclic cavity but is bound to a pyridyl nitrogen from two ligands. In 3, the Co(II) is occupies the macrocyclic cavity, being bound to the N_4-donor set of the macrocyclic ring. The remaining one site is occupied by a pyridyl nitrogen from a second ligand in one side of the macrocyclic plane axially, resulting in the formation of an infinite 1D structure. In addition, the reaction of H_2L with $Co(NO_3)_2{}^{\cdot}6H_2O$ in the presence of H_2bpdc resulted in the pillar-layered 3D framework, $[Co_4(L)_2(bpdc)_2]_n$ (4). In 4, the 3D framework was generated by pillaring the 2D layers formed by H_2bpdc with two macrocyclic complex units arranged side by side.



H_2**L**

3, $[Co(\mathbf{L})]_n$ (1D Zig-zag)

4, $[Co_4(\mathbf{L})_2(bpdc)_2]_n$ (3D pillar-layered)

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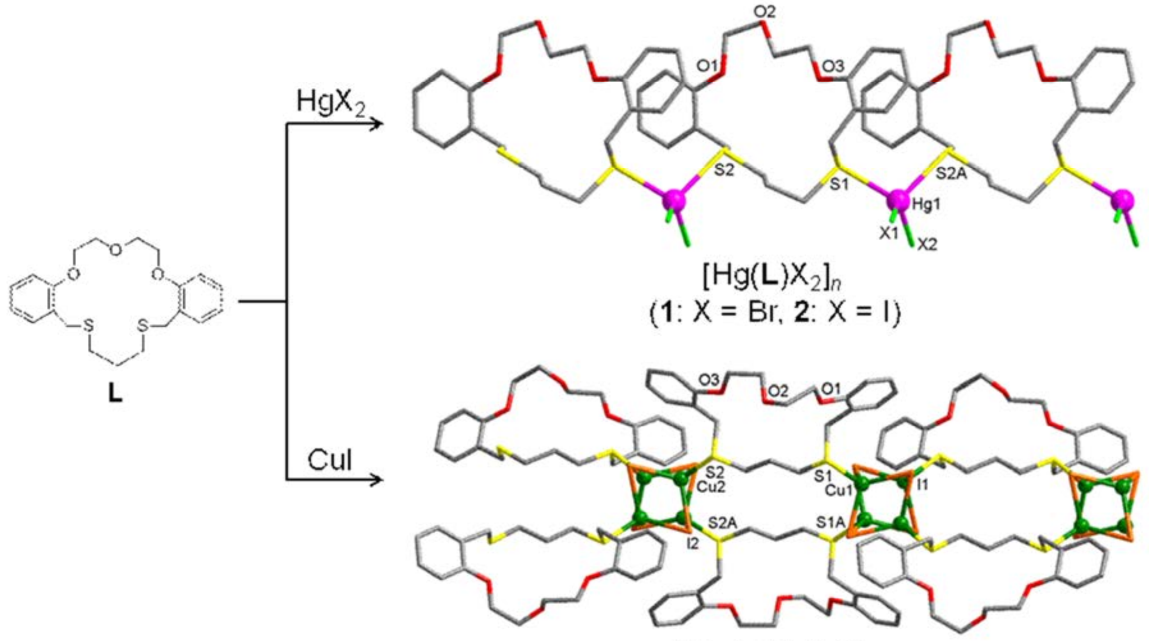
Supramolecular Soft Metal Complexes of an O_3S_2-Macrocycle with 1-D Polymeric Structures

최한별 류현수 이심성*

경상대학교 화학과

An 18-membered O_3S_2-macrocycle, L, and its thiaphilic soft metal complexes were synthesized and structurally characterized by X-ray analysis. Reactions of L with mercury(II) halides yielded isostructural one-dimensional (1-D) coordination polymer of type $[Hg(L)X_2]_n$ (1: X = Br and 2: X = I, *see below*), in which each tetrahedrally coordinated Hg(II) atom links two macrocycles via two Hg-S bonds to generate a chain structure. The remaining two sites are occupied by two halide anions. While, same reaction with CuI afforded an emissive double-stranded 1-D polymeric complex, $[Cu_4I_4(L)_2]_n$ (3). In 3, the successive ligand molecules are linked by a cubane-type Cu_4I_4 cluster via Cu?S bonds, with the macrocycle adopting a highly twisted configuration. Photoluminescence of compound 3 was also studied in solid state.



$[Hg(\mathbf{L})X_2]_n$
(**1**: X = Br, **2**: X = I)

$[Cu_4I_4(\mathbf{L})_2]_n$ (**3**)

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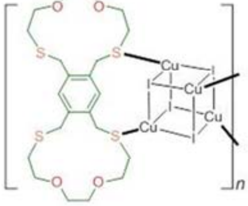
Cu_nI_n Cluster Complexes of Bis-thiamacrocycle Isomers

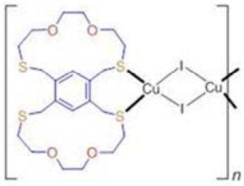
김슬기 이심성* Mari Ikeda[1] Yoichi Habata[2]

경상대학교 화학과 [1]Education Center, Faculty of Engineering, Chiba Institute of Technology, Japan [2]Department of Chemistry, Toho University, Japan

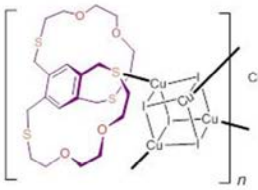
The self-assembly involving copper(I) iodide and multidentate ligands often leads the discrete complexes and continuous ones because the copper(I) iodide are capable of adopting a variety of structural motifs to form clusters such as rhomboid dimer, cubanes, prisms, 1D chains, and double-stranded stairs.[1] However, many of the copper(I) iodide cluster complexes have been obtained accidently, because of the difficulty of controlled synthesis of the specific cluster due to their similar energies. One of our targets is the selective stabilization of the copper(I) iodide clusters through the controlled ligand-directed approach by rational design and modification of the macrocycle system. Recently, we reported the regioisomers (*o*-L and *m*-L) of bis-dithiamacrocycle and the regioisomer-controlled endo- and exocyclic coordination behaviors of the silver(I) complexation depending on the intercyclic S···S distances.[2] As an extension of this concept, we isolated some exo-coordinated 1D coordination polymers (CPs) including $[(Cu_4I_4)o\text{-L}]n$ (1) and $[(Cu_2I_2)m\text{-L}]_n$ (2) in which 1 and 2 are connected by cubane and rhomboid dimer clusters, respectively.[3] More recently, we are successful to separate a para isomer, *p*-L, from the isomeric mixture. The *p*-L reacts with CuI to form an emissive 3D framework with an infinite suprastructure, $[(Cu_4I_4)p\text{-L}]_n$ (3), in which the *p*-L ligands are linked with cubane-type Cu4I4 clusters. In addition, we obtained an endocyclic Cu2I2 cluster complex, $[(Cu_2I_2)(L^2)]$ (4)[3], based on the 24-membered macrocycle, L^2, obtained from the 2:2 cyclization[4] as a first example of the endocyclic complex of this type.Reference1.S. Park, S. Y. Lee, K.-M. Park, S. S. Lee, *Acc. Chem. Res.* 2012, *45*, 391.2.A. D. Siewe, J.-Y. Kim, S. Kim, I.-H. Park, S. S. Lee, *Inorg. Chem.* 2014, *53*, 393.3.Unpublished results. 4.Y. Habata, J. Seo, S. Otawa, F. Osaka, K. Noto, S. S. Lee, *Dalton Trans*. 2006, 2202.



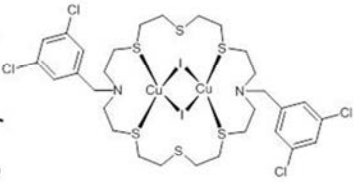
1 (1D)



2 (1D)



3 (3D)



4

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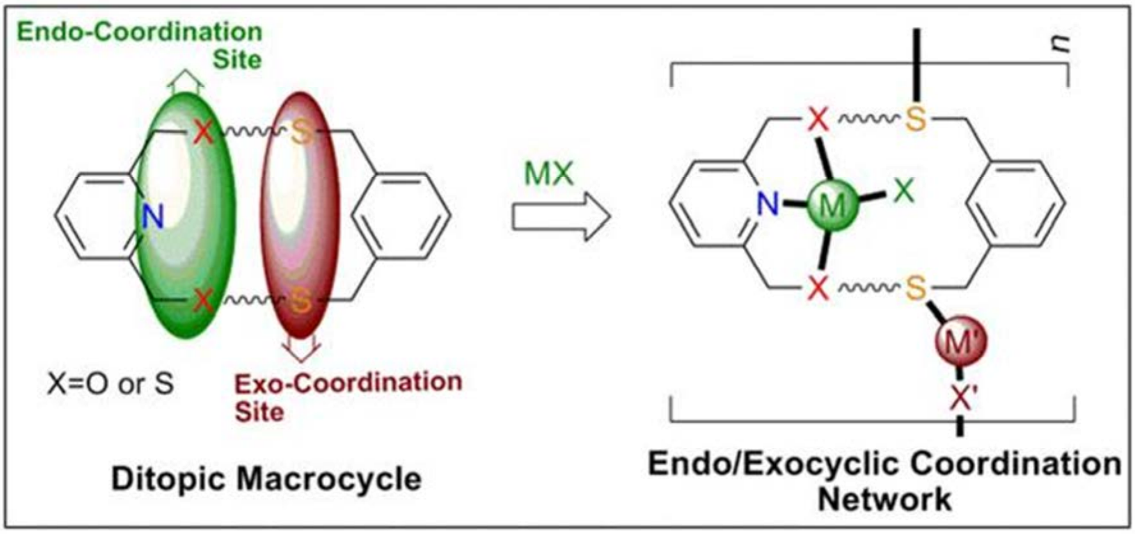
Crystal Engineering Approach toward Endo/Exocyclic Complexes of Macrocycles: Homo- and Heteronuclear Coordination Polymers

이은지 이심성*

경상대학교 화학과

Rationally designed NS_4-macrocycle L^1 and NO_2S_2-macrocycle L^2 which employ NX_2 donors (X= S or O) in one side to accommodate a metal cation in the cavity (endo-coordination) and the two sulfur donors as bridgeheads for the exo-coordination have been synthesized. The proposed approach allowed us to prepare several endo/exocyclic multi-dimensional coordination polymers. As might be expected, reaction of L^1 with $AgClO_4$ afforded an endo/exocyclic 1D coordination polymer (1). Exposure of 1 to different solvent induces a single-crystal to single-crystal (SCSC) transformation, resulting in a 1D coordination polymer (2) formed through rearrangement of the metal coordination environment coupled with a framework distortion. Meanwhile, reaction of L^2 with $AgClO_4$ afforded an endo/exocyclic 2D coordination polymer (3), in which the 2D network is made up of the cyclic dimer (Ag_4L_2) units and further bridged by the anion. In addition, reaction of HgI_2 with L^1 in the presence of CuI afforded a 1D Hg(II)/Cu(I) heteronuclear coordination polymer (4), in which each ligand is bridged by μ_2-Cu_2. On the other hand, the reaction of L^2 with a mixture of HgI_2 and CuI afforded a 1D Cu(I) coordination polymer (5), in which the square-type dimercury(II) hexa-iodide cluster exists as a separated counter anion.


Endo-Coordination Site
X
S
N
X
S
X=O or S
Exo-Coordination Site
Ditopic Macrocycle
MX
n
X
S
N
M
X
X
S
M'
X'
Endo/Exocyclic Coordination Network

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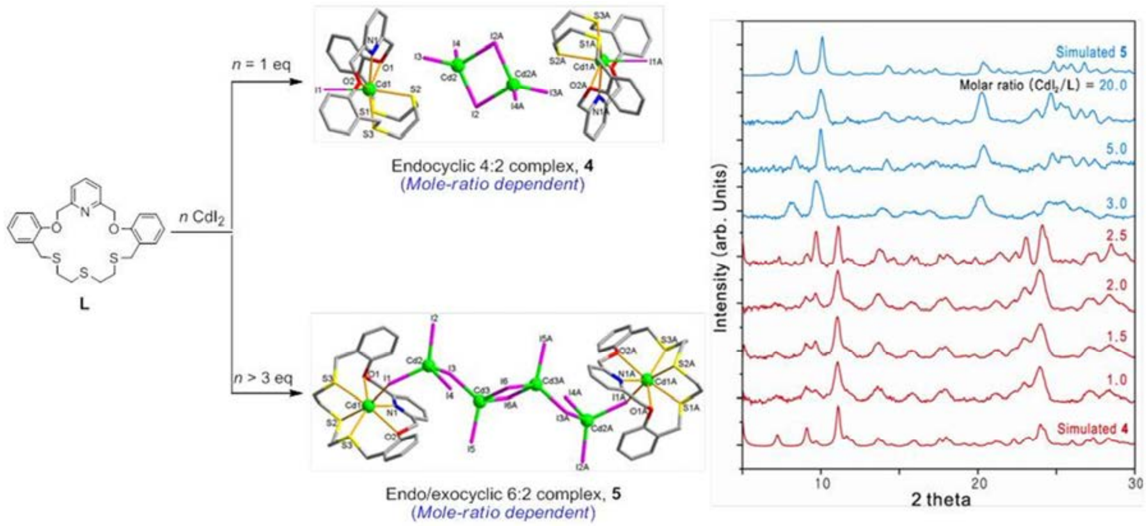
Complexation Behaviors of an NO_2S_3-Donor Macrocycle with Cadmium(II) Halides

이형환 박인혁 이심성*

경상대학교 화학과

Synthesis of an NO_2S_3-macrocycle (L, *see* below) incorporating a pyridine subunit and its anion and/or mole ratio-dependent coordination modes in the formations of cadmium(II) halide complexes are reported. The reaction of L with $CdBr_2$ afforded a bromo-complex, $[Cd(L)Br]_2[Cd_2Br_6]$ (1), showing three separated units: two macrocyclic complex cation units and one cadmium cluster complex anion unit. The complex 1 was filtered and the filtrate was collected. Complex $[Cd(L)Br]_2[CdI_4]$ (2) was formed by the slow diffusion into this resulting solution after a day. In the reaction of L with CdI_2, two endocyclic complexes, $[Cd(L)I]_2[CdI_4]\cdot(CH_2Cl_2)$ (3) and $[Cd(L)I]_2[Cd_2I_6]\cdot(CH_2Cl_2)$ (4), with different cadmium cluster complex anion unit were isolated as a kinetic (3) and thermodynamic controlled (4) products in neutral condition. In the mole-ratio variation experiments, notably, the use of three equivalents or above amount of CdI_2 in the same reaction condition gave a unique endo/exocyclic dumbbell-type complex, $[Cd_6(L_2)I_{12}]$ (5). To monitor the observed mole ratio-dependent endo-coordination products as well as their reactivities, the systematic powder X-ray diffraction (PXRD) analysis has also been applied (*see* below).


L
n CdI$_2$
n = 1 eq
n > 3 eq
Endocyclic 4:2 complex, **4**
(*Mole-ratio dependent*)
Endo/exocyclic 6:2 complex, **5**
(*Mole-ratio dependent*)
Cd1
Cd2
Cd3
Cd1A
Cd2A
Cd3A
Intensity (arb. Units)
2 theta
Simulated **5**
Molar ratio (CdI$_2$/L) = 20.0
5.0
3.0
2.5
2.0
1.5
1.0
Simulated **4**
10
20
30

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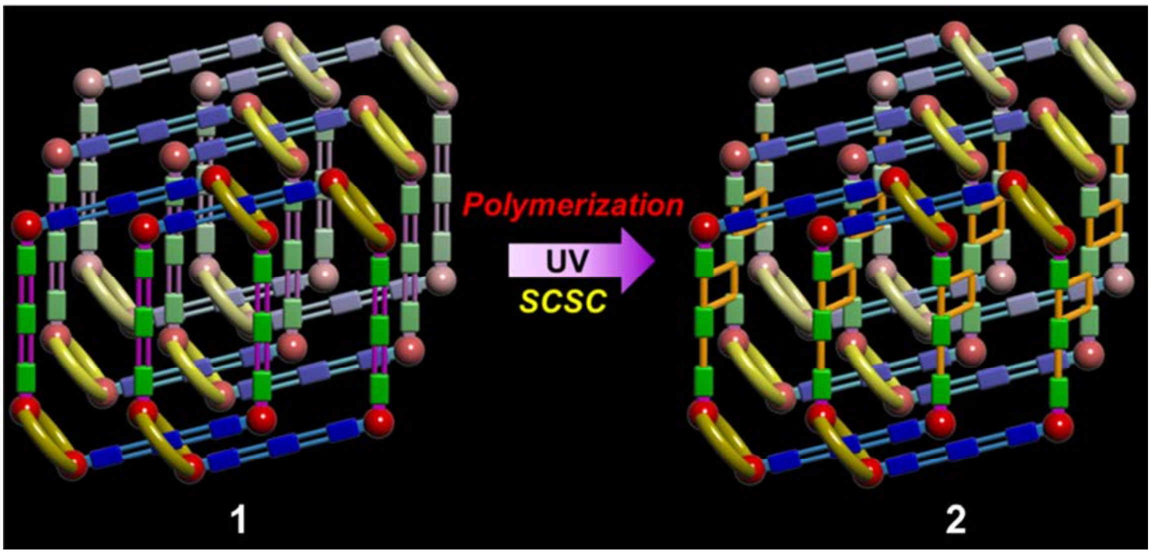
From 2D Polyrotaxane MOF to 3D Metal-Organo Polymeric Framework (MOPF) via [2+2] Cycloaddition Reaction in Solid-State

박인혁 Raghavender Medishetty[1] 이심성[*] Jagadese J. Vittal[1,*]

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

Molecular entanglement is one of the exciting fields of science. Of these rotaxane based organic systems as well as metal containing rotaxanes attracted enormous interest due their unusual structural topologies as well as potential applications, for example, as molecular motors, switching and sensing abilities. On the contrary, interpenetrating polyrotaxane structures in coordination polymers (CPs) were first reported by Robson in 1997. Stilbene based pseudorotaxanes have been found to undergo [2+2] cycloaddition reaction both in the solid state and solution. However, we are not aware of any photoreactive interpenetrated polyrotaxane based CPs, probably due to difficulty in combining two entirely different structural requirements in making it. In this work, the well-known [2+2] cycloaddition reaction has been used for the photo-polymerization of a conjugated diene ligand, bpeb. The polymerization observed in a metal-organic framework (MOF) has been assisted by the Cd(II) atoms which align the alternate bpeb ligands in the [Cd(bpeb)] zigzag chains to pack in a slip-stacked manner in a plane. This is a rare photoreactive 2D polyrotaxane MOF, [Cd(bpeb)(sdb)]?DMA (1), formed by 2-fold entanglement. The structural transformation readily occurs on the well-aligned alternate bpeb ligands under UV light yielding another 3D polyrotaxane MOPF, [Cd(bpeb)$_{0.5}$(*poly*-bppcb)$_{0.5}$(sdb)]?DMA (2), in an SCSC manner. Compound 2 is also a unique MOF containing an unusual organic polymer as a linker along with the conventional bent dicarboxylate ligand. This photo-dimerized structure 2 has both organic polymer ligand fused together with two-fold entangled rotaxane formed by [Cd(bpeb)$_{0.5}$(sdb)].


Polymerization
UV
SCSC
1
2

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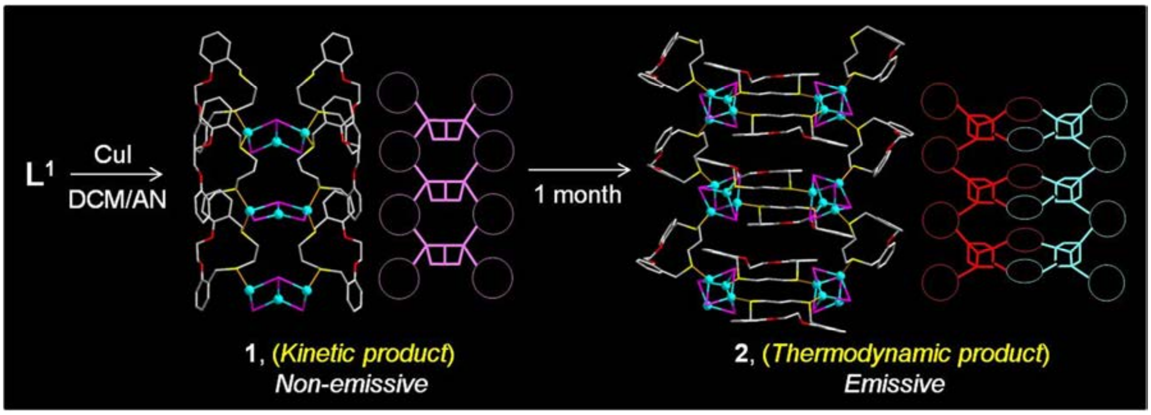
Regio-Isomers of 15-Membered O_2S_2-Macrocycle: Comparative Study for Their Supramolecular Soft Metal Complexes

천유경 김슬기 이심성*

경상대학교 화학과

Two regio-isomers of 15-membered O_2S_2-macrocycle, L^1 and L^2, were employed to prepare their supramolecular complexes with thiaphilic metal ions.[1,2] In the reaction of L^1 with CuI, two 1-D polymeric complexes $[(Cu_3I_3)(L^1)_2]$ (1) and $[(Cu_4I_4)(L^1)_2]$ (2) with different connectivity patterns were isolated as a kinetic (1) and a thermodynamic (2) products, respectively (*see below*). In 1, four macrocycles are bound to one Cu_3I_3 cluster at the center via Cu-S bond to generate a ladder from. While, four macrocycles in 2 are attached to one cubane Cu_4I_4 center via Cu-S bond to form an emissive double-ladder structure. Ligand isomer L^2 reacts with copper(I) halides and afforded isostructural dimer complexes $[(Cu_2X_2)(L^2)_2]$ (3: X = Br, 4: X = I) in which two exocyclic mononuclear complex units are linked with two bridging halide atoms. In the above CuI reaction, a double stranded 1D polymer complex, $[(Cu_2I_2)(L^2)]_n$ (5), was also isolated as a mixture with 4.

References
1.S. Park, S. Y. Lee, K.-M. Park, S. S. Lee, *Acc. Chem. Res.* 2012, *45*, 391.
2.S. Y. Lee, S. Park, S. S. Lee, *Inorg. Chim. Acta* 2009, *362*, 1047.


L^1
CuI
DCM/AN
1 month
1, (Kinetic product)
Non-emissive
2, (Thermodynamic product)
Emissive

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Synthesis of an $N_2O_2S_2$-Macrocyclic Ligand Possessing Hard Base and Soft Base Natures and Its Supramolecular Copper(ll), Mercury(ll), and Silver(l) Complexes

서수진 이은지 이심성*

경상대학교 화학과

We propose a ditopic macrocycle, L, which employs NO_2 and NS_2 donor sets in each side to accommodate one hard and/or one soft metal ion(s) in the cavity. Furthermore, two sulfur donors in the NS_2-side could provide the exo-coordination as bridgeheads which serve the metal ion coordination from outside the cavity. In this work, the pyridine-containing $N_2O_2S_2$-macrocycle, L, and its supramolecular complexes have been synthesized and structurally characterized. The results of the metal complexation behaviors of L both in solid and solution states are discussed. By using L, two complexes with silver(I) or copper(II) were prepared. First, the reaction of L with $AgClO_4$ afforded an exocyclic 1D coordination polymer, $\{[AgL]ClO_4\}_n$. (1). The structural and binding properties of the complex of L with $AgClO_4$ in solution were also monitored by ^{1}H-NMR. While, the reaction of HgI_2 with L in the presence of CuI afforded an endocyclic monocopper(II) complex, $[CuL][Hg_2I_6]$ (2), in which the square-type dimercury(II) hexa-iodide cluster exists as a separated counter anion (*see below*).

References[1] Teixidor, F.; Escriche, L.; Casabo, J.; Molins, E.; Miravitlles, C. *Inorg. Chem*. 1986, *25,* 4060.[2] Lee, E.; Lee, S. S. *Inorg*. *Chem*. 2011, *50,* 5803.[3] Lee, E.; Lee, S. S. *CrystEngComm*. 2013, *15*, 1814.

1, $\{[Ag\mathbf{L}]ClO_4\}_n$ **2**, $[Cu\mathbf{L}][Hg_2I_6]$

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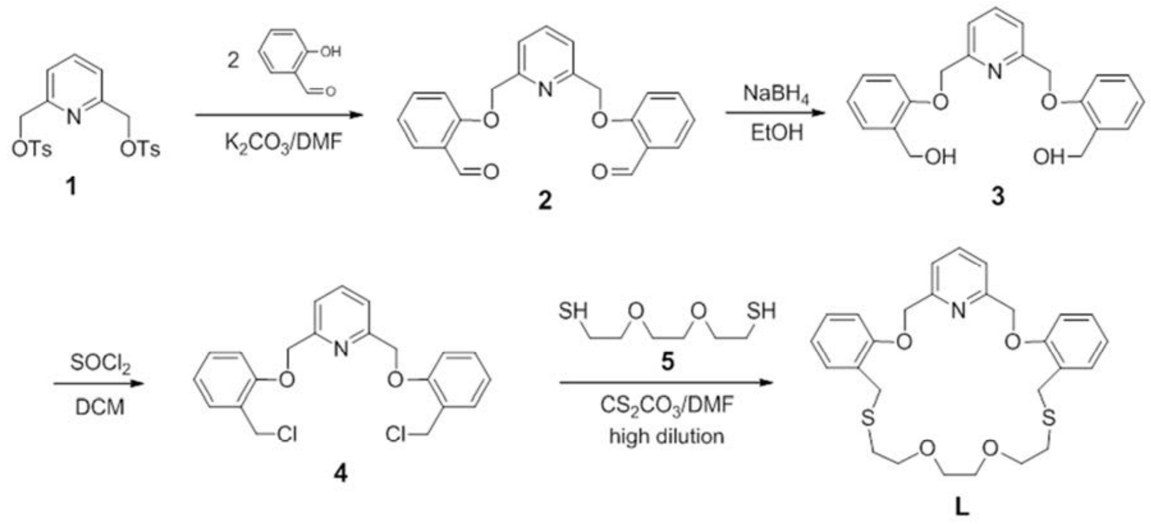
Synthesis of a 23-Membered NO_4S_2-Macrocycle and Its Complexation Behaviors

신민경 주희영 이심성*

경상대학교 화학과

We proposed a 23-membered NO_4S_2-donor macrocycle, L, which employs a pyridine subunit to accommodate one metal cation inside the cavity and two additional benzo subunits to enhance the structural rigidity. The ligand L is somewhat semi-flexible due to the consecutive thioether segment as bridge heads for the required exocyclic coordination, and this seems to induce the diversity of the coordination modes across their respective complexes. In this presentation, synthesis and structural characterization of the NO_4S_2-macrocycle L and its complexes are reported. The synthesis of the target macrocycle L involves four steps starting from ditosylate 1, with each step proceeding smoothly in reasonable yield. Dichloride 4 was prepared from dialdehyde 2 and dialcohol 3 using a known procedure.[1] L was obtained by coupling macrocyclization reaction between dichloride 4 and dithiol 5 in the presence of Cs_2CO_3 under high dilution condition. The ^{1}H NMR spectrum together with mass spectra was all in clear agreement with the proposed structures. Several soft and hard metal complexes of L wereisolated and their structural characteristics in solid state are discussed.Reference[1] Janssen, R. J. A.; Lindoy, L. F.; Matthews, O. A.; Meehan, G. V.; Sobolev, A. N.; White, A. H. *J. Chem. Soc., Chem. Commun.* 1995, 735.


2
OH
K$_2$CO$_3$/DMF
NaBH$_4$
EtOH
SOCl$_2$
DCM
SH
SH
5
CS$_2$CO$_3$/DMF
high dilution
OTs
OTs
N
O
Cl
S
1
2
3
4
L

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발표분야: 무기화학

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Copper(Ⅱ) Complexes with *N*-substituted Aspartic Acids : A New One-Pot Synthesis Method via in situ Michael Addition of Amines To Fumaric Acid

강재은 도정환[*]

건국대학교 화학과

The new copper complexes, Cu[(*rac*-*N*-benzyl-Asp)(benzylamine)(H_2O)] 1, Cu[*rac*-*N*-aminoethyl-Asp] 2, Cu[*rac*-*N*-aminopropyl-Asp] 3 and Cu[*rac*-piperazinyl succinate]$_2$ 4, have been synthesized and characterized by single-crystal X-ray diffraction techniques. Under mild hydrothermal conditions, Michael addition of benzylamine, ethylenediamine, 1,3-diaminopropane and piperazine to fumaric acid led to the formation of racemic mixtures of *N*-benzyl aspartic acid, *N*-aminoethyl aspartic acid, *N*-aminopropyl aspartic acid and piperazinyl succinic acid, respectively. We report a simple one-pot hydrothermal method of synthesizing *N*-substituted aspartic acid metal complexes in situ by utilizing the Michael addition of amines to fumaric acid.

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Hydrothermal synthesis, structure determination, and characterization of two new polymorphs of ternary sodium tellurites

이동우 옥강민*

중앙대학교 화학과

Single crystals and pure polycrystalline of two new sodium tellurium oxide materials, β-$Na_2Te_4O_9$ and $Na_2Te_2O_6\cdot1.5H_2O$, have been prepared through hydrothermal reactions using Na_2CO_3, TeO_2, and $H_2TeO_4\cdot2H_2O$ as reagents. The crystal structures of the two novel materials have been determined by single crystal X-ray diffraction. β-$Na_2Te_4O_9$ exhibits a three-dimensional framework structure containing only TeO_4 polyhedra. $Na_2Te_2O_6\cdot1.5H_2O$ reveals a layered structure composed of $Te^{6+}O_6$ octahedra and $Te^{4+}O_5$ polyhedra. Complete characterizations including thermogravimetric analyses, ion-exchange reaction, UV-vis diffuse reflectance spectra, IR spectra, elemental analyses, and dipole moment calculations are also presented

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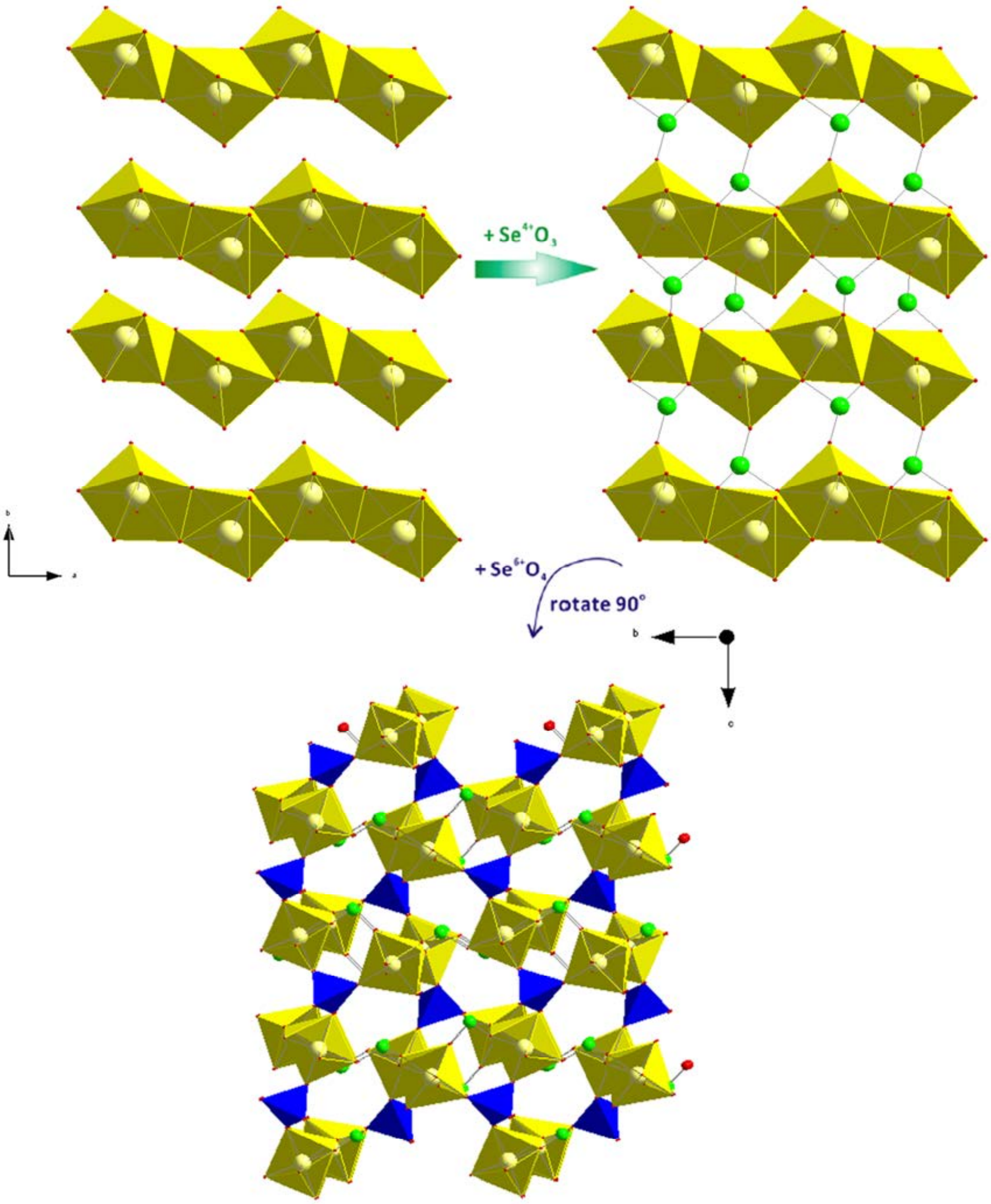
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrothermal synthesis and structural characterization of two new scandium selenium/tellurium oxides

송승윤 옥강민*

중앙대학교 화학과

Two scandium selenium/tellurium oxides, $Sc_2(SeO_3)_2(SeO_4)$ and $Sc_2(TeO_3)(SeO_3)(SeO_4)$, have been synthesized by hydrothermal reactions using $Sc(NO_3)_3$?xH_2O, SeO_2 (or TeO_2), and H_2SeO_4 as reagent. The two reported materials have been structurally characterized by single crystal X-ray diffractions. Isostructural $Sc_2(SeO_3)_2(SeO_4)$ and $Sc_2(TeO_3)(SeO_3)(SeO_4)$ are crystallographically centrosymmetric (CS) and reveal three-dimensional frameworks with ScO_7 pentagonal bipyramids, $Se^{4+}O_3$(and $Te^{4+}O_3$) trigonal pyramids, and $Se^{6+}O_4$ tetrahedra. The reported materials contain local asymmetric coordination environments attributable to the lone pairs on the Se^{4+} and Te^{4+} cations. Rich structural chemistry for the new oxides are originated from the combination of various polyhedral. Thorough characterizations including infrared, UV-vis diffuse reflectance spectroscopies, thermal analyses, elemental analyses, and dipole moment calculations for the new mixed metal oxides are presented.


+ $Se^{4+}O_3$
+ $Se^{6+}O_4$
rotate 90°
b
a
b
c

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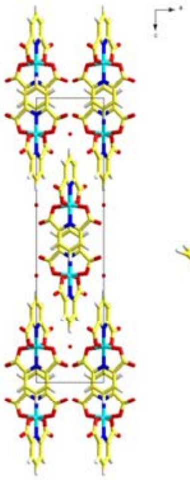
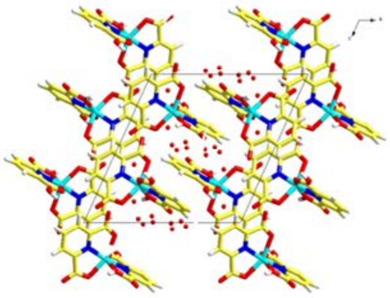
Hydrothermal Synthesis, Structure Determination, and Characterization of Three Co^{2+}-Organic Coordination Compounds

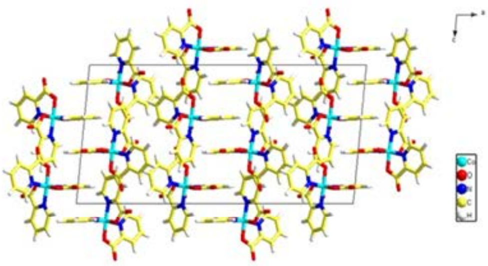
김샛별 옥강민[*]

중앙대학교 화학과

Three cobalt(II)-organic coordination compounds, namely, $Co(PDC)_2 \cdot H_2O$ (PDC = 2,6-pyridinedicarboxylato), $Co(PDC)_2 \cdot 3H_2O$, and $Co(PC)_3 \cdot H_2O$ (PC = pyridine-2-carboxylato) have been synthesized through a variety of hydrothermal reactions using $Co(NO_3)_2 \cdot 6H_2O$, CoO, $CoCl_2 \cdot 6H_2O$, and 2,6-pyridinedicarboxylic acid as reagents. Interestingly, isolated products vary depending on the reaction temperatures. While all of the reported materials crystallize in zero-dimensional molecular compounds, the crystal structures are different. In addition, the water-solubility of the materials is completely different: whereas $Co(PDC)_2 \cdot H_2O$ is water-soluble, $Co(PDC)_2 \cdot 3H_2O$ and $Co(PC)_3 \cdot H_2O$ are not soluble in water. Detailed characterization including thermogravimetric analysis, infrared spectroscopy, and elemental analysis are also presented.







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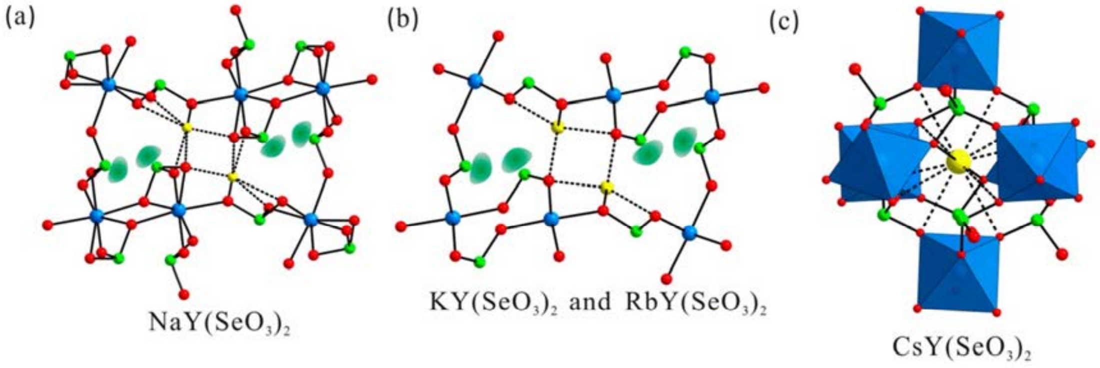
Synthesis, structure determination, and characterization of a series of new alkali metal yttrium selenites

방성은 옥강민*

중앙대학교 화학과

A series of alkali metal yttrium selenites, i.e., $AY(SeO_3)_2$ (A = Na, K, Rb, and Cs) have been synthesized through hydrothermal reactions using corresponding metal carbonates, $Y(NO_3)_3 \cdot 6H_2O$, and SeO_2 as reagents. Although all four materials exhibit three-dimensional framework structures, they show different backbone geometries. Noncentrosymmetric (NCS) $NaY(SeO_3)_2$ reveals chains of corner-shared YO_7 polyhedra and SeO_3 linkers, however, centrosymmetric (CS) $KY(SeO_3)_2$ and $RbY(SeO_3)_2$ exhibit channels consisting of YO_6 octahedra and SeO_3 groups. Finally, CS $CsY(SeO_3)_2$ shows a cage structure containing YO_6 and SeO_3 polyhedra. The cation size as well as coordination modes significantly influence the framework geometries. Nonlinear optical (NLO) property measurements on the NCS $NaY(SeO_3)_2$ will also be presented.



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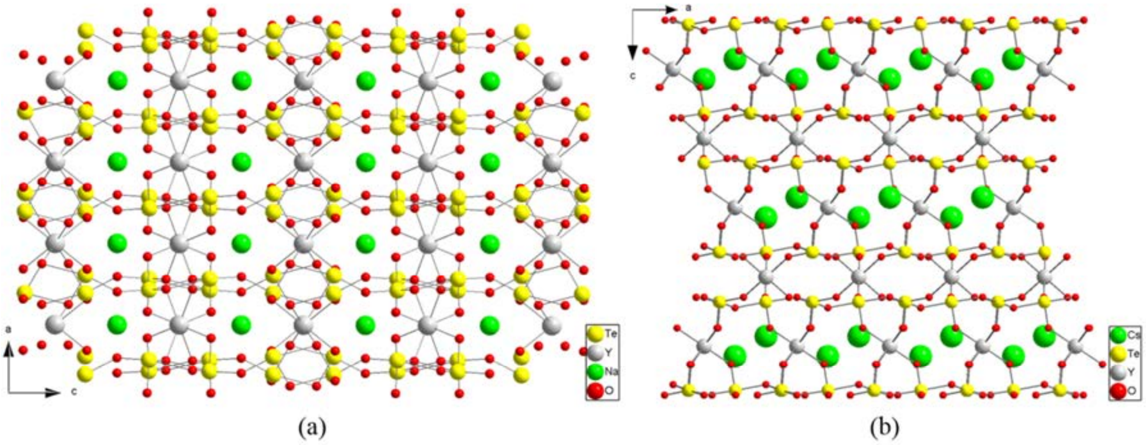
Syntheses and Characterization of Two New Three-Dimensional Quaternary Alkali Metal Yttrium Tellurites

김영권 옥강민*

중앙대학교 화학과

Two novel quaternary alkali metal yttrium tellurites, namely, $NaYTe_4O_{10}$ and $CsYTe_3O_8$, have been synthesized through hydrothermal and solid state reactions. Crystal structures of the reported materials were determined by single crystal X-ray diffraction. $NaYTe_4O_{10}$ is a new quaternary sodium yttrium tellurite that is crystallizing in a highly symmetric tetragonal space group, *P*42/*nbc* (No. 133). $NaYTe_4O_{10}$ exhibits a three-dimensional framework that is composed of YO_8 square antiprisms and TeO_4 seesaws. $CsYTe_3O_8$ crystalizes in the trigonal space group *R*-3 (No. 148) and reveals another three-dimensional framework structure. The framework of $CsYTe_3O_8$ consists of YO_6 octahedra and TeO_4 seesaws. Detailed characterization including energy-dispersive analysis by X-ray (EDAX), infrared and UV-vis diffuse reflectance spectroscopies, and thermogravimetric analyses (TGA) for the materials will be presented.

Figure 1. Ball-and-stick models of (a) $NaYTe_4O_{10}$ and (b) $CsYTe_3O_8$ in the *ac*-plane.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Syntheses, Structures, and Characterization of Four Novel Alkali Metal Indium Tellurites

배수환 옥강민*

중앙대학교 화학과

Four novel alkali metal indium tellurites, $NaIn(TeO_3)_2$, $KIn(TeO_3)_2$, $RbInTe_3O_8$, and $CsInTe_3O_8$, have been synthesized through both hydrothermal and standard solid-state reactions. The reported materials were fully characterized by TGA, FT-IR, and PXRD analysis and their crystal structures were determined by single X-ray diffraction. Interestingly, $NaIn(TeO_3)_2$ and $KIn(TeO_3)_2$ both have orthorhombic crystal systems, with different space groups, *Pbca* (No. 61) and *Cmcm* (No. 63), respectively, whereas isostructural $RbInTe_3O_8$ and $CsInTe_3O_8$ crystallize in triclinic space group, and *P*-1 (No. 2). Comparative structural study and UV-vis diffuse reflectance spectra were also suggested.

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Developing New Iridium catalyst for CO_2 Hydrogenation with the Anionic N-donor Ligand

윤예슬 윤성호[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

The increasing CO_2 concentration in the atmosphere, which has been attributed to the burning of fossil fuels, is considered as a major reason for global warming and the technology of CCS(Carbon Capture & Storage) can attribute to relieve this phenomenon. However, CCS is not cost-efficient and it has potential danger like the case of the explosion of CO_2-storage-lake in Cameroon. Instead of storage, the conversion of CO_2 into useful organic products is an intriguing and challenging subject. The formic acid, which is one of the materials that can be converted by CCU(Carbon Capture & Utilization), is used for essential substance of foundation of industry like a preservative and antibacterial agent in livestock feed. Recently, Himeda and co-workers studied the catalytic effect of $[Cp^*Ir(4DHBP)(OH_2)]^{2+}$ (4DHBP:4,4'- dihydroxy ? 2,2'- bipyridine) in basic condition. They reported that the catalyst shows higher conversion frequency donating (-) charge to N doner of neutral charge. Based on this study, we focused on designing bibenzimidazole (Bz) ligand with electron-rich N^- in neutral condition as against Himeda's group and confirmed the iridium catalyst ($(Cp^*IrBzCl)Cl^-$). Additionally the formation of formic acid from the reaction of the catalyst and CO_2 is identified. Furthermore, this catalyst can be used as a heterogeneous catalyst bounded with the surface of TiO_2 and the formation is confirmed. The catalytic activity of the $(Cp^*IrBzCl)Cl^-$-TiO_2 will be measured and analyzed.Acknowledgements: We acknowledged the financial support by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean government and also by the International Collaborative R&D Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by Korea government Ministry of Knowledge Economy.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A highly facile synthesis of hybrid nanomaterials and their applications

김미란 박강현*

부산대학교 화학과

The transition metal nanoparticles have been widely used as catalyst in various organic transformations. Being heterogeneous, the catalyst could be easily recovered and recycled, which significantly enhances the purity of the product. Recently, the concept of synergism in bimetallic nanoparticles is an emerging field in the area of nanocatalysis as evidenced from the number of publications increasing exponentially. So, we made an attempt to synthesize Fe_3O_4@Cu_2O core shell nanoparticle that enables to understand the synergistic effect and the catalyst recovery and recyclability by using an external magnet. In addition, we further incorporated palladium onto Fe_3O_4@Cu_2O and followed by oxidation to get Fe_3O_4@CuO/Pd nanoparticles in order to make highly catalytically efficient hybrid nanomaterials. The two-in-one nature of hybrid nanomaterials allows their use as catalyst in the organic synthesis.

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Facile Synthesis of FePd-Fe_2O_3 Catalysts for Sonogashira Coupling Reactions

이경호 박강현*

부산대학교 화학과

We report a facile synthesis of rod-like FePd-Fe_2O_3 nanocomposites via controlled thermal decomposition of $Fe(CO)_5$ and reduction of $Pd(OAc)_2$ followed by immobilization of FePd-Fe_2O_3 support. The morphology of these hybrid nanostructures can be easily controlled and synthesized FePd-Fe_2O_3 exhibited high catalytic activity and recyclability for the tandem synthesis of 2-phenylindoles.In recent years, numerous attempts have been made toward designing and synthesizing hybrid nanostructures with defined multicomponents via the size and shape control available through solution-growth fabrication.With the development of chemical sciences, new protocols bringing greater efficiency and simplicity to organic reactions are highly desirable. Among them, the catalytic synthesis of indole ring systems through cross-coupling/cycloadditions of 2-haloanilines with alkynes has proven to be the most powerful tool since indole nuclei which has unique biological activities is important as the building blocks in natural and pharmacological products.In this work, we report facile synthesis of rod-like FePd-Fe_2O_3 nanocomposites. These hybrid FePd-Fe_2O_3 nanostructures were used as catalyst for tandem synthesis of 2-phenylindoles and showed magnetic reusability by external magnet.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Series of Unique ruthenium arene complexes containing bidentate tetrazolyl ligand

박유진 이준승*

전남대학교 화학과

Rruthenium Arene complexes have been studied for a long time as an electron donor as well as a bridging system in the supramolecular assembly. To extend the library of ruthenium arene complexes and provide additional binding sites, 5-(2-hydroxyphenyl)-1-H-tetrazole)(**LH**) was chosen and used as a bridging unit to connect two ruthenium atoms. From the simple reaction of ruthenium arene precursor and **LH**, novel dimeric ruthenium arene having two bridging units, **LH** and Cl^- ion, was synthesized. More interestingly, use of AgOTf for chloride ion removal in the reaction resulted in totally different product. Hexa-ruthenium cluster complex was formed by the reaction of Ru complex and LH with the molar ratio of 2:3. In the molecule, unexpected ruthenium sandwich were observed. All complexes were characterized by various spectroscopic methods including ^{1}H-NMR, IR, and ESI-MASS spectrometry. Their solid state structures were confirmed by x-ray crystallography. With this concept, we can develop our strategy on the structural diversity and modulation using sotichiometic control of metal and ligands.

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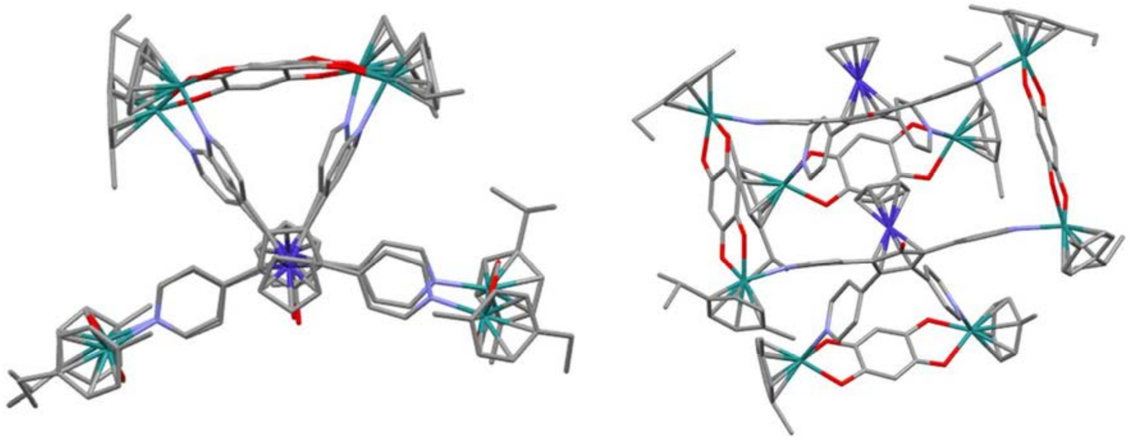
Synthesis of Co(Ⅰ)-Ru M_4L_2 supramolecular architecture via driven-coordination self-assembly

류지연 박유진 이준승*

전남대학교 화학과

Co(Ⅰ)-Ru M_4L_2 supramolecular architecture using [Tetrakis(4-pridyl)cyclopentadienone]cyclopentadienylcobalt and diruthenium donor of three types synthesized via driven-coordination self-assembly. Interestingly length of diruthenium donor controlled by oxalato, benzoquinone, naphthoquinone affects to structures of Co(Ⅰ)-Ru cages which look like stair, pocket, glove shape. These complexes were confirmed by IR, ^{1}H-NMR, high-resolution electrospray ionization mass spectrometry and single crystal X-ray crystallography. X-ray crystallography revealed they have small spaces surround by π-conjugation in cage which are suitable for host-guest chemistry with π-conjugated planar molecules.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Dimeric Iron(III) complexes having a different bonding environment and their catalytic performances in lactide polymerization

강이영 박형련 이준승*

전남대학교 화학과

Polylactide is a kind of biodegradable polymer and it has been spotlighted as an eco-friendly polymer. For a decades, metal complexes including such as Sn, Al, and Zn have been used as catalysts for the polymerization of lactide. Although iron is also attractive in the aspect of low toxicity and moderate prices, there are few reports of iron complexes for the polymerization of lactide due to their low activities.In this study, We synthesized novel Iron (III) complexes 1 - 2 [1 ; $Fe_2L^{Bu}{}_2acac_2$, 2 ; $Fe_2L_2acac_2$] bearing chiral tridentate Schiff base ligands LH [$L^{Bu}H$; R = tert-Bu, LH ; R = H], derived from (1S,2R)-(-)1-aminoindanol, using a simple one step reaction. These complexes were characterized by various spectroscopic methods such as IR, EA, mass spectrometry. We confirmed that complex 2 is a dimeric structure containing two iron atoms in the different bonding environment by X-ray crystallography. Complexes 1 - 2 were tested as catalysts in the polymerization of lactide and complex 2 showed highest activity among reported Fe complexes. Colored polylactide polymer were obtainied in the rac-lactide polymerization. We will present the detailed study.

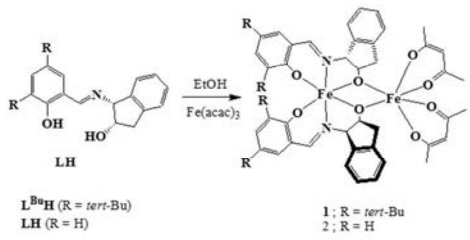

Figure 1: Sythesis of iron (III) complexes **1 – 2**

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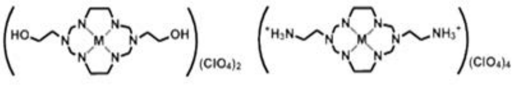
Preparation and Structure of Supramolecules Obtained from the Combination of Polyazamacrocyclic Complexes and Aromatic Polycarboxylic Acids

서민지 곽지훈[1,*]

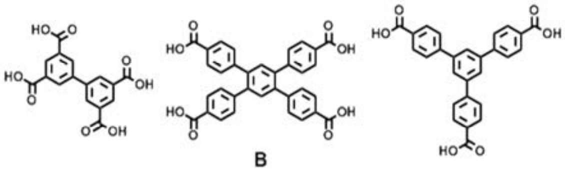
순천대학교 화학과 [1]순천대학교 화학교육과

It has been interested in the preparation and properties of supramolecules obtained from the combination of macrocycles and polycarboxylate ligands because they form interesting multidimensional structure and show intrigue properties. These multidimensional frameworks have been attracted many attentions because of their potential applications in energy and environment materials. Especially, by the fabrication of various metal nanoparticles in frameworks, for example, that materials can selectively adsorb carbon dioxide from the industry flue gas. Here, we report the synthesis, characterization and X-ray structure of the complexes obtained from the attempted preparation using polyazamacrocyclic complexes (A) with aromatic polycarboxylic acids (B).



A

(M = Ni(II) or Cu(II))



B

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Reaction of Malononitrile($CH_2(CN)_2$) with *N*-Cyanomethyl Pendant Arms of Tetraaza Macrocyclic Complexes

김현자 강신걸* 곽지훈[1]

대구대학교 화학과 [1]순천대학교 화학교육과

The reaction of $[Ni(L^1)]^{2+}$ (L^1 = 2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) with malononitrile($CH_2(CN)_2$) produces $[Ni(L^2)]^{2+}$ bearing two *N*-$CH_2C(=NH)CH(CN)_2$ pendant arms. However, $[Cu(L^1)]^{2+}$ reacts with $CH_2(CN)_2$ to form $[Cu(L^3)]^{2+}$ bearing one *N*-$CH_2C(=NH)CH(CN)_2$ and one *N*-CH_2CN pendant arms. Interestingly, $[Ni(L^2)]^{2+}$ oxidizes to the nickel(Ⅲ) complex $[Ni(L^2\text{-}2H)]^+$ in acetonitrile containing HNO_3. The hydrolysis of $[Cu(L^3)]^{2+}$ in basic aqueous solutions produces $[Cu(L^4)]^{2+}$ containing one *N*-$CH_2C(=NH)CH(CN)_2$ and one *N*-CH_2CONH_2 pendant arms. The pendant arms of $[Ni(L^2\text{-}2H)]$, $[Ni(L^2\text{-}2H)]^+$, $[Cu(L^3\text{-}H)]^+$, and $[Cu(L^4\text{-}H)]^{2+}$ are coordinated to the metal ions in the solid state, whereas those of $[Ni(L^2)]^{2+}$, $[Cu(L^3)]^{2+}$, and $[Cu(L^4)]^{2+}$ are not involved in coordination. Synthesis, characterization, and chemical properties of the functionalized macrocyclic compounds are presented.

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Phosphorescent Iridium(III) Complexes with Ancillary Carbene Ligands for Organic Light?Emitting Diodes (OLEDs)

<u>김민지</u> 송영광 윤성재 최지혜[1] 강성권[2] 진성호[1] 김영인[1,*]

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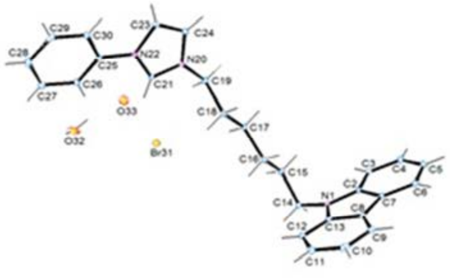
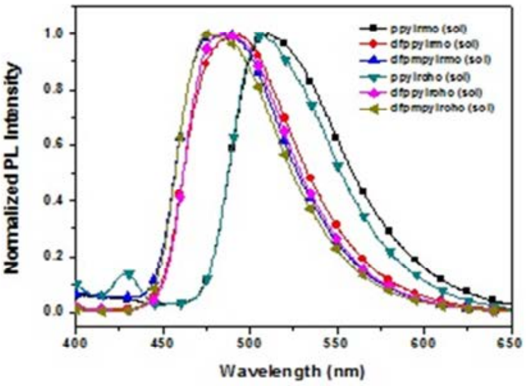
Phosphorescent organic light-emitting diodes (OLEDs) based on heavy transition-metal complexes have attracted extensive attention in recent years because of their potential to improve device brightness and performance. The efficient cyclometalated iridium(III) complexes with carbene as ancillary ligands were synthesized and characterized ; ppyIrmc (1), dfppyIrmc (2), dfpmpyIrmc (3), ppyIrchc (4), dfppyIrchc (5) and dfpmpyIrchc (6) (ppy = 2-phenylpyridine ; dfppy = 2-(2,4-diflorophenyl)pyridine ; dfpmpy = 2-(2,4-diflorophenyl)-4-methylpyridine ; mc = 1-phenyl-3-methylimidazolin-2-ylidene and chc = 1-phenyl-3-hexylcarbazolylimidazolin-2-ylidene). The structures were determined using single crystal X-ray method. These complexes showed sky-blue phosphorescent emissions between 480 and 511 nm in PL spectra and exhibited quantum yields of 3~78.5 % in dichloromethane solution. The complex 1~6 showed a blue-shift in the order of 1<4<2<3<5<6.





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Hydrogenation of CO_2 by a New Iridium catalyst with the Anionic N-donor Lingand

박광호 윤성호*

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Owing to usage of fossil fuels as main energy source since the industrial revolution, mankind faced problems including fast depletion of energy resources based on fossil fuel and global warming caused by the increased concentration of carbon dioxide in the atmosphere. Reductive conversion of carbon dioxide by catalytic hydrogenation has received much attention because it could diminish the atmospheric CO_2 level and also regenerate useful chemicals. Recently, highly effective catalytic conversions by $[Cp^*Ir(4DHBP)(OH2)]^{2+}$, where 4DHBP is 4,4’- dihydroxy-2,2’- bipyridine and Cp* is pentamethylcyclopentadienyl, in basic condition have been reported. With the improved catalytic effect and of interest, it has been proposed to originate from the increase electron density on N atoms of 4,4’-dihydroxy-2,2’- bipyridine ligand.Herein, we report the synthesis and characterization of new Ir complexes with the ligand based on the dipyrrole motif. In addition, catalytic activity of the compound at sc CO_2 and high-pressure H_2 condition for the formation of formic acid has been reported.Acknowledgements: We acknowledged the financial support by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean government and also by the International Collaborative R&D Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by Korea government Ministry of Knowledge Economy [20118520010020].

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개미산 생산을 위한 N,N$^-$,C$^-$리간드를 이용한 Iridium(III) 화합물의 중심금속의 전자밀도 변화에 대한 연구

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수소와 이산화탄소를 이용한 개미산 형성 반응 촉매인 [Cp*Ir(III)(4,4’-dihydroxy-2,2’-bipyridine)Cl]Cl 는 염기성 환경하에서 활성이 증가된다 보고되어왔다. 이러한 효과는 염기에 의한 4,4’-dihydroxy 작용기의 탈수소 반응에서 기인되며 탈수소 반응은 리간드의 전기적 음성도를 증가시켜 중심금속의 더 많은 전자밀도를 공여하게 한다. 본 연구에서는 (N,N$^-$,C$^-$)1,5,9-triphenyldipyrromethene^{2-} 의 음전하를 띄는 리간드를 이용하여 금속화합물 [Cp*Ir(III)(1,5,9-triphenyldipyrromethene-N,N$^-$,C$^-$)]를 합성하였다. 합성된 화합물 중심금속의 전자밀도를 알아보기 위해 cyclovoltametry 환원 전위를 측정하였고, 개미산 형성 반응의 촉매로서 활성을 측정하였다. Acknowledgements: We acknowledged the financial support by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean government.

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Zinc oxalate 고체화합물의 형상과 반응조건에서의 물 함량과의 관계성 규명

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Zinc oxide(ZnO) 나노구조체는 큰 exciton binding energy, 높은 열적 안정성, harsh 한 환경에서의 oxidation resistance 를 가지고 있을 뿐만 아니라 저가의 물질로서 많은 응용분야에 가능성을 가지고 있다. 나노구조체의 크기과 형상 조절은 분산성 및 반응성을 변화시킬 수 있기 때문에 중요한 의미를 갖고 있다. 최근 ZnO 나노구조체는 Zinc oxalate precursor 물질의 간단한 소성을 통해 형상될 수 있다고 발표되고 있다. 따라서 Zinc oxalate 의 크기 및 모양을 조절하는 것은 향후 ZnO 크기 및 형상 조절로 연결될 수 있기 때문에 중요하다. 본 연구에서는 precursor 합성단계에서 반응조건의 물 함량을 조절함에 따라 얻은 다양한 형상구현 결과를 보고하고자 한다. Acknowledgements: We acknowledged the financial support by grants from Korea CCS R&D Center, funded by the Ministry of Education, Science and Technology of Korean government, by a grant from the Fundamental R&D program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea and also by the Industrial Technology Development Program funded by the Ministry of Knowledge Economy (MKE, Korea)

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폴리아닐린 유도체를 이용한 대면적 은 나노플레이트의 합성연구

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은 나노플레이트는 특이한 촉매적, 광학적, 전기적 성질이 나타나기 때문에 화학,생물센서에 응용가능성에 대한 많은 연구가 이루어지고 있다. 대표적인 은 나노플레이트 합성법으로 광화학적인 방법, 리간드를 이용한 환원법, 전기화학 합성, 템플레이트 방법, 초음파를 이용한 방법 등 여러가지 방법이 있다. 그러나 이러한 기존 방법들은 대면적 은 나노플레이트를 합성하는데 한계를 보인다. 본 연구에서는 설포네이트 그룹 (-SO_3H group)과 카복실그룹 (-carboxyl group)이 있는 폴리아닐린 유도체(PANi-D)와 설포네이트 그룹만 있는 폴리아닐린 유도체(PANi-SO_3H)를 이용하여 3μmx3μm 이상의 대면적을 갖는 은 나노플레이트를 합성하였으며 폴리아닐린 유도체에 따른 온도조절실험을 통해 은 나노플레이트의 합성메커니즘을 연구하였다. Acknowledgements: We acknowledged the financial support by the International Collaborative R&D Program of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by Korea government Ministry of Knowledge Economy [20118520010020], by a grant from the Fundamental R&D program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea and also by the Industrial Technology Development Program funded by the Ministry of Knowledge Economy (MKE, Korea)

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Methanolysis of *N*-alkynyl Groups Attached to a Tetraaza Macrocyclic Nickel(Ⅱ) Complex

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Two $N\text{-CH}_2\text{C}\equiv\text{CH}$ pendant arms of the nickle(Ⅱ) complex $[\text{Ni}(C\text{-}racemic\text{-L}^1)(\text{OAc})]^+$ (L^1=1,8-bis(propargyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane) react with methanol to yield the *cis*-octahedral complex $[\text{Ni}(C\text{-}racemic\text{-L}^2)]^{2+}$(green) bearing two coordinated $N\text{-CH}_2\text{C(=CH)-OMe}$ pendant arms. The complex $[\text{Ni}(C\text{-}racemic\text{-L}^2)]^{2+}$(green) is isomerized to the square-planer form $[\text{Ni}(C\text{-}racemic\text{-L}^2)]^{2+}$(red) in basic aqueous solution at pH 12, but to $[\text{Ni}(C\text{-}racemic\text{-L}^2)]^{2+}$(yellow) at pH 7. In acidic aqueous solution, however, the nickel(Ⅱ) complex is hydrolyzed to give $[\text{Ni}(C\text{-}racemic\text{-L}^3)]^{2+}$ (L^3=1,8-bis(1-propenol)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane) bearing two $N\text{-CH=C(OH)-CH}_3$ pendant arms. Synthesis and reactions of $[\text{Ni}(C\text{-}racemic\text{-L}^2)]^{2+}$ are presented.

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

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The nickel(Ⅱ) complex $[\mathrm{NiL^1}]^{2+}$ ($\mathrm{L^1}$=2,13-bis(propargyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) bearing two N-propargyl pendant arms undergo hydrolysis/hydroamination at pH 12 to form $[\mathrm{NiL^2}]^{2+}$; one of the two functional groups is hydrolyzed, whereas the other reacts with coordinated secondary amino group of the macrocycle. On the other hand, $[\mathrm{CuL^1}]^{2+}$ undergoes C-N bond cleavage to form $[\mathrm{CuL^3}]^{2+}$($\mathrm{L^3}$=3,14-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) under the similar basic conditions. One of the two N-$\mathrm{CH_2C{\equiv}CH}$ pendant arms on $[\mathrm{NiL^1}]^{2+}$ readily react with salicylaldehyde to yield $[\mathrm{NiL^4}]^{2+}$ bearing a heterobicyclic pendant arm. Synthesis and chemical properties of the functionalized macrocyclic complexes are presented.

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Thermally Robust 3D Co-DpyDtolP-MOF with Hexagonally Oriented Micropores

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A new porphyrin-based Co-MOF, $[Co(DpyDtolP)]_6?12H_2O$ (I) composed of DpyDtolP (5,15-di(4-pyridyl)-10,20-di(4-methylphenyl)porphyrin) was prepared in a high yield and structurally characterized by X-ray crystallography.Unlike the pyridyl groups, the 4-tolyl groups in DpyDtolP could not be involved in coordination toward the metal ion. Nevertheless, the presence of these two 4-tolyl groups led to a new infinite three-dimensional framework: Co-MOF (I) with exceptionally high thermal stability at elevated temperature. The robust framework of I contained micropores that were periodically arranged in a hexagonal symmetry. While the evacuated I moderately sorbed N_2 at 77 K, it sorbed 142.8 $cm^3\ g^{-1}$ (6.37 mmol g^{-1}) of CO_2 at 196 K. Furthermore, the crystal structure of CO_2 captured I (I_CO_2) revealed that the linear arrangement of the CO_2 molecules occupying the inside of micropores, thereby indicating the effective CO_2 capture by evacuated I. The evacuated I was also found to be ideal for the encapsulation of iodine molecules in cyclohexane to provide iodine-captured I (I_I_2), which was also characterized by X-ray crystallography. The linear arrangement of polyiodine chains in the micropores was observed, and a single crystal of I_I_2 exhibited electrically conducting behavior. The encapsulation amount of iodine was dependent on the crystal sizes of I. Additionally, the separately prepared micro-scale sample, micro-I, with a much reduced particle dimension than the bulk I exhibited an enhanced uptake of iodine under the same conditions.

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Investigation on the phase transitions in $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) using optical microscope and thermal analysis

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The title compound belongs to the layered inorganic-organic systems of general formula AMX_4, where A = organic cation, M = divalent metal and X = halides. These systems have attract special interest, because of their low-dimensional magnetic properties (de Jongh, 1986). Recently the multi-ferroic properties in Cu-PEA was reported, although Cu-PEA crystallized in an orthorhombic Pbca structure (No.61), with a = 7.2099(9), b = 7.2664(9), c = 38.238(5) and Z = 4 at room temperature (Polyakov et al., 2012). It is well know that a crystal cannot be ferroelectric if the crystal possesses the inversion center in the crystal structure. To verify this fact, we investigated Cu-PEA employing temperature dependent domain changes under optical microscope and DSC method. In Cu-PEA, three phases are observed. Our findings and the group-subgroup relationship strongly suggest that Cu-PEA is non-ferroelectric but ferroelastic.

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Steric effects on the reactivity of Ni-O_2 complexes toward organic substrates

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대구경북과학기술원(DGIST) 신물질과학

Mononuclear metal-O_2 (M-O_2) adducts, such as metal-superoxo and peroxo species, are key intermediates in the catalytic reactions of dioxygen activation reactions in biology. Thus, the study of the biomimetic models of M-O_2 is important in chemistry. Herein, we report the preparation of different type of pyridinophane ligands: *N*,*N′*-di-tert-butyl-2,11-diaza[3.3](2,6)pyridinophane (TBDAP) and *N*,*N′*-cyclohexyl-2,11-diaza[3.3](2,6)pyridinophane (CHDAP) in order to investigate the steric effect on the reactivity of Ni-O_2 complexes toward external substrates. The Ni(III)-O_2 complexes containing pyridinophane type ligands were successfully generated and characterized with various physicochemical methods. The reactivity of Ni(III)-O_2 species bearing CHDAP toward organic substrates is higher than that of Ni(III)-O_2 species bearing TBDAP.

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Host-Guest Chemistry of Metallacyclodimeric of Zinc(II) Complexes: Recognition of Dihalomethane Molecules

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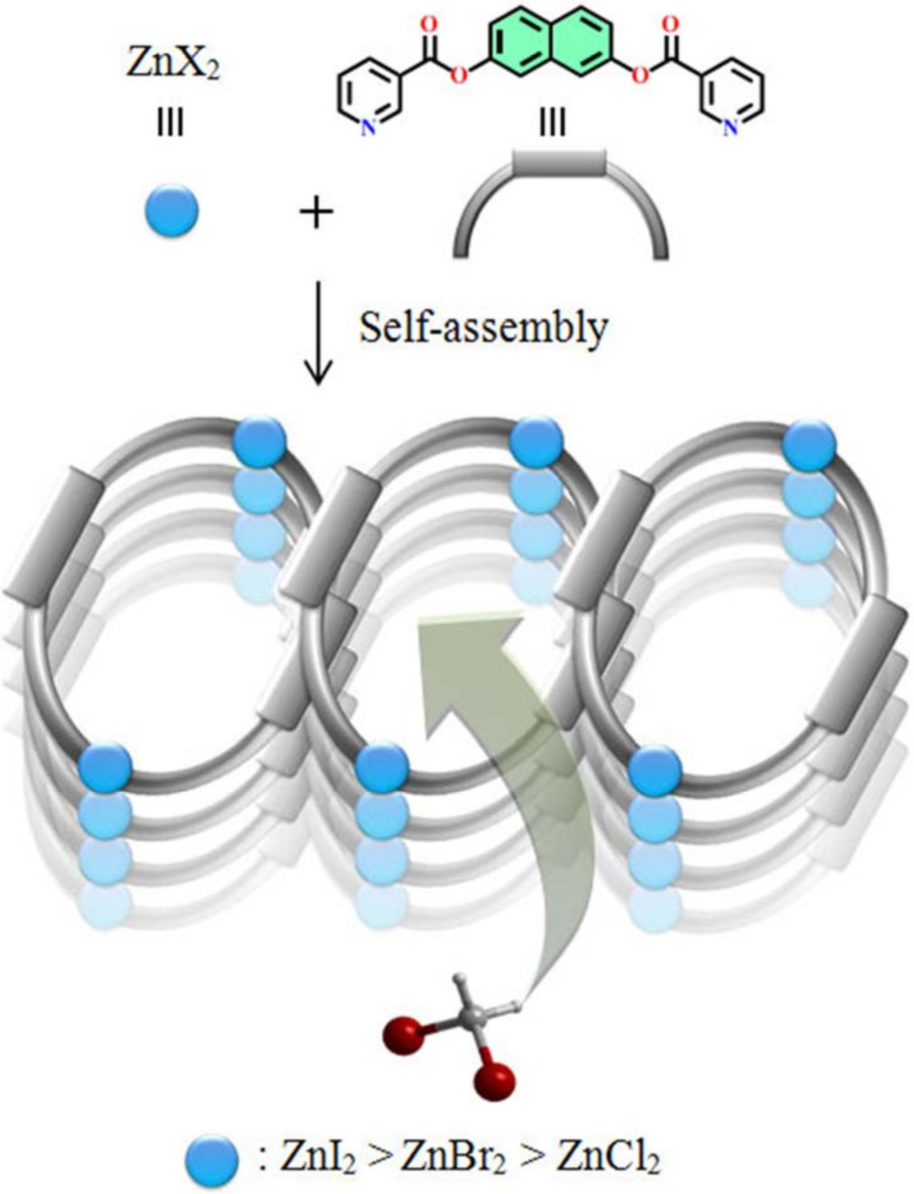
부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with 2,7-bis(nicotinoyloxy)naphthalene (L) as a hemi-circular bidentate ligand containing chromophore moiety yields a systematic metallacyclodimeric unit, $[ZnX_2(L)]_2$. These basic skeletons constitute, via interdigitated π???π interactions, a unique columnar ensemble forming a suprachannel. This can then be employed as an unusual "diiodomethane within the suprachannel" host-guest system, $CH_2I_2@[ZnX_2(L)]_2$. Specifically, the suprachannel significantly stabilizes the CH_2I_2 molecules in the order $[ZnI_2(L)]_2 > [ZnBr_2(L)]_2 > [ZnCl_2(L)]_2$. This suprachannel has significant halogen effects on the photoluminescence (PL), thermal properties, and host-guest inclusion.


ZnX$_2$
O
O
N
N
+
Self-assembly
●: ZnI$_2$ > ZnBr$_2$ > ZnCl$_2$

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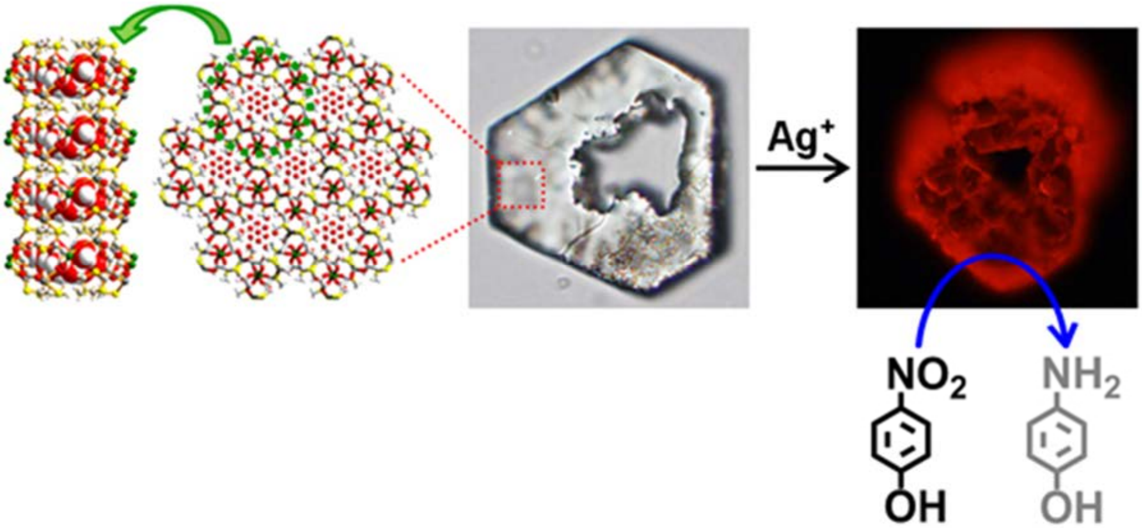
Crystal Morphology and Physicochemical Properties of Zeolite L-Mimic Heterometallic Ni^{II}/Ag^{I} Compound

노태환 정옥상*

부산대학교 화학과

Research on construction, morphology, and functions of a novel zeolite L-mimic metal-organic framework (ZLMOF) has been carried out. The present ZLMOF consisting of $[Ag_4Ni(L)_3]?3.5H_2O$ has been produced via reaction of $AgNO_3$ with $[K_2Ni(L)_2(H_2O)_3(CH_3OH)_2]$ as a metallo-ligand without any template. The ZLMOF with the caterpillar-shape channels of the internal diameter of 11.97 ? and the aperture of 7.55 ? that is very similar to the dimensions and shape of zeolite L has been efficiently constructed. Unique water clusters of $(H_2O)_{13}$ were nestled in the channels of ZLMOF in a line, and were reversibly encapsulated. Truncated trigonal prismatic tubular crystals with dimension of 90 μm width × 280 μm length and with average 50 μm inner diameter form through the successive growing of stick crystals and the dumbbell-type bundles of prism rods. The surface of the trigonal prism morphology is smoothly coated by silver(0) nanoparticles from direct treatment of trigonal prismatic crystals with $AgBF_4$ in acetone at 40 °C, which exhibit red PL with λ_{max} at 636 nm and catalytic activity in reduction of *p*-nitrophenol.


Ag+
NO2
OH
NH2
OH

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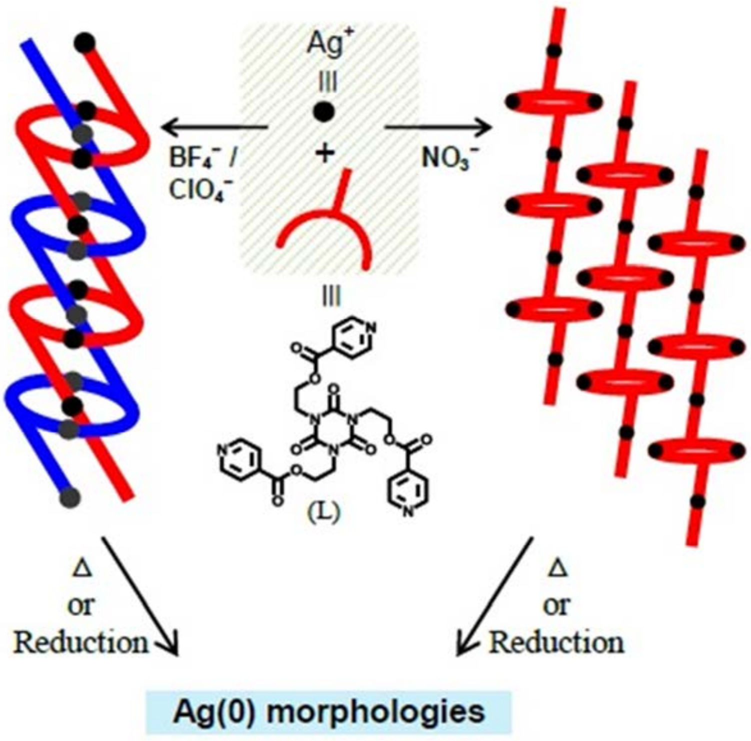
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anion Role on Formation of the Super-arrays of Loop-and-chain Silver(I) Coordination Polymers and Their Physicochemical Properties

장재성* 정옥상

부산대학교 화학과

Self-assembly of AgX^- (X^-= BF_4^-, ClO_4^-, and NO_3^-) with C_3-symmetric 1,3,5-tris(isonicotinoyloxyethyl)cyanurate (L) leads to 1D → 1D polyrotaxaned loop-and-chains (X^-= BF_4^-, ClO_4^-) and 1D → 2D π???π? interdigitated loop-and-chains (X^-= NO_3^-) in the solid state. Structural formation, thermal and reactivity were elucidated based on nature of anions: calcination of $[Ag_3(L)_2](X)_3$ (X^-= BF_4^- and NO_3^-) crystals at 600 °C produces micro-sized silver(0) materials whereas the same treatment of $[Ag_3(L)_2](ClO_4)_3$ crystals affords the mixture materials of silver(0) and silver(I) chloride. Formation of Ag(0) nanoparticles via reduction using ascorbic acid at room temperature is in the order of $ClO_4 > BF_4 > NO_3$.


Ag⁺
|||
●
+
BF₄⁻ /
ClO₄⁻
NO₃⁻
|||
N
O
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O
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N
O
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O
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N
(L)
Δ
or
Reduction
Δ
or
Reduction
Ag(0) morphologies

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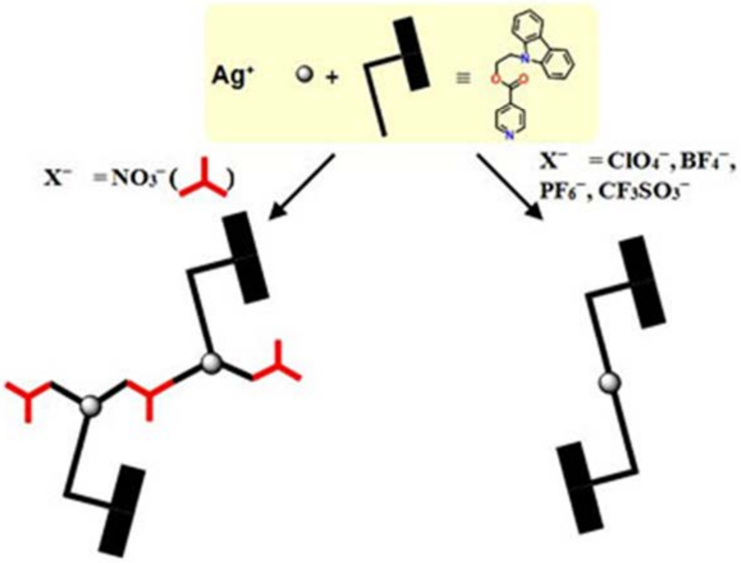
Anion Effects on Construction and Photoluminescence Properties of Silver(I) Complexes

김정균 정옥상*

부산대학교 화학과

N-Donor carbazole-containing silver(I) complexes were synthesized. And their photophysical properties have been extensively investigated. After construction of silver(I) complexes containing 9-(2-isonicotinoyloxyethyl)carbazole as a new ligand, x-ray crystal structures were determined. The crystal structures of the present silver(I) complexes were different depending on the nature of anions. According to single crystal x-ray diffraction, $[Ag(NO_3)(L)]?CH_2Cl_2$ is a 1D linear coordination polymer while the others are discrete molecules, $[Ag(L)_2](X)$ ($X^- = BF_4^-$, ClO_4^-, PF_6^- and $CF_3SO_3^-$). Investigations into the anion effects on construction and photoluminescence (PL) of a series of AgX compounds with 9-(2-isonicotinoyloxyethyl)carbazole (L) were carried out. Their physicochemical properties were fully characterized by means of FT-IR, UV-Vis spectroscopy, and photoluminescence. For $[Ag(NO_3)(L)]?CH_2Cl_2$, a luminescence was observed at 502 nm, for the others, 481-495 nm were observed in solid state. Upon gradual addition of pyrocatechol to the supramolecules in solid state, supramolecular structures showed strong quenching effect.


Ag⁺
+
≡
N
O
O
X⁻ = NO₃⁻ ( )
X⁻ = ClO₄⁻, BF₄⁻,
PF₆⁻, CF₃SO₃⁻

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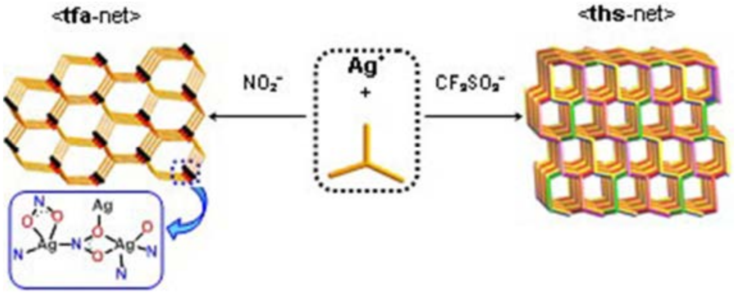
Construction of Unique Trinodal 3,3,4-Connected tfa Net Topology by Unusual Coordinating Ability of Nitrite

김은이 정옥상*

부산대학교 화학과

Self-assembly of AgX (X^-=NO_2^- and $CF_3SO_3^-$) with C_3-symmetric *N*,*N*',*N*''-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L) produces an unusual nitrite-bridged 3-D coordination polymer, $[Ag_2(NO_2)_2L]$?H_2O, with trinodal 3,3,4-connected tfa net topology and a unique 3D coordination polymer, $[Ag_3L_2](CF_3SO_3)_3$?CH_2Cl_2?$4H_2O$, with 6-fold interpenetrating uninodal 3-connected ths net topology, respectively. The L/M ratios of the products are significantly dependent upon the coordinating ability of anions: trifluoromethanesulfonate anions act as simple counteranions whereas nitrite anions take part in coordination. Specifically, $[Ag_2(NO_2)_2L]$?H_2O shows the unprecedented coordination mode of nitrite anions with both a μ^3-1κ^2-O,O':2κ-O:3κ-*N* mode and a κ^2-O,O' mode. The κ^2-O,O' nitrite anion was more easily exchanged than μ^3-1κ^2-O,O':2κ-O:3κ-*N* nitrite. Their structure-related thermal behavior, anion exchangeability, and photoluminescence have been investigated.



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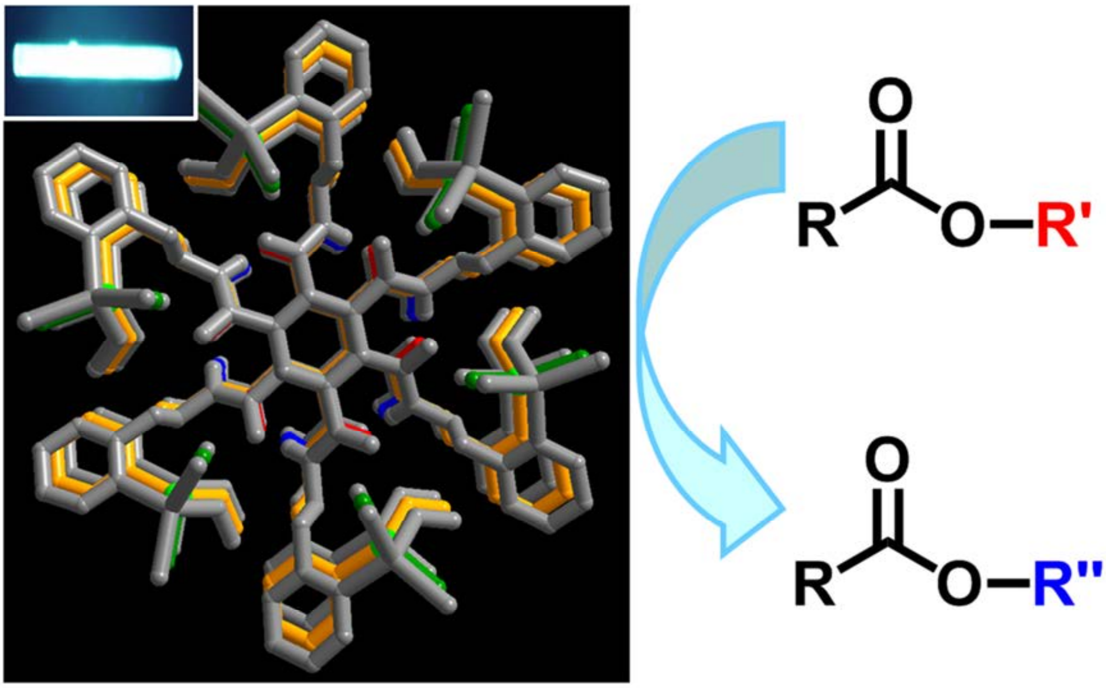
발표종류: 포스터, 발표일시: 수 16:00~19:00

Halogen Effects on Catalytic Activities and Photoluminescence of Columnar Zinc(II) Structures

이해리 정옥상*

부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with C_3-symmetric tridentate *N*-donor ligand, *N*,*N'*,*N"*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L), yields discrete trimetallic zinc(II) complexes, $[Zn_3X_6L(MeOH)_3]$. These form, via inter- and intra-molecular interactions, an ensemble constituting a columnar stacking structure in abab??? staggered fashion. For this series of complexes, the halogen effects on the photoluminescence, catalysis, and thermal properties were investigated. For $[Zn_3Cl_6L(MeOH)_3]$, a blue luminescence was observed at 462 nm (λex = 369 nm). The transesterification catalysis showed significant halogen effects in the order $[Zn_3I_6L(MeOH)_3] > [Zn_3Cl_6L(MeOH)_3] > [Zn_3Br_6L(MeOH)_3]$ in methanol, whereas in a mixture of methanol and acetonitrile, the order was $[Zn_3I_6L(MeOH)_3] > [Zn_3Br_6L(MeOH)_3] > [Zn_3Cl_6L(MeOH)_3]$. Such notable different effects among the three complexes might be explained by the halogens' electronic effects and dissociation properties. This catalysis work reveals that both direct halogen effects and solvent systems play significant roles in transesterification. Calcination of the materials results in formation of different morphologies of zinc(II) oxide. More systematic studies, for example on the synthesis of related ligands, are in progress. Further experiments, moreover, will provide more detailed information on the enormous potentials of the complexes' catalytic properties and photoluminescence.


O
R
O–R'
O
R
O–R''

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Structure of Multinuclear Complexes of Cyclic/Non-Cyclic Polyaza Ligands Containing μ-Carbonate or μ-Oxalate Ligand

김성민 곽지훈[1,*]

순천대학교 화학전공 [1]순천대학교 화학교육과

Generally, multinuclear metal complexes is formed by linking over two complexes with bridging ligands. The multinuclear complexes with carbonate or oxalate have been prepared and explored relating to the mimic of metalloenzymes. Futhermore, carbonate or oxalate is an elegant ligand to design and produce 2-D or 3-D molecular network relating to molecular magnetic materials and molecular tectonics as well. Numbers of Metal(II)-polyaza networks incorporated carbonate of oxalate have been reported and it has been revealed that their structure and properties are strongly depend on the nature of polyaza ligands. In this presentation, we will discuss the preparation and x-ray structures of multinuclear complexes by the reaction of cyclic/non-cyclic polyaza complexes, and carbonate and oxalate.

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Hollow Porous Carbon Particles Made by Pyrolysis of Core-Shell Type Metal-Organic Framework (MOF) and Their Sorption Properties

최소라 이희정 오문현*

연세대학교 화학과

Porous carbon materials are very important materials due to their useful applications in adsorbents, supercapacitors, and catalyst supports. Among them, hollow porous carbon materials have received special attentions because of their interesting properties such as low density, high surface-to-volume ratios, and good chemical stabilities. Herein, we report a simple approach for the production of uniform hollow porous carbon materials. The direct pyrolysis of core-shell type MOF (polystyrene@ZIF-8) resulted in well-defined hollow porous carbon particles through a transformation of ZIF-8 shell into porous carbon and the concurrent elimination of the polystyrene core.

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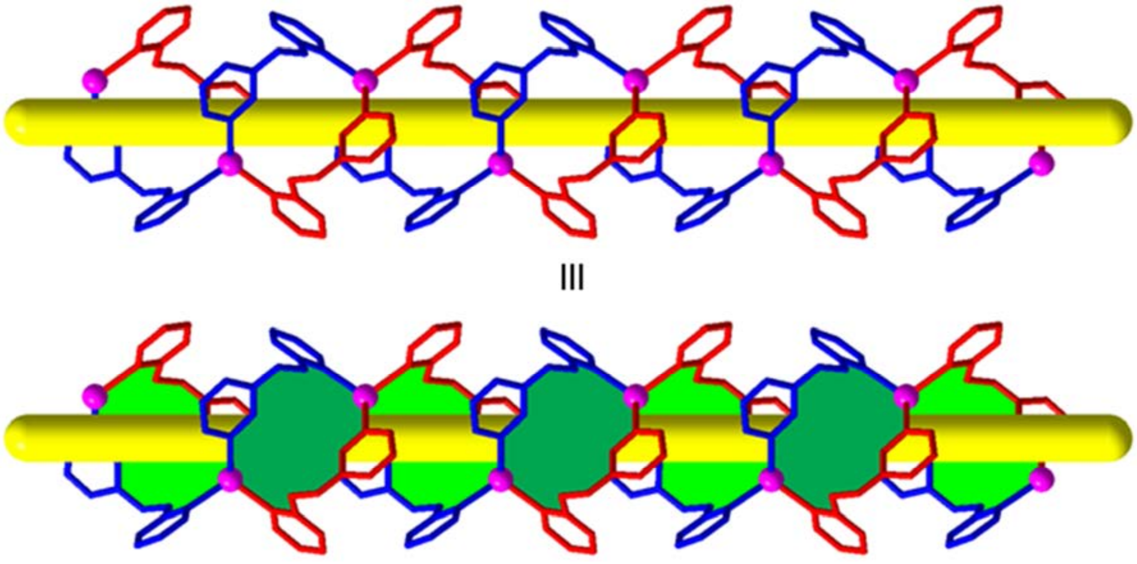
Silver(I) Coordination Polymer with Helical Looped-Chain Topology

주희영 이은지 박기민[1,*]

경상대학교 화학과 [1]경상대학교 기초과학연구소

Recently, a large number of coordination polymers with helical structures have received much attention in owing to not only their intriguing architectures but also their practical applications as functional materials in catalysis chemistry, biomimetic chemistry, molecular recognition, and nonlinear optics. In this area of research, symmetrical dipyridyl ligands consisting of two terminal pyridines with same substituted nitrogen positions have been used mainly for the synthesis of coordination polymer because of their easy preparation and the constructability of predictable coordination polymer. On the other hand, a few of novel coordination polymers based on unsymmetrical dipyridyl ligands composed of two terminal pyridines with different substituted nitrogen positions were reported. Especially, the unsymmetrical dipyridyl ligand with 2- and 3-pyridyl terminal groups exhibits a tendency to form helical coordination polymers or metallomacrocyclic compounds through the reaction of Ag(I) ion with linear geometry. In extending this work on interesting helical Ag(I) coordination polymers, *N*-(pyridine-2-ylmethyl)pyridine-3-amine (L) as an unsymmetrical dipyridyl ligand was prepared according to the previously reported method. The reaction of Ag(I) ion with the unsymmetrical ligand L afforded a Ag(I) coordination polymer (1) with an intriguing infinite helical framework made up of looped-chain. Herein we report crystal structure and physical properties of 1.



Helical looped-chain structure of Ag(I) coordination polymer **1**.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual Changes in Conformation and Optical Properties of Fluorophores within a Metal-Organic Framework (MOF)

조원 이희정 최소라 오문현*

연세대학교 화학과

Rational design of metal-orgabic frameworks (MOFs), which have the specific binding sites to interact with specific analytes, is vital for selective recognition and sensing events. Two well-known approaches to provide the specific binding sites are the incorporation of unsaturated Lewis acid metal sites and the immobilization of Lewis basic sites within the MOF structures. Herein, we report a fluorescent turn-off sensor based upon a functional MOF for Cu^{2+} sensing. In addition, the interesting dual changes in optical property and conformation of fluorophores within a MOF structure during framework construction and sensing event are demonstrated.

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One-Pot Synthesis of Fluorescent and Magnetic Nanochains of Fe_3O_4@Coordination Polymer

이희정 오문현*

연세대학교 화학과

There are many demands for the construction of dual-functional (especially, magnetic and fluorescent) materials since they are useful in many biological applications, for example imaging and separation. Herein, we report a facile solvothermal approach for the construction of well-organized Fe_3O_4@coordination polymer (Fe_3O_4@CP) nanochains with fluorescent and magnetic properties. Fluorescent and magnetic properties are associated with the fluorescent coordination polymer shell and magnetic magnetite (Fe_3O_4) core.

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Magnetic Particles-Embedded Porous Carbon Composites Made from Metal-Organic Frameworks (MOFs) and Their Sorption Properties

이희정 조원 오문현*

연세대학교 화학과

Porous carbon materials have received many attentions because of their useful applications such as adsorbents, supercapacitors, and as catalyst supports. In order to enhance their usefulness, the fusion of carbon materials with other functional materials is an essential strategy. Especially, magnetic carbon materials are useful in lithium ion batteries, supercapacitors, and separation of pollutants Herein, we report a unique method for one-pot synthesis of nano- and micro-sized hybrid composites, which contain porous carbons and magnetic particles (γ-Fe_2O_3, Fe_3C and/or α-Fe), through a simple thermal treatment of iron-containing MOFs as precursors.

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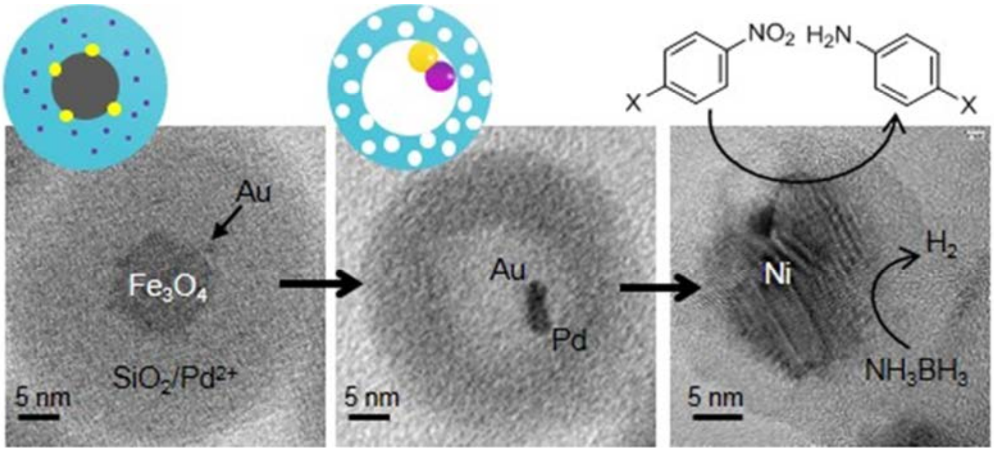
Seed-engineering Approach toward Hollow Nanoreactor Suitable for the Confined Synthesis of Less-noble Ni-based Nanocrystals

정관용 이인수*

포항공과대학교(POSTECH) 화학과

Yolk@shell nanoparticles, which encapsulate a movable metal core within a hollow shell, have been proved to be promising candidates as nanoreactor systems that confine the seed-mediated growth of metal nanocrystals inside the cavity as well as selectively and repeatedly catalyze the organic reaction. I would like to present recent findings in our efforts to extend the utility of the hollow nanoreactor approach, which templates the synthesis of metal nanocrystals, toward producing the less-reducible and, therefore, less confinable non-noble metal nanocrystals beyond the noble metals. A hollow nanoreactor suitable for the cultivation of Ni-nanocrystals was developed through a distinct seed-engineering strategy, which involved an assembly of a catalytically active Au/Pd-heterojunction-nanocrystal inside the hollow silica nanoshell. The engineered hollow nanoreactor demonstrated targeted performance in the growth of the Ni nanocrystal within the confines of its cavity. The nanoreactor-synthesized Ni-nanocrystals exhibited the active and recyclable performance in catalyzing hydrogen generation from NH$_3$BH3$_3$ and the chemoselective reduction of nitroarenes in aqueous solutions at room.


Au
Fe3O4
SiO2/Pd2+
5 nm
Au
Pd
5 nm
NO2
H2N
X
X
Ni
H2
NH3BH3
5 nm

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Schiff base type of bimetallic metal complex building blocks

김부현 허정석*

충남대학교 화학과

As demonstrated in many reports, bimetallic complex shows superior catalytic activities compared to monometallic metal complexes and of great interest in organic synthesis and conversions. To take advantage of this feature, development of bimetallic building blocks, easy to couple with nanoparticles or any substrate, is highly desirable. We have developed synthetic route which allows one step synthesis of bimetallic building block. The target building block contains two intact aldehyde groups, afterward these are available to reacted with either a primary amine functionalized compound, surface or nanoparticles. In the poster session, detailed synthesis and characterization results of the bimetallic metal complex will be presented.

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Gas adsorption and Chemical recognition with a Luminescent Zr-MOF

김성민 허정석*

충남대학교 화학과

Since porous coordination polymers exhibit high surface area and selective adsorption properties, they allow us promising applications. Among several MOFs composed of same organic component and different metal components, only Zr(4+)-MOF retained structural stability and permanent porosity. Zr-MOF also found to be very stable even in aqueous and acidic condition allowing us useful potential applications not only gas adsorption but also molecular sensing. Due to the fact that any amount of water or vapor surround us, it is important that MOF exhibit water stable for applications. We prepared Zr-MOF has carbonyl functional group between two phenyls. Its adsorption properties, X-ray structure, thermal analysis data and host-guest chemistry in aqueous solution will be presented in the poster session.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Regenerable Covalent Organic Framework for CO2 Capture after Soaking in Water

김영훈 허정석*

충남대학교 화학과

Series of Covalent Organic Frameworks (COFs) have been investigated using imine condensation reaction with aldehyde and amine compounds. Among them, I-COF-1 (Imine-coupled COF) has a unique property of regeneration for gas adsorption. N_2 and CO_2 adsorption amount was recovered as much as the amount that the COF can adsorb at first, or even higher than it, although the gas adsorption amount was decreased by approximately 58 % after soaking in H_2O for a day. Detailed characterization results will be presented in the poster session.

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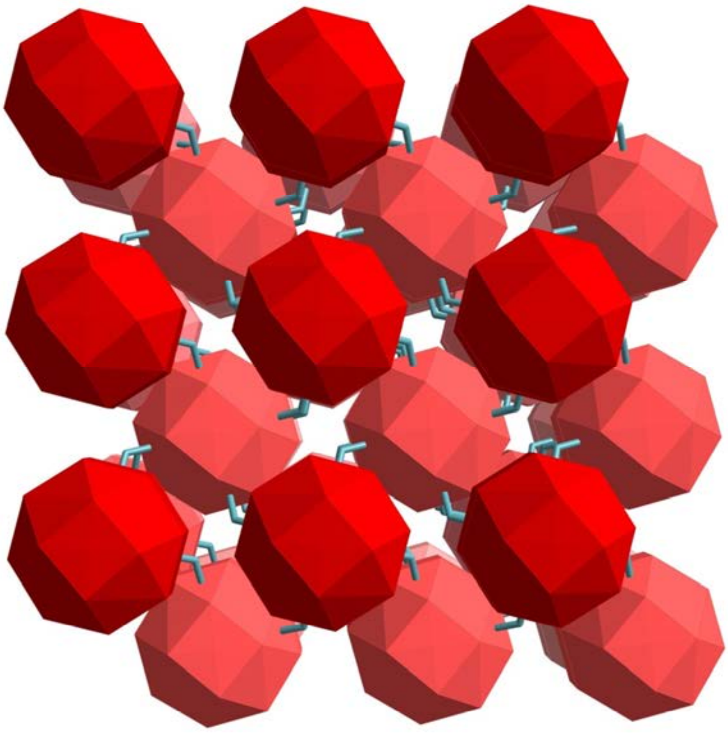
Nanocage as a Structure Building Unit for Porphyrinic Metal-Organic Frameworks

진은지 최원영*

울산과학기술대학교(UNIST) 화학과

Metal-organic frameworks (MOFs), assembled from metal nodes and organic linkers, are an important new class of nanoporous materials with potential applications such as gas storage and heterogeneous catalysis. Ever-increasing popularity of such MOFs partly stems from wide selection of metal nodes and organic linker, thus creating virtually limitless structures. An interesting approach to create robust MOFs is to utilize polyhedron as a structure building unit. In this presentation, we report a new series of polyhedral-based MOFs, built from porphyrinic nanocages and new Zn4O(COO)6 metal nodes, with high density of open metal centers.



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Biomimetic zinc complexes for CO_2 fixation

박예훈 조재흥*

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CO_2 fixation by metal complexes is of great interest from the issue of global warming, because the fundamental understanding may lead to some of practical means to eliminate CO_2 in air. The carbonic anhydrases are zinc containing enzymes that catalyze the reversible hydration of CO_2 and dehydration of HCO_3^-. In this work, we would like to prepare a series of zinc complexes bearing various *N*-donor ligands to understand the mechanism of CO_2 fixation by zinc center. The mechanistic information was obtained by electrospray ionization mass spectrometer. Kinetic studies on the CO_2 fixation by the biomimetic zinc complexes will show the relations between coordination environment and reactivity.

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Peptide Unit Based Dinuclear Copper Complex as a Model of Catechol Oxidase: Synthesis, Kinetics and Mechanism

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경북대학교 화학과

Catechol oxidase, a type-3 copper enzyme, that contains dinuclear copper(II) center in its active site. This enzyme mediates a two electrons transfer reaction during the oxidation of a wide range of catechols to corresponding *o*-quinones by the molecular oxygen. General interest in investigating the functioning of carboxamide processing proteins and enzymes is due to their important roles in the biological chemistry. Synthetic models for the active site of catecholase have been prepared mostly with amines and imines pyridine type nitrogen donors. Our interest is in the preparation and investigation of more biotic model complex for catecholase in an attempt to discover the minimal peptide binding motif that spectroscopically and functionally represents the protein active site. 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 catechol to the corresponding *o*-quinone. The complex was characterized by various spectroscopic techniques and the catalytic activities were monitored by the ESI-Mass, UV-kinetics and EPR spectroscopy.

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Synthesis and characterization of bimetallic Metal/Graphitic Carbon nanocrystals and Metal@Carbon nanocomposites

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서강대학교 화학과

We have synthesized bimetallic fct-FePt/Graphitic Carbon (fct-FePt/GC) nanocrystals and fct-FePt@Mesoporous Carbon (fct-FePt@MC) nanocomposites by a chemical vapor deposition (CVD) method. The fct-FePt/GC nanocrystal is composed of a fct-FePt alloy core and a graphitic carbon shell and the fct-FePt@MC nanocomposites are mesoporous carbon embedded with fct-FePt alloy nanocrystals. The nanocrystals and nanocomposites have been characterized by XRD, TEM, EDX, ICP-Mass, SAED pattern, and Raman. We expect the nanocomposites to be useful as recyclable catalysts for the reduction of nitro compounds due to the catalytic function of the FePt nanocrystals and the ability to be attracted to an external magnetic field.

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Synthesis, Characterization and Reactivity of a Mononuclear Ni-O_2 Complex with Macrocyclic Ligand, Me_3-TPADP

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Mononuclear metal-active oxygen adducts (M-O_2), such as metal-superoxo and -peroxo species, have been implicated as important parts in the catalytic cycles of biological reactions. Biomimetic compounds of M-O_2 species have been structurally and spectroscopically characterized and investigated in nucleophilic and electrophilic oxidation reactions. Here we report the synthesis of Me_3-TPADP (3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane) which gives an electronically tunable site on the para position of the pyridyl group. The starting complex, $[Ni^{II}(Me_3\text{-TPADP})(CH_3CN)]^{2+}$ (1), and Ni-O_2 intermediate, $[Ni^{III}(Me_3\text{-TPADP})(O_2)]^{+}$ (2), were prepared and successfully characterized by various physicochemical methods. We are going to investigate the reactivity of 2 toward external organic substrates and then compare the results with those of the previously reported Ni-O_2 complexes.

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Synthesis and Molecular Structure Of Copper(II) Complex With Tetradentate Ligand Contain Pyridine and Hydroxyl Group

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Multidentate ligands are considered to form interesting metal complexes with transition metals. The mononuclear $[\mathrm{Cu^{II}(L)Cl_2}]$ was synthesized from $\mathrm{CuCl_2.2H_2O}$ and 3-({[(pyridin-2-ylmethyl)amino]methyl}amino)propan-1-ol (L, PMDAE) in methanol. Copper(II) ion in this complex has one pyridine group of PMDAE whose an aminoethanol groups coordinates adjacent copper(II) ion. This complex was characterized by spectroscopic methods and X-ray single crystal diffraction. The molecular structure of this complex has five coordination numbers and trigonal bipyramidal geometry involved non-coordination of the oxygen atom of the hydroxyl group and the copper(II) center. The detailed synthesis, crystal structure, and physical properties of $[\mathrm{Cu^{II}(L)Cl_2}]$ will be discussed in this poster presentation.

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Synthetic Flavonoids, Aminoisoflavones: Interaction and Reactivity with Metal-Free and Metal-Associated Amyloid-β Species

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Metal ion homeostasis in conjunction with amyloid-β (Aβ) aggregation in the brain has been implicated in Alzheimer's disease (AD) pathogenesis. To uncover the interplay between metal ions and Aβ peptides, synthetic, multifunctional small molecules have been employed to modulate Aβ aggregation in vitro. Naturally occurring flavonoids have emerged as a valuable class of compounds for this purpose due to their ability to modulate both metal-free and metal-induced Aβ aggregation. Although flavonoids have shown anti-amyloidogenic effects, the structural moieties of flavonoids responsible for such reactivity have not been fully identified. In order to understand the structure-interaction-reactivity relationship within the flavonoid family for metal-free and metal-associated Aβ, we designed, synthesized, and characterized a set of isoflavone derivatives, aminoisoflavones (1-4), that displayed reactivity (i.e., modulation of Aβ aggregation and control of reactive oxygen species generation) in vitro. NMR studies revealed a potential binding site for aminoisoflavones between the N-terminal loop and central helix on prefibrillar Aβ different from the non-specific binding observed for other flavonoids. The absence or presence of the catechol group differentiated the binding affinities and enthalpy/entropy balance between aminoisoflavones and Aβ. Furthermore, having a catechol group influenced the binding mode with fibrillar Aβ. Inclusion of additional substituents moderately tuned the impact of aminoisoflavones on Aβ?aggregation. Overall, through these studies we obtained valuable insights on the requirements for parity among metal chelation, intermolecular interactions, and substituent variation for Aβ interactions.

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Gold nanoparticle-based Norovirus detection

김근석 정윤재[1,*]

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Human noroviruses (NoV) is a genetically diverse group of non-enveloped RNA viruses and regarded as the main reasons of nonbacterial acute gastroenteritis worldwide. Various routes of infection exist and only ~ 20 NoV can cause manifestation. Therefore point-of-care detection of NoV becomes one of the most important issues in public health science. In this research, we develop rapid immunological diagnostic system for Human NoV using gold nanoparticle. One of the effective methods is using chromatography that distinguishes nanoparticles with and without NoV. Another method is classifying different colors of nanoparticle clusters according to the existence level of NoV. Distinct red color of gold nanoparticles allows us to detect Human NoV in a short time.

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Synthesis and Characterization of Macrocyclic Complexes containing 4-(Phenylazo)benzoate

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Two metal-organic complexes, $[Ni(C_{18}H_{42}N_6)(C_{13}H_9N_2O_2)_2]?2CH_3CN?H_2O$ (1) and $[Cu(C_{18}H_{42}N_6)(H_2O)_2](C_{13}H_9N_2O_2)_2$ (2) were obtained by the reaction of nickel(II)/copper(II) hexaaza macrocyclic complex with deprotonated 4-(phenylazo)benzoic acid. The complexes were characterized by elemental analysis, IR, UV-Vis, fluorescence and single X-ray diffraction. In complex 1, nickel(II) macrocyclic unit binds two 4-(phenylazo)benzoate ions in trans position, while copper(II) ion in 2 coordinates two water molecules in axial positions. In 2, 4-(phenylazo)benzoate ions exist as anions in the crystal lattice are involved in Hydrogen bonding interactions with coordinated water moleculer. Complex 1 is soluble in most organic solvents, and complex 2 is soluble in most solvents except for water and acetone. The detailed synthesis, crystal structure, and physical properties of complexes 1 and 2, respectively, will be discussed in this poster presentation.

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Fe-Porphyrin Microporous Network@Fe3O4 Nanoparticles: Magnetic Heterogeneous Catalytic System for Carbene Insertion to N-H Bond

유진 손성욱* 김민철 김보룡 강성아 강나래

성균관대학교 화학과

Microporous organic networks (MONs) are a new class of porous materials. This study shows the application of MON chemistry for the preparation of heterogeneous catalysts with a core-shell structure. Core part consists of magnetic nanoparticle (Fe3O4) with an average size of ca. 200 nm. The Fe-porphyrin microporous network shells were prepared via Sonogashira coupling of tetra(4-ethynylphenyl) Fe(III)-porphyrin and 1,4-diiodobenzene. The Fe3O4 nanoparticles were coated successfully with Fe-porphyrin microporous networks. The materials were characterized by the powder X-ray diffraction studies, N2 isotherm analysis, scanning electron microscope and transmission electron microscope. The average thickness of shells was a 17 nm and the Fe-porphyrin network coating exhibited amorphous and microporous characteristics. The microporous Fe-porphyrin networks on the Fe3O4 nanoparticles showed good catalytic performance for the carbene insertion into N-H bond of amines. The catalyst was easily recycled from the reaction mixture via magnetic separation.

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Metal-Organic Framework@Microporous Organic Network: Hybrid Hydrophobic Adsorbents with Crystalline Inner porosity

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This presentation will show the synthesis of metal-organic framework(MOF)@microporous organic network (MON) hybrid materials and their application for the adsorption of organic adsorbate on the water. Metal-organic framework, UiO-66-NH2, has good wettability and outstanding stability in water which might be caused by Zr-carboxylate bonds. Because of good wettability, many MOFs including UiO-66 series sink into the water. The microporous organic networks display different properties from those of MOFs. They have hydrophobic properties so that they can be used as a hydrophobic coating against water. As a result, the MOF@MON hybrid materials float on water surface and show excellent adsorption ability for the removal of organic adsorbates on the water. To investigate the adsorption property of MONs, UiO-66-NH2 in hybrid materials was chemically removed and then adsorption ability was tested. MONs shows poor adsorption ability toward toluene which implies that the inner crystalline MOFs are the key to adsorb toluene. Also chemically etched hybrid materials showed hollow structure of MONs and this indicates that MOFs can be used as a template for shape controlled MONs.

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Porphyrins in the Microporous Organic Hollows: Detection of Organic Pollutants in Water porphyrin-MOH

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성균관대학교 화학과 [1]성균관대학교 자연과학대학 화학과

Microporous organic networks (MONs) are a new class of functional materials. For expanding the application fields, the discovery and undersanding of new nature of MONs is desirable. This work reports on the controllable trapping and releasing guest molecules of MON hollow spheres. Controllable trapping and releasing of guests by hollow carriers is an important research issue for ultimate practical applications including chemical delivery and storage. The fundamental chemistry in this work originates from the unexpected discovery of a high and controllable wall permeability of MON hollow spheres. Zn-porphyrins with systematic alkyl chains were entrapped in the MON hollow spheres. The resultant materials showed organic solvent-responsive release behavior in water. In this work, considering the fluorescent properties of Zn-porphyrins, we studied the potential of Zn-Por@MOH-B as a fluorescent alerting systems for the model organic solvents discarded in water. Conventional luminescence detection systems for organic pollutants in water operate for emissive organic analytes. Although non-emissive and water soluble organic solvents commonly used in chemical synthesis are high potential water pollutants, reports focusing on this issue are quite rare. To detect non-emissive organic solvents in water, chromatographic equipment is ultimately required, which is not suitable for prompt recognition of contamination. Thus, more diverse colorimetric detection strategies for non-emissive organic solvents in water should be explored. In this work, the response sensitivity (0.22 mol% organic solvent) of Zn-Por@MOH-B toward organic solvents is superior to that of organic solvent responsive systems in literatures. The organic solvent-responsive release behavior of guest@MOH-B can be a new strategy for the water soluble organic solvent detection in water.

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Microporous Organic Network on the Fe3O4 Nanosphere: High Performance Anode Materials for Lithium-Ion Batteries

김민철 유진 강성아 김보룡 강나래 손성욱*

성균관대학교 화학과

Fe3O4 is well known as an anode material for lithium ion batteries. However, volume expansion during charge/discharge can cause serious problems such as a capacity loss. Carbon coating is one of the most used surface modification techniques for anode materials. The carbon coating can give significantly effects on the electronic conductivity of electrode materials and play an important role as a structural buffer. Microporous organic networks (MONs) are a new class of porous materials. Thin microporous organic networks were formed on the surface of Fe3O4 nanospheres using Sonogashira coupling reaction of tetra(4-ethynylphenyl)methane and 1,4-diiodobenzene. The thickness of MON coating was controlled by screening the amount of building blocks. Through carbonization, Fe3O4@C composites were obtained. The Fe3O4@C composites were characterized by powder X-ray diffraction studies, transmission and scanning electron microscopes, and N2 adsorption isotherm analysis based on the Brunauer-Emmett-Teller theory. Consequently Fe3O4@C composites showed promising reversible discharge capacities of up to 807 mA h g-1 and enhanced electrochemical stability.

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Production of Iron oxide hydroxide/reduced graphene oxide composites and its application as electrochemical catalyst for oxygen reduction reaction

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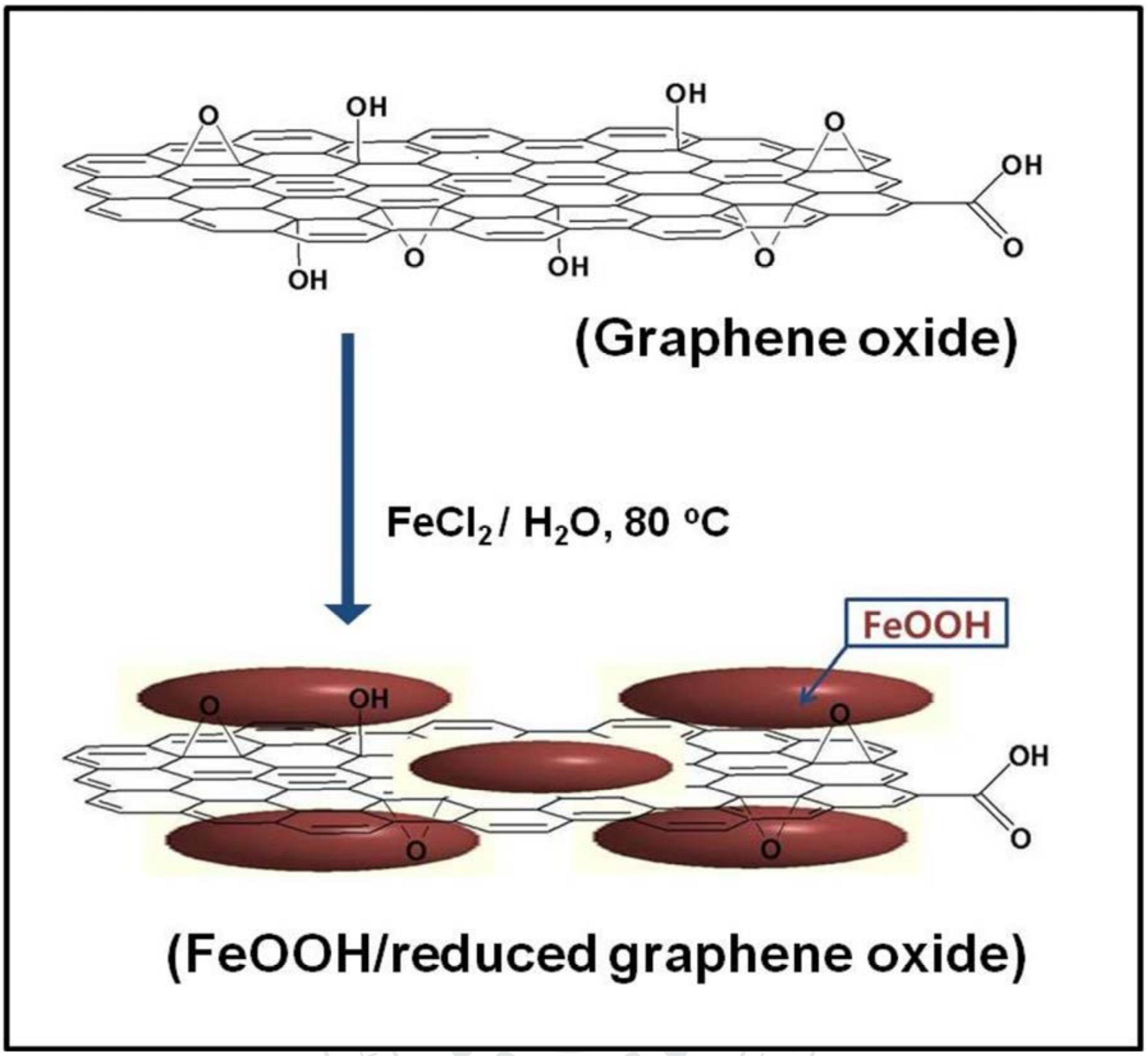
Fe-based hybrid systems have been suggested as promising candidates for oxygen reduction reaction (ORR) catalysts owing to their good catalytic performances and feasibilities for mass production at low cost. In this work, we develop means of producing novel hybrids containing FeOOH particles well-dispersed on graphene-based materials using a one-pot solution process. The hybrid materials show good electrochemical catalytic activity for ORR, such as, an on-set potential of 0.76 V (vs. the reversible hydrogen electrode), a near four electron pathway, excellent stability against methanol poisoning during durability test. This is the first report of the use of FeOOH/reduced graphene oxide hybrid materials as ORR catalysts.


O
OH
OH
O
OH
O
OH
O
OH
O
(Graphene oxide)
FeCl$_2$/ H$_2$O, 80 °C
FeOOH
O
OH
O
OH
O
O
O
(FeOOH/reduced graphene oxide)

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Precise control of Ag nanoparticle synthesis using two phytochemicals

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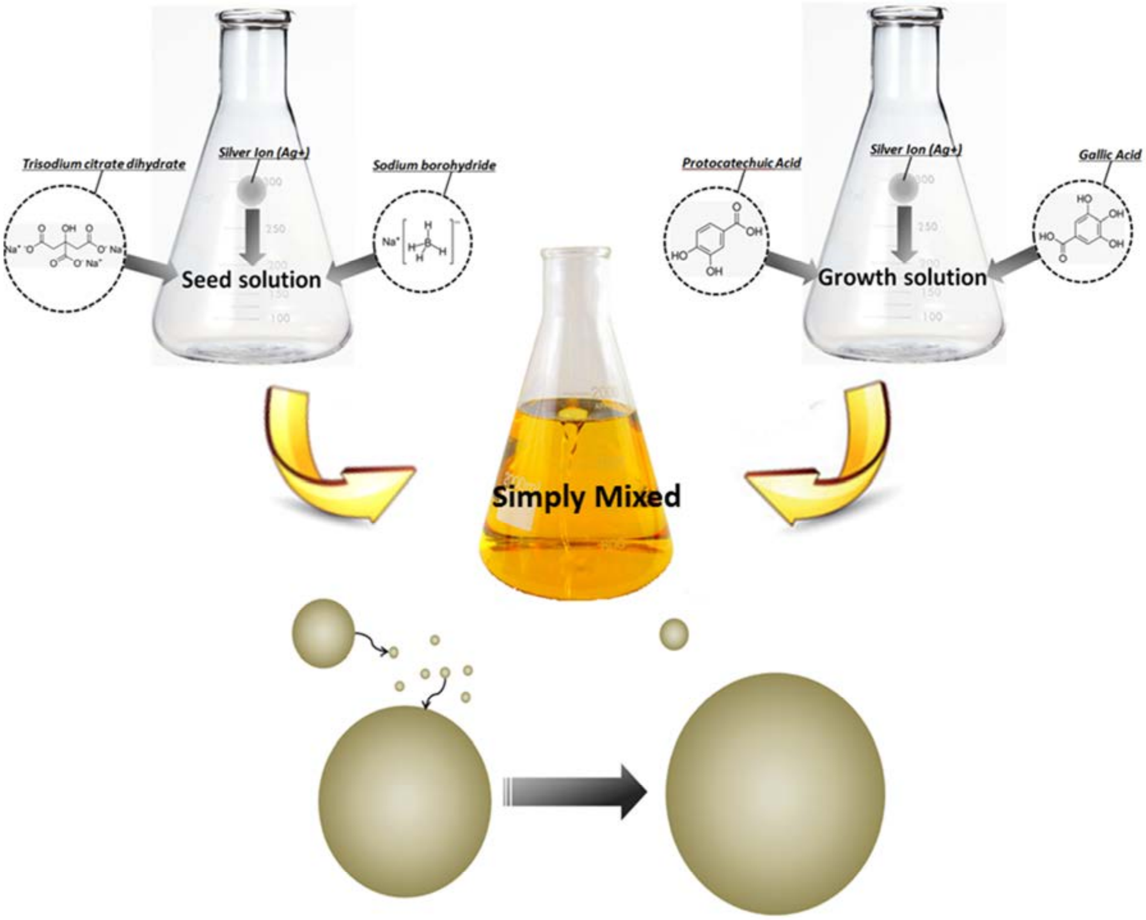
Precise control of size and shape of nanoparticles is of scond-to-none importance since their electronic and optical characteristics are directly related with them. In this study, we demonstrate a simple growth approach to obtain precise size control using silver precursors and two kinds of phytochemicals, i.e., gallic acid (GA) and protocatechuic acid (PCA). These phytochemicals have similar chemical structure and characteristic except for one different OH- functional group, inducing different reducing ability to metallic precursors. So, their composition and concentration were precisely varied to induce optimized condition for nucleation and growth of NPs. The whole steps of NP synthesis were carefully monitored by UV-Vis spectrophotometer and electron microscopy. Ag NPs with diameters in the range of 10-20nm were readily controlled by altering concentrations of precursor and phytochemicals.



Ostwald ripening is major mechanism to grow the NPs in the growth step.

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Isoreticular and Polymorphic Metal-Organic Frameworks via Combination of *de novo* synthesis and Postsynthetic modification

정석 나명수*

울산과학기술대학교(UNIST) 화학과

The metal-organic frameworks (MOFs), [Ni(HBTC)(pz)] (3) (hms net topology) (where, H3BTC = 1,3,4-benzenetricarboxylicacid; pz = pyrazine) and [Ni(HBTC)(bipy)] (4) (gra net topology) (where, bipy = 4,4'-bipyridine) that were unattainable via conventional synthetic approach, were prepared via the postsynthetic ligand exchanges of 3-D MOFs, [Ni(HBTC)(bipy)] (1) (hms net topology) and [Ni(HBTC)(pz)] (2) (gra net topology), respectively. The MOFs, [Ni(HBTC)(pz)] (5) (gra net topology) and [Ni(HBTC)(bipy)] (6) (gra net topology) that are the same as 2 and 4, respectively, were prepared via the postsynthetic ligand insertions into 2-D MOF [Ni(HBTC)(DMF)] (hcb net topology). 1 and 4 (or 6) are the polymorphic MOFs of the same 3,5-connected but of different net topologies, hms and gra net topologies, respectively, with the same [Ni(HBTC)(bipy)] formula. 2 (or 5) and 3 are also the polymorphic MOFs of the same formula unit, [Ni(HBTC)(pz)]. 1 and 3 are the isoreticular structures of the same hms net topology and 2 and 5 also are the isoreticular structures of the same gra net topology.

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Catecholase Activity of a Cobalt Complex with pyridylcarboxamide ligand

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경북대학교 화학과

Catechol oxidase is an enzyme catalyzing two electron oxidation of a wide range of catechols to corresponding *o*-quinones by oxygen molecules. This enzyme contains dicopper center in its active site. Numerous mono- or multi-copper model complexes have been developed to elucidate the mechanistic reaction pathway of the enzyme’s catalytic action. As one of the such efforts, we have previously synthesized copper complexes, containing distant two or four copper ions, with carboxiamide ligand groups and shown their catecholase activity. In this study, we expand our view to search the catecholase activity catalyzed by non-copper metal ions. We have synthesized a cobalt complex with H_2L ligand (H_2L = (N,N'-(ethane-1,2-diyldi-*o*-phenylene)-bis(3-methylpyridine-2-carboxamide)). Indeed, the cobalt complex exhibited the catalytic ability to oxidized 3,5-di-*tert*-butylcatechol to 3,5-di-*tert*-butyl-1,2-benzoquinone. In this poster, we present the crystal structure and the evidences of the catecholase activity of the complex to propose the mechanistic reaction pathway of the catalytic reaction.

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Efficient Hydrolysis of Phosphate Esters Mediated by Binuclear Cu Complexes

김정희

선문대학교 화학과

A series of unsymmetrical binucleating ligands has been synthesized. Binuclear Cu complexes of 1-(3-(1,4,7-triazonan-1-yl)propyl)-1,4,7,10-tetraazacyclododecane(L1), 1-(3-((1,4,7-triazonan-1-yl)methyl)benzyl)-1,4,7,10-tetraazacyclododecane(L2) have been prepared and their efficiency in hydrolyzing phosphate esters such as BDNPP, NPP, BNPP, and HPNPP was tested. The catalytic reactivities were compared to those obtained with Cu(II) complexes of the corresponding symmetrical binucleating ligands, 1,3-di((1,4,7-triazonan-1-yl)propane(L3) and 1,3-bis((1,4,7-triazonan-1-yl)methyl)benzene(L4). The binuclear Cu2(L1) hydrolyzed BDNPP and HPNPP more than 10 times efficiently than the Cu2(L3) complex, and the binuclear Cu2(L2) mediated hydrolysis of BNPP and NPP with 10-100 times rate enhancement compared to those by the Cu2(L3) and Cu2(L4) complexes under mild conditions.

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Isoreticular metal-organic frameworks (MOF) based on quadruply interlinked a rhombic dodecahedral metal-organic polyhedron (MOP) as a tertiary building unit

김동욱 나명수*

울산과학기술대학교(UNIST) 화학과

The reactions of two different covalent linked tetracarboxylate ligands containing two 1,3-benzenedicarboxylate (BDC) residues with Zn(II) ion generated the two isoreticular MOP-based MOFs, PMOF-4 and PMOF-5, with a 3,3,4-c zjz topology, in which the MOP is a 3,4-c rhombic dodecahedron based on 3-c [$Zn_2(COO)_3$] and 4-c 4-c [$Zn_2(COO)_4$] secondary building unit. The MOP with 24 branching edges served as a 24-c rhombicuboctahedral tertiary building unit (TBU), which was quadruply linked to six neighboring rhombicuboctahedral TBUs in an underlying pcu topology. Although the underlying topology of PMOF-4 and PMOF-5 was the same as that of PMOF-3 with a 3,3,4,4-c zmj topology and of the PCN-12 with a 3,3,3,3,4,4,4,4-c b>zhc topology, the mode of the quadruple linkage in PMOF-4 and PMOF-5 is different from those of the other MOFs with different net topologies.

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BODIPY functionalized inorganic motif for low-energy photosensitization

이아랑* 한원식*

서울여자대학교 화학과

A new type of organic/inorganic dyad that can induce low-energy photosensitization has been developed; electron donor and electron acceptor units are boron dipyrromethene (BODIPY) and inorganic motif, respectively. New dyads consist of V-shaped molecular array in which two BODIPY units are substituted onto inorganic motif. In the presence of inorganic motif, significant fluorescence quenching was observed to compare with BODIPY derivatives without inorganic motif. In other words, photoinduced electron transfer (PET) had occurred from the end-on BODIPY units to the inorganic motif with PET efficiencies of 63-71%. As a result, corresponding cationic and anionic species that are responsible for the CT state were detected by the serial spectroelectrochemical studies; cationic BODIPY radicals at 400 nm at the applied voltage of 1.44 V and broad absorption bands of anionic radical for inorganic motif in the range of 250 ~ 490 nm at ?1.84 V. Transient absorption studies further confirmed the BODIPY radical anion at 540 nm and the radical anion for inorganic motif at 350?475 nm with structureless broad band.

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Copolymerizations between 2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole and Dichlorodisubstitutedsilanes or Dichlorotetrametyldisilane using *n*-Butyllithium

장지훈 민용기 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole as monomers were prepared by the intramolecular reductive cyclizations of diethyl bis(phenylethynyl)silane with treatments of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide *in situ*. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diethyl-3,4-diphenyl-2,5-silole and disubstitutedsilanes or dichlorotetramethyldisilane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diethyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane or dichlorotetrametyldisilane using *n*-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, ^1H, ^{13}C, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular

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Copolymerizations between 2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole and Dichlorodisubstitutedgermanes using *n*-Butyllithium

장지훈 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole as monomers were prepared by the intramolecular reductive cyclizations of diethyl bis(phenylethynyl)silane with treatments of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide *in situ*. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diethyl-3,4-diphenyl-2,5-silole and disubstitutedgermanes along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diethyl-3,4-diphenylsilole with several dichlorodisubstitutedgermanes using *n*-butyllithium. The obtained polycarbosilanes containing disubstitutedgemanes are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, ^1H, ^{13}C, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular

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Purification of Dye-Contaminated Water Using Metal-Organic Frameworks

김성준 윤민영[1,*]

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Water is one of the most important and essential components for vital activities of living organisms. However, water can be easily deteriorated because of its good solubility for possible pollutants such as colorful dyes, which may be tremendously increased by growth of population, civilization and industrialization. Water purification, thus, has become one of the most important issues in the present. For the purification of water by adsorption, porous materials such as activated carbon have been widely used. Recently, a new type of porous material, metal-organic framework (MOF) has been studied for various applications including gas storage, separation and catalysis. MOFs, however, were scarcely used for water purification due to their vulnerability to water. Herein we reported an application of MOFs for the purification of dye-contaminated water. Several MOFs that are stable in water, such as UiO-66, UiO-67 and MIL-100(Fe), have been employed for decolorization of water by adsorption of colorful dyes. Decolorization was evaluated by UV absorption spectra and adsorbed dye amount was also calculated by UV absorption change. Although the dyes showed different adsorption kinetics depending on their size and MOF pore size, the dye-contaminated water was clearly decolorized in several minutes or in an hour. In addition, thermogravimetric analysis (TGA) data quantitatively demonstrates adsorption of dye molecules on MOF surface. Details of our recent work will be presented.

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Synthesis of Copolymers Containing 1,1-Diisopropyl-3,4-diphenylsilole and Disubstitutedsilane along the Main Chain and their Applications to Lithium-ion Battery

정영민 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diisopropyl-3,4-diphenylsilole as monomer was prepared by the intramolecular reductive cyclization of diisopropylbis(phenylethynyl)silane with treatment of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide in situ. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diisopropyl-3,4-diphenyl-2,5-silole and disubstituted silane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diisopropyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane using n-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular. In order to study the electrochemical properties of the synthesized materials, we also prepared a composite of the obtained polycarbosilanes with silicon nano powder, and examined the characteristics as a lithium-ion battery.

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Synthesis of New TaN Precursors for MOCVD

이상찬 박보근[1] 정택모[2] 홍창섭[*] 김창균[1,*]

고려대학교 화학과 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학소재연구단

Metal-organic complexes of early trasition metals, bearing nitrogen-containing ligands have received increasing attention over the last decades. Major application of these compounds is their use as precursors for thin films by MOCVD and ALD techniques. Tantalum nitride (TaNx) films have been an attractive candidate as a diffusion barrier, gate electrode for CMOS (complementary metal oxide semiconductor), and electrodes for capacitors used in memory devices. Also tantalum carbo-nitride (TaCxNy) films have been studied as a gate electrode in the next generation nano-CMOS technology for its low resistivity, proper work function, and high reliability.We synthesized novel Ta precursors for TaNx and TaCxNy thin film deposition using MOCVD process. All compounds have been characterized by means of NMR, FT-IR spectroscopy, elemental analysis, and TGA.

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Synthesis and Characterization of Group Ⅳ Transition Metal Precursors

김다혜 박보근[1] 전동주[2] 김창균[1] 손성욱[*] 정택모[3,*]

성균관대학교 화학과 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학물질연구단 [3]한국화학연구원 화학소재연구단

The oxides of group Ⅳ transition metals such as titanium, zirconium, hafnium have many important current and future application, including protective coatings, sensors and dielectric layers in thin film electroluminescent (TFEL) devices. Especially, group Ⅳ transition metal oxide films have been intensively investigated as replacements for SiO2 due to high permittivities (k ~ 14-25) compared with SiO2 (k ~ 3.9), large band-gaps, large band offsets and high thermodynamic stability on silicon. The novel group Ⅳ transition metal precursors have been synthesized by partially replacing the amido groups of the complexes [M(NMe2)4] and [M(NEtMe2)4] (M= Ti, Zr, Hf), using β-diketone ligands such as acetylacetone and 1,1,1-trifluoro-2,4-pentanedione. The complexes were characterized by FT-IR, 1H NMR, 13C NMR and thermogravimetric analysis (TGA). It is thought that the newly synthesised compounds are suitable for atomic layer deposition (ALD) precursors to grow group Ⅳ transition metal oxide thin films.

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Post-synthetic Modification of Fluoro-functionalized HKUST-1

홍지수 심재웅 오유진 김자헌*

숭실대학교 화학과

HKUST-1 is one of the most investigated metal-organic frameworks (MOFs) due to its easy preparation, good water stability, and optimum pore properties especially for methane adsorption. Recently, other research group reported prepared fuloro-functionalized form (UHM-31) from copper nitrate and 2-fluoro-1,3,5-benzenetricarboxylic acid (H_3BTC-F), and studied its gas (N_2, H_2, CO_2, CH_4) adsorption properties. We also could prepare UHM-31 or HKUST-1-F using a potassium salt of H_3BTC-F instead of the free acid ligand. In this presentation, we show its water sorption behavior and chemical reactivity with various nucleophiles. For example, benzylamine reacts with HKUST-1-F via aromatic nucleophilic substitution under mild conditions, which has been verified by various physical and chemical analyses including ^{1}H-NMR measurements.

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Water Sorption Properties of Functionalized Cr-MIL-101 Metal-Organic Frameworks

최판규 유래경 홍지수 김자헌*

숭실대학교 화학과

Cr-MIL-101 has superior water stability and a large water uptake capability of 1.2 g g^{-1} at 298 K and P/P_0 = 0.9. However, its steep water uptake take places at higher pressure than $P/P_0 = 0.4$, limiting its practical applications for adsorptive heat transformation such as thermally driven adsorption chillers. Thus, there have been great interests to improve its water adsorption properties at $0.05 < P/P_0 < 0.4$, more preferably $0.1 < P/P_0 < 0.3$. A plausible strategy is to introduce some hydrophilic groups to the organic linker so that they can attract water molecules by forming hydrogen bonds with water at low pressure. In this presentation, we show the preparations and characterizations of various Cr-MIL-101 derivatives functionalized with $-NH_2$, UR2, -NH-Mal, $-NH-Pr-SO_3H$, and ?COOH. The water sorption measurements indicated that most functionalized Cr-MIL-101s improved the water uptake capacity at P/P_0 = 0.1~0.3 except for Cr-MIL-101-UR2 containing ethyl urea group.

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A New Zeolitic Imidazole Framework Having Large Channels

임나래 홍지수 김태민[1] 김자헌*

숭실대학교 화학과 [1]숭실대학교

Zeolite imidazole frameworks (ZIFs) tend to mimic the zeolite structures due to their tetrahedral metal centers and bent ditopic imidazolate linkers. So far, among the 41 ZIF structural types, 10 types are exactly same as those found in zeolites. In the course of searching for new ZIF structural types, we could prepare a new one exhibiting zeolite AFI topology by low-temperature routes from the reactions between zinc salt and imidazole or purine. A single crystal X-ray diffraction analysis revealed that the new ZIF had a similar structure as gme ZIFs with large straight one-dimensional channels. Nitrogen adsorption measurements resulted in a Type-I isotherm, and a BET surface area was estimated to about 1900 m^2/g which is the second largest among the known MOF. In this presentation, we also report the gas adsorption and guest inclusion properties of the new ZIF.

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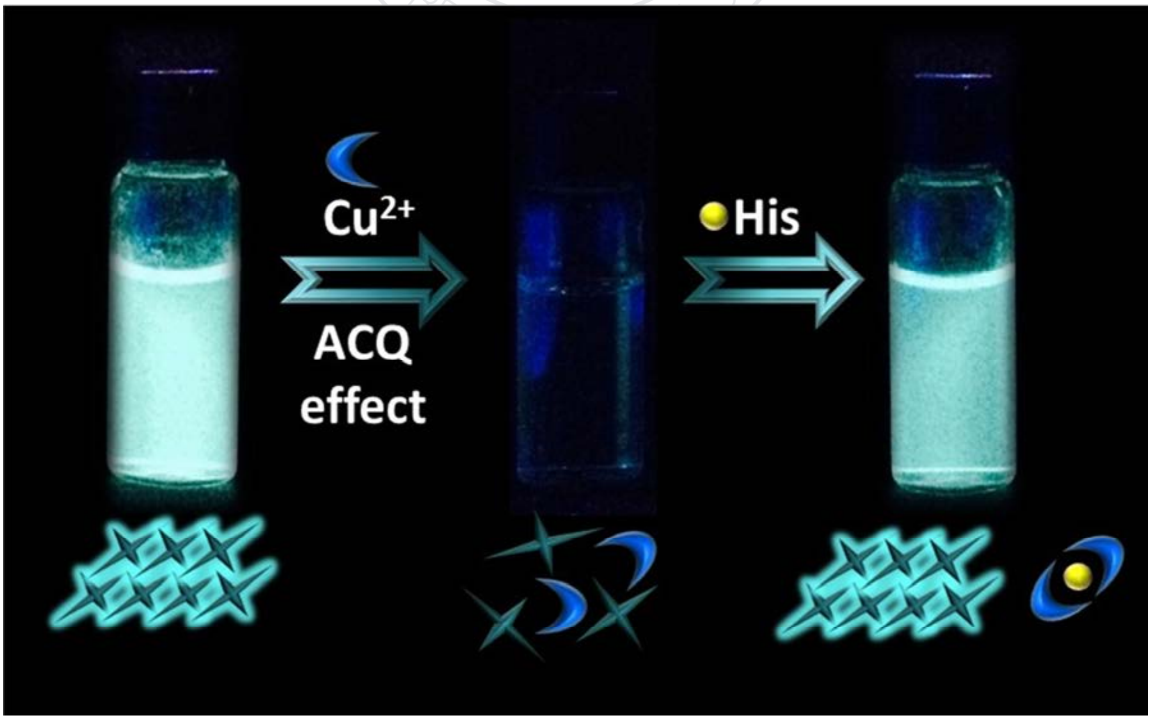
Imidazole-appended p-phenylene-Cu(II) ensemble as a chemoprobe for histidine in biological samples

김가영 정종화* 정성호

경상대학교 화학과

A tetra-imidazole-appended tetrakis(p-phenylene)ethylene 1-Cu^{2+} ensemble was found to enhancement fluorescence upon addition of histidine, but not with any other amino acids. The 1-Cu $^{2+}$ ensemble also selectively detected proteins containing histidine residues in a mixture of water and methanol (90:10, v/v%). The 1-Cu^{2+} ensemble-coated filter paper could also detect histidine quantitatively. Furthermore, the fluorescence emission recovery upon addition of five concentrations of His was ~80% with good linearity.



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Arabidopsis thaliana **SPL14전사인자 결합성 DNA가 도입된 금 나노입자 응집체를 이용한 단백질 검출**

안준호 이준화 정종화*

경상대학교 화학과

본 연구는 단백질과 DNA 간의 복합체 형성을 통한 금 나노입자의 신호변화에 기반한다. 말단에 싸이올 기를 지니는 상보적 DNA 를 각 금 나노입자 표면에 salt aging 방법으로 도입하였다. 단백질 및 DNA 간의 결합 형성으로 야기되는 신호는 각 DNA 가 도입된 금 나노입자를 혼합 함으로써 제조된 이중나선 DNA 가 형성된 금 나노입자 응집체가 이용되였다. 상보적 염기서열을 지니는 DNA 가 도입된 두 종류의 금 나노입자는 혼합 함에 따라 DNA 간 수소결합에 의해 입자간 응집을 일으키며 변색되는데, 이를 UV-Vis 분광기, 임도분포 측정기, 투과전자현미경을 통하여 분석하였다. 이중나선을 형성한 채 응집된 금 나노입자는 SPL12 의 첨가로 UV-Visible 영역 내에서 파장의 이동이 관찰되었다. 관찰된 파장의 이동은 라만 스팩트라, 투과전자현미경, 입자크기분포를 통해 단백질-DNA 의 결합을 이루어 유발된 것임을 확인하였다. 첨가되는 단백질 양에 따라 파장이동의 변화를 UV-VIS 분광기로 확인 하였으며, 대조군 단백질로 BSA(Bovine serum albumin)을 사용하여 단백질-DNA 간의 선택적 결합이 이루어진다는 것을 UV-Vis 분광기, 라만 스팩트라, 투과전자현미경 및 입자크기분포 분석을 통해 증명하였다.

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Hollow Metal-Organic Frameworks via Using Metal-Organic Polyhedra as Crystalline Sacrificial Hard Templates

김혜현 나명수*

울산과학기술대학교(UNIST) 화학과

While the Zn-MOF [$Zn_{24}(mip)_{24}(dabco)_6(H_2O)_{12}$] (where H_2mip = 5-methylisophthalic acid; dabco = 1,4-diazabicyclo[2.2.2.]octane) based on the cuboctahedral MOP [$Zn_{24}(mip)_{24}(H_2O)_{12}$], as a 12-connected node could only be prepared via one-pot solvothermal reaction, similar attempts to prepare isoreticular Cu-MOFs via conventional one-pot synthetic approach in presence of 5-hydroxylisophthalic acid (H_2hip) and various linkers between the potential MOP intermediate, [$Cu_{24}(hip)_{24}(H_2O)_{12}$], only produced metal-organic polyhedron (MOP), [$Cu_{24}(hip)_{24}(DMF)_{12}(H_2O)_{12}$]. A series of isostructural and isoreticular Cu-MOFs, [$Cu_{24}(hip)_{24}(L)_6(H_2O)_{12}$] (where L = dabco; pz = pyrazine; bipy = 4,4'-bipyridine), could only be obtained via stepwise reactions using the cuboctahedral MOP, [$Cu_{24}(hip)_{24}(DMF)_{12}(H_2O)_{12}$], as a molecular precursor. Especially, single crystalline hollow metal-organic frameworks (MOFs) with cavity dimensions in the order of several micrometers and hundreds of micrometers were prepared using a MOP single crystal as a sacrificial hard template.

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발표코드: **INOR.P-206**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

미토콘드리아를 타겟으로 하는 트리페닐포스페이트 유도체의 합성과 형광 특성 연구

백영은 정성호 정종화*

경상대학교 화학과

본 연구에서는 미토콘드리아를 타겟으로 하는 트리페닐포스페이트와 형광 유도체인 쿠마린을 도입한 화합물 1 을 합성하였다. 화합물 1 을 PH=7 에서 적당한 열을 가하여 마이셀을 제조하였다. 마이셀의 크기는 입도분석기와 SEM 을 이용하여 분석하였다. 그 결과 대략 50~200 nm 정도의 구형 모양을 가지고 있었다. 그리고 마이셀의 형광 특성을 형광분석기로 연구하였다.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **INOR.P-207**

발표분야: 무기화학

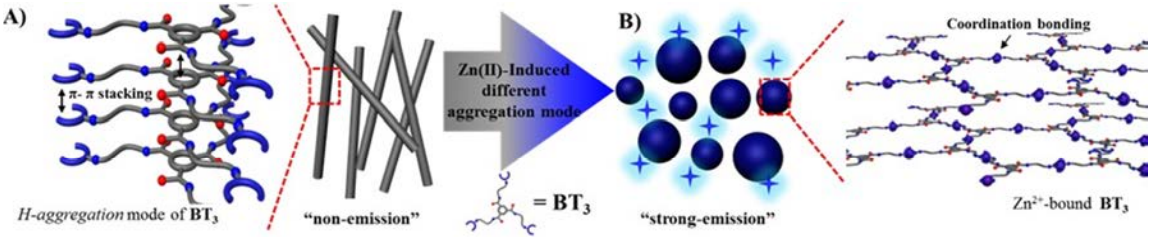
발표종류: 포스터, 발표일시: 수 16:00~19:00

A turn-on fluorogenic Zn (II) chemoprobe based on a terpyridine derivative with aggregation-induced emission (AIE) effects through nanofiber aggregation into spherical aggregates

정성호 권기영 정종화*

경상대학교 화학과

The self-assembly of terpyridine-based ligand (BT_3) in a DMSO/water solvent mixture (1:99 v/v) with a high content of water formed a nanofibrillar structure and showed a non-emissive process, which resulted due to the π-π?stacking between the terpyridine groups of BT_3 (ACQ). On the other hand, the self-assembly of the terpyridine-based ligand exhibited a strong emission in the presence of Zn^{2+} due to the formation of coordination bonds between the terpyridine moieties and the Zn^{2+} by aggregation-induced emission effect (AIE). The morphology of this aggregate represented a spherical structure (Zn^{2+}-bound BT_3).



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **INOR.P-208**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermochromic Luminescent Properties of Copper(I) Coordination Polymers Based on Dithioether Ligands with Pyromellitic Diimide

강기행 전영은 조성화 이상진 김태호* 김진은*

경상대학교 화학과

Recently, we have explored coordination polymers based on dithioether ligands and $(CuI)_x$. As an extension of our efforts to investigate Cu(I) coordinaion polymers of dithioether ligands, N,N'-bis[2-(*tert*-butylthio)ethyl]pyromellitic diimide, (L^1), N,N'-bis[2-(cyclohexylthio)ethyl]pyromellitic diimide, (L^2) were synthesized. Three Cu(I) coordination polymers 1-3 based on the ligands were prepared by self-assembly reaction between CuI and L^1, L^2. Structural and photophysical studies of CPs 1-3 in solid state are reported. CPs 1-3 are composed of cubane Cu_4I_4 cluster nodes, emitting red-orange light under UV-irradition. The shift of the emission color of CPs 1-3 in comparison with the yellow color of other Cu_4I_4 complexes is attributed to halogen- π interactions.

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

Reversible Transformation between Cubane and Stairstep Cu_4I_4 Clusters Using Heat or Solvent Vapor

조성화 이상진 전영은 강기행 김태호* 김진은*

경상대학교 화학과

The controlled self-assembly of CuI and an asymmetric ligand with mixed N/S donors, 2-(*tert*-butylthio)-*N*-(pyridin-3-yl)acetamide (**L**), afforded three CuI coordination polymers (CPs), $[Cu_4I_4L_2(MeCN)_2]n$ (**1**), $[Cu_4I_4L_2]n$ (**2**), and $\{[Cu_4I_4L_2]\cdot MeOH\}n$ (**3**). X-ray analyses showed that CPs **1**-**3** are supramolecular isomers with one-, two-, and three-dimensional structures, respectively. CP **1** adopts a stairstep Cu_4I_4 cluster, whereas CPs **2** and **3** are composed of cubane-like Cu_4I_4 clusters. Crystal-to-crystal transformations of **1** to **2** and **3** showed reversible transformations between different Cu_4I_4 clusters using heat or solvent (acetonitrile or methanol) vapor. CP **2** was reversibly transformed to **3** by the addition of methanol and heat. Therefore, the transformations between supramolecular isomers **1**, **2**, and **3** are completely reversible.

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발표코드: **INOR.P-210**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] Immobilization of a Benzothiazole-Based Receptor on Filter Paper and on Silica Nanoparticles

이진혁 이지하 정종화*

경상대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **INOR.P-211**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Crystal Transformations of Cu(I) Coordination Polymers with an N/S Donor Ligand: Novel 1D Triple Stranded Ladder Structure, Luminescence Solvatochromism and Thermochromism by Influence of Intermolecular Interactions or Heat

전영은 조성화 이상진 강기행 김태호* 김진은*

경상대학교 화학과

Four copper(I) coordination polymers, $\{[Cu_4I_4L_2]\cdot H_2O\}_n$ (1), $\{[Cu_4I_4L_2]\cdot 2CH_3CN\}_n$ (2), and $\{[Cu_4I_4L_2]\}_n$ (polymorphs 3 and 4) with 2-(2-benzylthio)ethyl)pyrazine (L), have been prepared by self-assembly reaction between CuI and L. Four coordination polymers 1-4 show supramolecular isomerism by solvent molecules. Compounds 1-3 interconnected by stair-step Cu_4I_4 units are 1D looped chain structures. Remarkably, the crystal structure of CP 4 is 1D triple stranded ladder composed of 1D zigzag chain $(CuI)_n$ and stair-step $(Cu_2I_2)_n$ polymer units. The color of CP 1 changes from red at 298K to yellow at 77K and the color of CP 2 changes from orange at 298K to yellow at 77K. In addition, crystal transformation between 1-4 occurred reversibly by removal of solvent molecular or addition of solvents. The results of our investigation including synthesis, structural characterization, thermal and luminescent properties of four new Cu(I) coordination polymers are presented.

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발표코드: **INOR.P-212**
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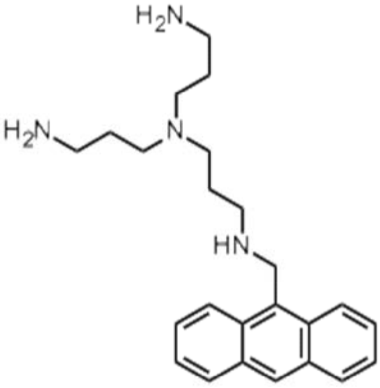
발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of the Phosphate in hydrogel

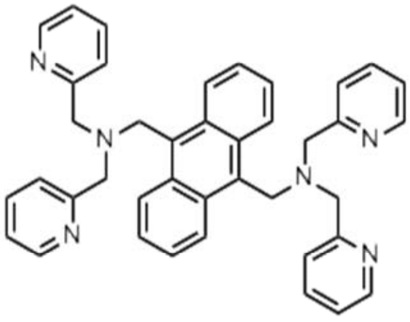
박재현 이지하 신수비 정종화*

경상대학교 화학과

본 연구에서는 인을 포함하는 음이온을 센싱할 수 있는 안트라센유도체 1 과 2 를 합성하였다. 인을 포함하는 음이온 수용체를 하이드로 젤에 1 또는 2 을 내포시켜 특정 음이온에 대한 센싱연구를 수행하였다. photoinduced electron transfer (PET)효과에 의해서 형광특성이 매우 약했다 반면에 특정음이온이 (ATP, ADP, AMP 등)이 첨가시 하이드로젤 강한 형광 특성을 나타내었다. 따라서 화합물 1 또는 2 가 내포되어 있는 하이드로젤은 인을 포함하는 음이온 센싱 물질로 활용이 가능할 것으로 예상된다. 본 심포지움에서는 하이드로 젤을 이온 센싱에 대한 연구결과를 소개한다.



1



2

일시: 2014년 10월 15~17일(수~금) 3일간
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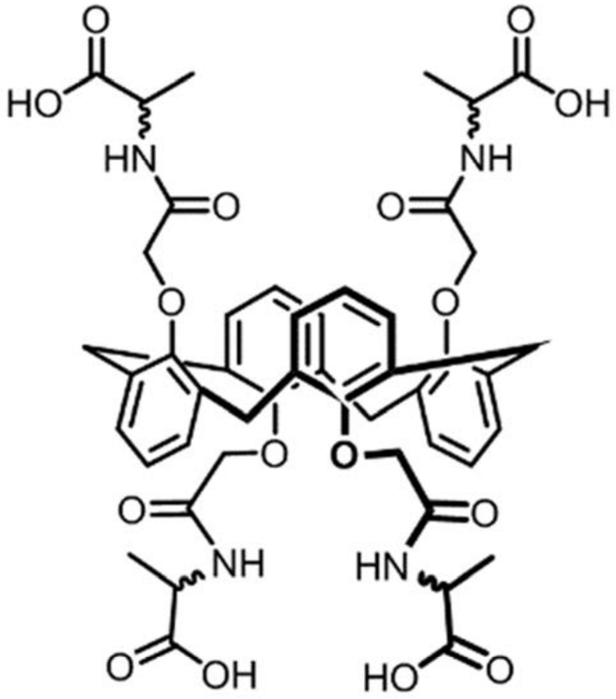
발표코드: **INOR.P-213**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Roles of both amines and acid in supramolecular hydrogel formation of tetracarboxylic acids-appended calix[4]arene gelator

최희경 이지하 정성호 정보라 정종화*

경상대학교 화학과

A tetracarboxylic acids-appended calix[4]arene derivative (1) showed completely different self-assembly behaviors depending upon the sequence of addition of amines and acid. The number of amino group involved in amines and concentration of amines played an important role in supramolecular hydrogel formation.



1

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **INOR.P-214**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Green luminescent Ir(III) complexes with sulfur containing ancillary ligands

이상진 김태호* 김진은*

경상대학교 화학과

In recent years, iridium(III) complexes have been studied intensively due to their wide applications in OLEDs, biosensors, oxygen sensitizers etc. In general, there are two major kinds of iridium(III) complexes according to the category of ligands bound to Ir center: homoleptic $Ir(C^{\wedge}N)_3$ and heteroleptic $Ir(C^{\wedge}N)2(L)$ complexes ($C^{\wedge}N$ denotes a cyclometalating ligand and L denotes an ancillary ligand). The cyclometalating ligands such as 2-phenylpyridine and its derivatives are used frequently while the most popular ancillary ligands include picolinate, acetylacetonate, and others. However, there is no study of bis-cyclometalated iridium(III) complexes with sulfur containing ancillary ligands, (L^1= 2-methylthioacetate and L^2= 2-benzylthioacetate). Green-emitting Iridium(III) complexes$[(ppy)_2IrL^1]$(1) and $[(ppy)_2IrL^2]$(2) were synthesized from bis 2-phenylpyridine Ir(III) complex $[(ppy)_2IrCl]_2$ and the ancillary ligands. The results of our investigation including syntheses, structural characterization, thermal and luminescent properties of two new Ir(III) complexes are presented.

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

De novo Synthesis of Metal-Organic Frameworks based on Terbium(Ⅱ) via Acidic Condition Control

박정인 정석 김동욱 나명수[*]

울산과학기술대학교(UNIST) 화학과

Various Tb-metal-organic frameworks (MOFs) of different network structures were obtained in the same solvothermal reaction condition but with different amounts of acid. Tb-MOFs, (cation)$_2$[Tb(btec)(formate)] (1), [Tb$_2$(btec)(formate)$_2$(H$_2$O)$_2$] (2) (cation)$_3$[Tb$_6$(Hbtec)$_2$(btec)$_3$(formate)$_3$] (3) (where, H$_4$btec = 1,2,4,5-benzene tetracarboxylic acid) could be prepared via one-pot de novo solvothermal reaction combining terbium(III) nitrate precursor and H4btec in DMF/MeOH mixed solvent. The amount of acid plays an important role in the formation of the network structures because it controls the amount of cation and formate generated in-situ. 3 is very stable in hydroscopic condition. The PXRD pattern of 3 stood in boiling water for 1 day is the same as that of the as-synthesized structure. 3 is even stable in both acidic and basic conditions. The structures, the properties and the potential applications of the Tb-MOFs will be discussed.

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발표코드: **INOR.P-216**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of volatile Cu(II) precursors containing β-ketiminate ligands with bulky alkyl group

원욱경 이익모* 박성진

인하대학교 화학과

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Department of Chemistry, Inha University
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Cu(II) complexes containing substituted β-ketoiminate ligand has been successfully synthesized by using a microwave with moderate yields.

Reactions between $CuCl_2$ and Na[OC(Me)CHC(Me)N(R)] in THF produced brown liquid, which resulted in $Cu[OC(Me)CHC(Me)N(R)]_2$.

Since the copper(II) complexes are paramagnetic, characterization of the complexes has been done by melting point, TGA, MS, and elemental analysis. Iso thermal TG curves have been obtained to check the volatility of the copper precursors and other properties of these compounds will be discussed.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **INOR.P-217**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasound-assisted synthesis of Li_2MnSiO_4 nanoparticles for Li-ion battery

황차환 이경구[1,*] 옥강민[*]

중앙대학교 화학과 [1]군산대학교 화학과

Li_2MnSiO_4 (LMS) has been regarded as a promising cathode material for lithium ion battery because of its higher theoretical capacities (333mAh g^{-1}) and thermal stability compared to lithium metal oxides. However, due to its poor electronic conductivity and slow Li-ion diffusion, particles of LMS are required to be nano-sized and carbon coated. By doing so, high rate capability and discharge capacity can be easily achieved. In this study, ultrasound-assisted reaction was adopted for the synthesis of LMS nanoparticles. The high power sonochemical reaction can induce an effective surface coating on template materials homogenously in a short reaction time. LMS precursors (nanosized-SiO_2/$Mn(OH)_2$/LiCOOH/carbon source) were prepared under ultrasound field for 40~60 min. The precursors were calcined at 700 ^{o}C for 12h under Ar atmosphere to obtain carbon coated crystallites. The synthesized LMS/C nanoparticles (20~50nm) crystallized in orthorhombic space group, $Pmn2_1$. The first cycle discharge capacity of synthesized LMS/C was about 200 mAh g^{-1} in the voltage range of 4.7~2 V and the current density was 16.5 mAh g^{-1}.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Correlation between structural evolution and spectral change during Galvanic replacement reaction at a single-particle level

박영찬 송현준*

한국과학기술원(KAIST) 화학과

In recent years, Galvanic replacement reaction is widely used to synthesize complex hollow structures, which are expected to apply for various optical applications due to their unique structures and optical properties. Since the optical properties are dictated by structures, better understanding of the correlation between structure and optical property is required. To this aim, we have combined transmission electron microscopy, single-particle dark-field spectroscopy, and FDTD calculations to investigate structural evolution and spectral change in the course of the reaction. Galvanic replacement reaction is found to proceed continuously as a function of time, but the structural change does not directly reflected in spectral shift because gold deposition on the surface has a great effect on the peak position while the hole formation exhibits little influence. Based on these observations, details of hollow formation mechanism will be proposed in this presentation.Such integrative monitoring techniques can potentially be applied to study various kinds of chemical reactions at a single-particle level.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-step construction of a covalently alkylamine-tethered metal-organic framework for enhanced CO_2 binding affinity

김윤경 김태경[1] 문도현[2] 문회리[*]

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) 친환경에너지공학부 [2]포항가속기연구소 빔라인부

To enhance CO_2 capture capabilities of metal-organic frameworks (MOFs), amine functionalization of those pore surfaces has been actively studied. In general, amine-functionalized MOFs have been synthesized via post-synthetic modifications. Herein we introduce the one-step construction method of a MOF, $\{[(NiL_{ethylamine})(BPDC)]\cdot 3H_2O\}$ ($MOF_{NH2\text{-}as}$, $BPDC^{2-}$ = biphenyldicarboxylate), in which alkylamine groups are covalently tethered. To see the effect of amine group on CO_2 adsorption, an isostructural but different pore-functionalized MOF was also synthesized as $\{[(NiL_{propyl})(BPDC)]\cdot 2.5H_2O\}$ ($MOF_{CH3\text{-}as}$). Single crystal X-ray diffraction data showed that $MOF_{NH2\text{-}as}$ and $MOF_{CH3\text{-}as}$ have honeycomb-like 1D channels and the interior of MOFs is covalently decorated with ethylamine and propyl group, respectively. Unlike the CO_2 adsorption behavior of MOF_{CH3}, which shows physisorbing properties, MOF_{NH2} showed the chemical interaction with CO_2 molecules, as evidenced by large hysteresis. Due to narrow channels, upon CO_2 uptake the pores of MOF_{NH2} are blocked. Therefore, grinding MOF_{NH2} crystals significantly enhanced CO_2 sorption performances by increasing external surface area. Importantly, the chemisorbed CO_2 molecules in MOF_{NH2} can be regenerated under mild temperature, 100^oC.

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발표분야: 무기화학
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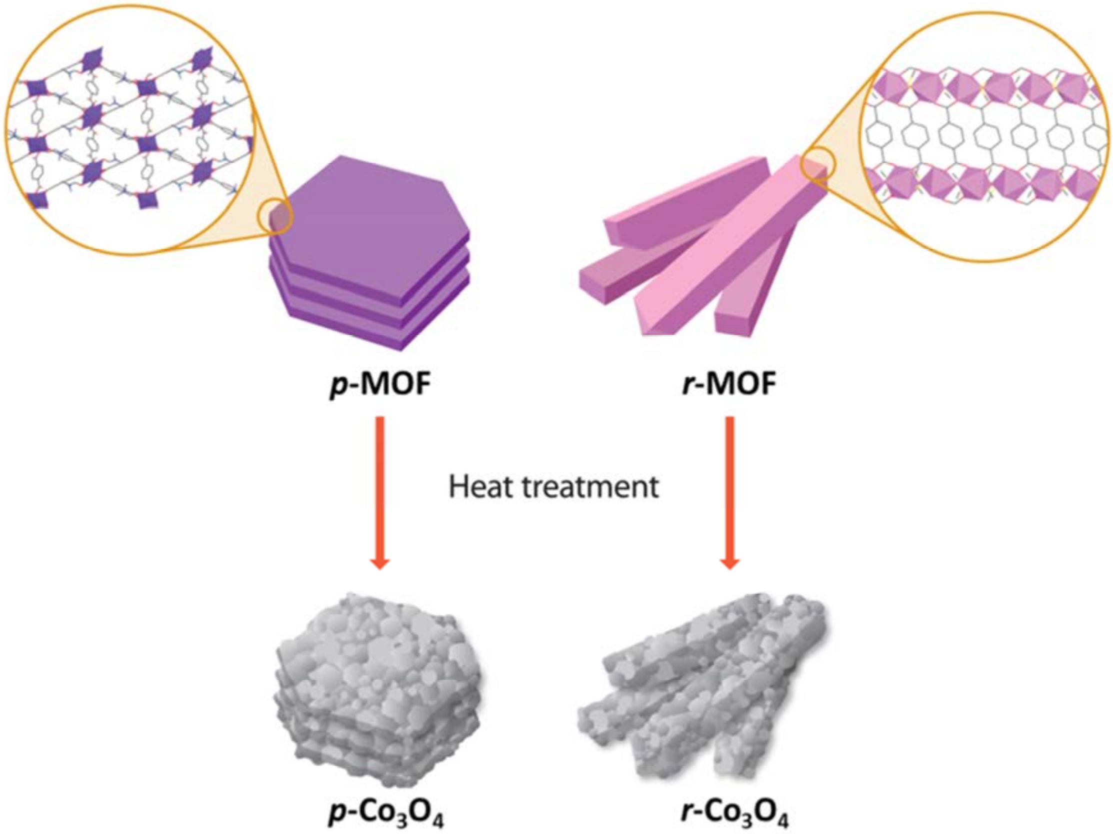
Preparation of Co_3O_4 electrode materials with different microstructures via pseudomorphic conversion of Co-based metal-organic frameworks

이경주 김태경[1] 문회리[*]

울산과학기술대학교(UNIST) 화학과 [1]울산과학기술대학교(UNIST) 친환경에너지공학부

To develop high-performance nanostructured metal oxide electrodes, it is important to understand their structural effects on electrochemical performances. Thus, the preparation of metal oxide materials that have well-tailored nanostructures is crucial for studies. However, while synthetic strategies to control the size of metal oxide nanoparticles are well-developed, the control of the higher level structures, namely microstructure, is not very well established. Herein, we present the synthesis of the two kinds of Co_3O_4 nanomaterials through pseudomorphic conversion so that the macroscopic morphologies of parent MOFs, such as plate-like and rod-like shape, are well-maintained.[1] Both Co_3O_4 nanomaterials are composed of almost identical 10 nm-sized primary nanocrystals but with different nanoporous secondary structures and macroscopic morphologies such as plate and rod shapes. These Co_3O_4 nanomaterials were utilized as an electrode in lithium ion batteries (LIBs), and their electrochemical properties were comparatively investigated. It was revealed that the different cyclability and rate capability are attributed to their different microstructures. The pseudo-monolithic integration of primary and secondary structures at higher level was the governing factor, which determined the electrochemical performances of the Co_3O_4 electrode.

1.Lee, K. J.; Kim, T.-H.; Kim, T. K.; Lee, J. H.; Song, H.-K. and Moon, H. R., *J. Mater. Chem. A* 2014, 2, 14393.


p-MOF
r-MOF
Heat treatment
p-Co_3O_4
r-Co_3O_4

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Single Redox Shuttle for Electrochemical Photovoltaics: Reveal-ing Unrevealed Photoelectrochemistry via a Ruthenium Complex-Based Electrolyte

김정윤 손호진[1] 정낙천[*]

대구경북과학기술원(DGIST) 신물질과학과 [1]고려대학교 소재화학과

Dye-sensitized solar cells (DSCs), distinctively those comprising of molecular chromophores and redox shuttles, have shown potential promise as a type of electrochemical photovoltaic devices. Ruthenium complexes, with chemical modification to various types, have proven their excellence as chromophores in the DSCs, but never been considered as redox shuttle. Here we report a most primitive version of ruthenium complex, $Ru(bpy)_3^{2+}$. In contrast to that all redox shuttles, which have been discovered or developed so far, are conspicuously the shape coupled with the forms mixing both reduced and oxidized ones, this ruthenium-based shuttle performs high photovoltages although it operates solely without an oxidized pair. Exploiting this new “single shuttle”, we find unexpected, interesting features: (i) abnormal shape of IPCE curves; (ii) gigantic IPCEs relative to photocurrent density; (iii) discordance between the photocurrent density and the overlap integral of IPCE; (iv) non-linearity of photocurrent density change versus light intensity change; (v) relative higher efficiency under lower power illumination. Especially from the last one, we caught a hint that this type of cells is better to use in modest light or in-door light condition. In fact, the efficiency was even 5.8-fold enhanced by reducing illumination power. We believe these new findings will prove transferable and thereby, advancing developing new redox shuttles as well as yielding high performance devices.

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Chemical Vapor Deposition Growth of Graphene Domains on Copper with Liquid Carbon Source

강청 이진석*

숙명여자대학교 화학과

Graphene is a two-dimensional carbon material whose structure is one-atom-thick planar sheet of sp2-bonded carbon atoms densely packed in a honeycomb crystal lattice. It has drawn significant attention with its distinguished structural and electrical properties. Extremely high mobility and a tunable band gap make graphene potentially useful for innovative approaches to electronics. Although mechanical exfoliation of graphite and decomposition of SiC surfaces upon thermal treatment have been the main method for graphene, they have some limitations in quality and scalability of as-produced graphene films. Solution-phase and solvothermal syntheses of graphene achieved a major improvement for processing, however for device fabrication, a reproducible method such as chemical vapor deposition (CVD) growth yielding high quality films of controlled thickness is required. In this research, we synthesized rectangular graphene flakes on Cu foils by CVD method using liquid carbon source and controlled its coverage, density and the size of graphene domains by changing reaction parameters. It is important to control these parameters of graphene growth during synthesis in order to achieve tunable properties and optimized device performance.

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Molecular Layer Deposition of Organic-Inorganic Alucone Films using Trimethylaluminum and Alkanediols with Different Alkyl Chains

박이슬 조보람[1] 이진석*

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Molecular layer deposition (MLD) is sequential, self-limiting surface reaction to form conformal and ultrathin polymer film. This technique typically uses bifunctional precursors for stepwise sequential surface reaction and entirely organic polymer films. Also, in comparison with solution-based technique, because MLD is vapor-phase deposition based on ALD, it allows epitaxial growth of molecular layer on substrate and is especially good for surface reaction or coating of nanostructure such as nanopore, nanochannel, nanwire array and so on.We fabricated organic-inorganic nanohybrid thin films using trimethylaluminum and alkanediols by a sequential, self-limiting surface chemistry process known as molecular layer deposition (MLD). Using ellipsometry, we confirmed linear growth of the films versus number of MLD cycles at all same temperature. But this tendency of linear growth of the films versus number of MLD cycles is confirmed to reduce with increasing of the number of alkyl chains. Atomic force microscopy was also used to check the roughness of the films that showed the roughness increased with increasing of the number of alkyl chains. Contrary, the film density decreases with increasing of the number of alkyl chains.

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Stabilization of Metal-Organic Framework *via* Linking Additional Ligands between the Metal-Cluster Nodes

원소미 김동욱 나명수*

울산과학기술대학교(UNIST) 화학과

The disadvantage of the MOF with 4-c zinc paddle wheel secondary building unit (SBU) is its poor stability in ambient condition. To increase the stability of the Zn-MOF in ambient condition, an additional ditopic linker, 4,4’-bipyridine, was introduced between the zinc paddle wheel SBUs of the pre-existing Zn-MOF structure [$Zn_{24}L_8(H_2O)_{24}$] (where, H_6L=5,5’,5’’-[1,3,5-benzenetriyltris(carbonylimino)tris-1,3-benzene-dicarboxylic acid) *via* one-pot solvothermal reaction. Furthermore, it would be possible to control the pore sizes by controlling the position and type of the additional linkers attached inside the cage.

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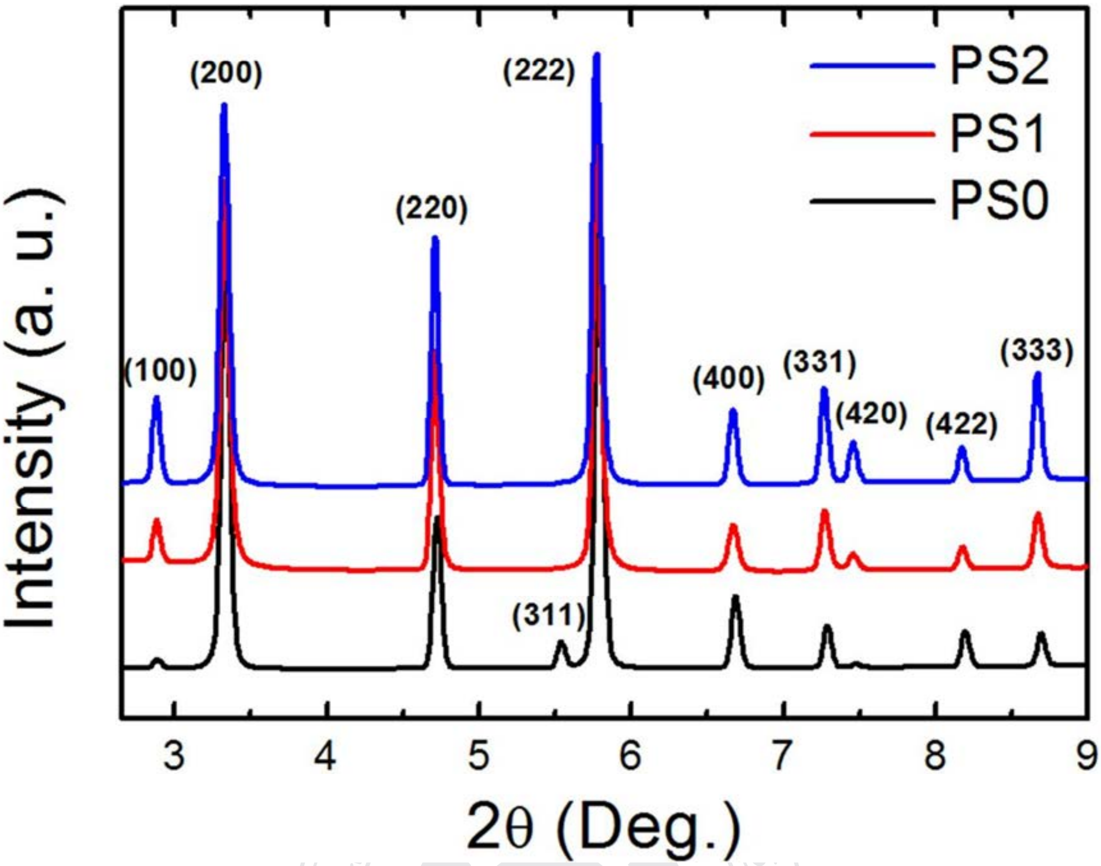
Effects of solvent on infiltrated LiBH$_4$ into HKUST-1: in situ x-ray diffraction study

조인화 임대운 이희주 김태민[1] 김성준[2] 최용남*

한국원자력연구원 중성자과학연구부 [1]숭실대학교 [2]가천대학교 글로벌캠퍼스 나노화학과

One fancy way of nano-confining LiBH$_4$ is to infiltrate it into nanoporous materials such as HKUST-1, one of metal organic framework. By confining LiBH$_4$ monomers into its cage with ~ 15 A in diameters, remarkable lowering of dehydrogenation temperature (110C) has been reported [1]. We change the solvent for the infiltration from diethyl ether to tetrahydrofuran in order to investigate the effect of solvents on the infiltration of LiBH$_4$ and dehydrogenation process since THF has high polarity (THF 4.0, Ethyl ether 2.8). In situ x-ray diffraction patterns at high temperatures shows adsorbed molecules on Cu^{2+} ions of HKUST-1 frame desorbed from it as temperature rises. In addition, ex situ UV-VIS and in situ FT-IR spectroscopy are used to elucidate how LiBH$_4$ monomer interacts with HKUST-1 during dehydrogenation.[1] Weiwei Sun et al., 40 (2011) 5673, Dalton Trans. Figure 1. X-ray diffraction patterns of samples. PS0 is activated HKUST-1 (black) and PS1 and PS2 are samples of LiBH$_4$ infiltrated into HKUST-1(PS0) by solvent infiltration. Diethyl ether is used as a solvent for PS1 and tetrahydrofuran for PS2.



PS2
PS1
PS0
(100)
(200)
(220)
(222)
(311)
(400)
(331)
(420)
(422)
(333)
Intensity (a. u.)
2θ (Deg.)
3
4
5
6
7
8
9

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synthesis of ZrO2-SiO2 sheets doped WO3 nanoparticles and their electrochemical property

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아주대학교 분자기술학과 [1]아주대학교 응용생명화학공학부

We report on the first synthesis of porous ZrO2-SiO2 sheets doped WO3 nanoparticles for energy storage performance. synthesized samples were characterized by transmission electron microscopy (TEM), powder X-ray diffraction (XRD), atomic force microscopy(AFM), cyclic voltammetry(CV), and Brunauer-Emmett-Teller(BET) methods.porous ZrO2-SiO2 ,as tamplate, sheets were fabricated by graphene oxide. binary composite oxides like ZrO2- SiO2 are important to obtain materials that exhibit chemical, thermal and mechanical stabilities. And WO3 is an attractive electrode materials because of its multiple oxidation states. Therefore, ultrasmall WO3 NPs is synthesized on the porous ZrO2-SiO2 sheets by the impregnation.The synthesized electrode material is approximately 20 nm thick, had 10 nm pores, and had a maximum specific capacitance of 313 F/g at a current density of 1 A/g and a minimum specific capacitance of 160 F/g at a current density of 30 A/g. additionally, over 90% of its initial specific capacitance value was retained after 2500cycle charge- discharge operation.

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Preparation of ansa-metallocenes for production of poly(α-olefin)

어성찬 이분열*

아주대학교 분자과학기술학과

Recently, the application of metallocene catalysts has been expanded to the production of poly(α-olefin) (PAO) lubricants or fuels. α-Olefins are produced through the selective oligomerization of ethylene. ExxonMobil has announced the construction of a metallocene catalyst-based PAO plant for the production of lubricant base stocks. PAO is typically produced on industrial scale through the cationic oligomerization of α-olefins such as 1-decene. The cationic initiator produces a mixture of branched oligomers with a distribution that peaks around a trimer. After hydrogenation, these products become outstanding lubricants with excellent viscosity indices, low pour points, and high oxidative stabilities. In the preparation of PAO lubricants using metallocene catalysts, controlling the degree of polymerization is a key factor, which is dependent on the catalyst structure. α-Olefin polymerizations have been previously investigated using various metallocene, half-metallocene and post-metallocene catalysts, which typically aim to produce high-molecular-weight polymers. Most of the experiments in these studies generated PAO with Mw > 10 000, which are not useful as lubricant base stocks. α-Olefin polymerizations to produce lubricant base stocks have been disclosed in patents. It was reported that the unbridged zirconocene (η5-RC5H4)2ZrCl2 (R = H, Me, iPr, nBu) primarily produced dimers (～50%) in the polymerization of 1-decene at 110 °C. The isolated dimer was further oligomerized with 1-decene using a cationic initiator for use as a lubricant base stock. A doubly bridged ansa-metallocene [(1,1′-Me2Si)(2,2′-Me2Si)- (η5-C5H3)ZrCl2] was also disclosed for the preparation of PAO lubricants.

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Synthesis and Characterization of Lanthanide Oxide Precursors for Ln_2O_3 Thin Films

조아라 김창균[1,*] 정덕영 정택모[2] 박보근[1]

성균관대학교 화학과 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학소재연구단

Rare-earth oxide thin films are emerging materials for applications in many different fields such as wear and corrosion-resistant coatings, optoelectronics and high-k materials of microelectronics, due to their high thermal stability, high refractive indices(1.91-1.98) and high dielectric constants, respectively. Especially, thin film growth of rare-earth oxides by MOCVD and ALD have been of great importance. However, suitable precursors are little known except Ln(β-diketonate)$_3$, Ln(Cp)$_3$, and Ln(mmp)$_3$. Herein we report the synthesis and characterization of Ln(tmma)$_3$, (Ln = Dy , Yb) , (tmma = N,N,N',N' -tetramethylmalonamide) compounds.

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Photoactivated NO-releasing Ru(ebpp)(NO) Complexes : Its Derivatives and Physical Properties

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경북대학교 화학과 [1]부산대학교 화학과

Nitric oxide plays important roles in a wide variety of physiological processes, including neurotransmission, immune response, blood pressure control, and inhibition of tumor growth. For the purpose of controlling the physiological processes, compounds that selectively release nitric oxide have attracted considerable interest. Among them, nitrosyl ruthenium complexes have been proposed as attractive photodynamic therapeutic agents in biomedicine and in tumor treatment. This research aims at developing nitrosyl ruthenium complexes which absorb long wavelength visible light to release NO with high quantum yield. Previously, we have developed a new Ru-nitrosyl bis-pyridyl/biscarboxamide compound, [Ru(III)(ebpp)(Cl)(NO)], where H_2ebpp = N,N'-(ethylene di-p-phenylene)bis(pyridine-2-carboxamide) to be tested as a model NO-releasing agent. Here, we present the strategies to develope visible-light sensity NO-releasing Ru complexes with higher quantum yield. We will show the alteration of the ligands, firstly, by substitution on the ligand frames (R=H, 4-CH_3, 4-OCH_3, 5-butyl), and secondly by extent of conjugation (R=1-isoquinoline (1-IQ) and 3-isoquinoline (3-IQ)). In this study, we describe our progress in designing photoactive ruthenium nitrosyls there other evidences of photoactivated NO-releasing and other properties monitored by UV-VIS, EPR, X-ray crystallography and Femtosecond Mid-IR Spectroscopy.

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Development of Efficient Hole-Transporting Materials for Inorganic-Organic Hybrid Perovskite Solar Cells

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고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과

The organometal halide perovskite ($CH_3NH_3PbX_3$) perovskite has used as light harvesters for solar cells. The perovskite-based solar cell has many components, such as substrate, TiO_2, lead halide perovskite, and HTM. Among the perovskite solar cell components, the hole transporting material (HTM) is an important component for efficient inorganic-organic hybrid perovskite solar cells. Here we report the synthesis and characterization of novel HTMs, and their application in inorganic-organic hybrid perovskite-based solar cells.

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Efficient Star-Shaped Hole Transporting Materials with Diphenylethenyl Side Arms for an Efficient Perosvkite Solar Cell

박소진 도광석 최혜주 조현준[1] 이혜정[1] 심장근[2] 김기동[1] 고재중[*]

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

Two symmetrical star-shaped hole transporting material (HTMs), FA-MeOPh and TPA-MeOPh with a fused triphenylamine or triphenylamine core and diphenylethenyl side arms were synthesized. FAMeOPh showed a strong molar absorption coefficient and a red-shifted absorption compared with TPA-MeOPh due to its planar configuration. The power conversion efficiency (PCE) of the perovskite solar cells based on FA-MeOPh and TPA-MeOPh is about 11.86 and 10.79%, in which the efficiency of former is comparable to that (12.75%) of spiro-OMeTAD based cell. The high photocurrent (18.39 mAcm-2) of FA-MeOPh based solar cell relative to TPA-MeOPh based one may be attributable to the enhanced and red-shifted absorption of mp-TiO2/CH3NH3PbI3/FA-MeOPh based cell. In addition, the FA-MeOPh based cell showed a relative stability under light soaking for 250 h. The high efficiency, relative stability, synthetically simple and inexpensive materials as the HTMs hold promise to replace the expensive spiro-OMeTAD.

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Star-shaped hole transporting materials with a triazine unit for efficient perovskite solar cells

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

ye-sensitized solar cells (DSSCs) have been considered a promising alternative to the silicon-based solar cells due to their low-cost production and simple device fabrication. DSSCs using liquid electrolytes of Co^{II}/Co^{III} redox couples have shown efficiencies surpassing 12%. However, the stability issues of the DSSCs devices arise from leakage and evaporation of liquid electrolyte. Many efforts have been made to replace liquid electrolytes with quasi-solid-stateelectrolytes or solid-state hole conductors to alleviate the stability issues. However, the photovoltaic power conversion efficiency of solid-state DSSCs (ssDSSCs) remains significantly below that of liquid electrolyte-based devices. Recently, the organometal halide perovskites ($CH_3NH_3PbX_3$, X = Cl, Br, I) have attracted great attention due to their direct band gap, large optical absorption and high mobility. An impressive photovoltaic performance was achieved over 15% power conversion efficiency using 2,2′,7,7′-tetrakis[*N*,*N*-di(4-methoxyphenyl)amino]-9,9′-spirobifluorene (spiro-OMeTAD) as a hole transporting material (HTM). The most effective HTM for the hybrid solar cells is spiro-OMeTAD, even though another small molecule HTMs such as 3,4-ethylenedioxythiophene-, pyrene-, linear π-conjugated structure, butadiene-, and swivel-cruciform thiophene- based HTMs gave high conversion efficiencies of 10~13%. However, the high synthetic cost of spiro-OMeTAD gives another problem for the commercialization. Therefore, the development of cost-effective HTMs with high efficiency and long stability is very important. We report new types of hole transporting materials with donor-π-acceptor (D-A) systems by incorporating an electron-deficient 1,3,5-triazine core and an electron-rich diphenylamino unit.

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Synthesis, Characterization, and Reactivities of Mononuclear Cobalt(III)-Hydroperoxo Complex

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대구경북과학기술원(DGIST) 신물질과학

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

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Synthesis and Structure of New 1D-chain Cu Complex

KhanMohammadSherjeelJaved **shuranjan sarkar** 이주은 조장훈 이홍인*

경북대학교 화학과

Tetrathiafulvalene (TTF) and its derivatives are renowned organic π donors which have been largely studied for distinct applications, in particular, in the area of conducting organic materials including intermolecular charge-transfer interactions with several π -accepting molecules (A). An array of mono- or polydentate coordinating functional groups has been adhered to the TTF moiety and the interrelated metal complexes have been divulged. Tetrathiafulvalene (TTF) has proven to be an excellent electron donor in the preparation of highly conductive charge transfer compounds. The structural and electronic properties of TTF are considered to be important determinants of electrical-transport properties in crystals of conductive materials. Transition metal complexes are very helpful in the synthesis of charge transfer compounds because of change in their oxidation states by the adaptation of the chemical environments around the metal ions. In this study, we have done the synthesis of the transition metal coordination polymer containing a tetrathiafulvalene (TTF) moiety substituted with a dicarboxylic group of the formula [CuL] BCDT-TTF (L = 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hezaazacyclotetradecane) (BCDT = Bis(4,5-carboxy-1,3-dithiolidene). It has been characterized by various analytical methods.

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Synthesis and characterization of novel indium gallium zinc oxide precursors

오현지 박보근[1] 정택모[2] 김창균[1,*]

한국화학연구원 박막재료연구그룹 [1]한국화학연구원 화학소재연구본부 [2]한국화학연구원 화학소재연구단

In recent years, a variety of solution-processed oxide semiconductors have been studied for oxide-based TFTs. Metal oxide semiconductors such as zinc oxide (ZnO), indium gallium zinc oxide (IGZO), zinc tin oxide (ZTO), and zinc indium tin oxide (ZITO) have been explored using various metal salt precursors and implemented into TFT structures. Heterometallic alkoxides could be excellent precursors to control stoichiometry and lower annealing temperature for multi-metal oxide semiconductors. Herein, we report on the synthesis and characterization of new heterometallic tin-gallium, zinc-gallium, and zinc-indium complexes containing designed functional alkoxide ligand.

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Synthesis and characterization of heteroleptic cobalt complexes

한성호 정택모[1,*] 김창균[2] 박보근[2] 손성욱

성균관대학교 화학과 [1]한국화학연구원 화학소재연구단 [2]한국화학연구원 화학소재연구본부

Cobalt oxide has interesting properties such as high catalytic activity, antiferromagnetism, and electrochromism. Therefore cobalt oxides offer a great potential for their applications in the various fields such as optical gas sensor, catalysts for oxidation reaction, electrochromic devices, high temperature solar selective absorbers, magnetic materials, and negative electrodes for lithium-ion batteries.We have synthesized novel heteroleptic cobalt complexes with simple substitution reactions using cobalt(II) bis(trimethylsilyl)amide as a starting material. All these complexes were characterized by single crystal X-ray analyses, FT-IR and Mass spectroscopic analyses. The studies to prepare cobalt oxide thin films using novel heteroleptic cobalt complexes by various deposition techniques are ongoing.

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Synthesis and Properties of Low Bandgap Star Molecules for Solution Processed Bulk Heterojunction Organic Solar Cells

심장근 도광석[1] 최혜주[1] 박소진[1] 김기동[2] 고재중[1,*]

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

Two symmetrical planar star shaped organic small molecules TPA[DTS-PyBTTh3]3 (1) and DMM-TPA[DTS-PyBTTh3]3 (2) with TPA and fused TPA core donors, respectively and three branched DTS-PyBTTh3 units were synthesized and characterized. These small molecules were used donor materials along with PC71BM acceptor for solution processed bulk heterojunction (BHJ) solar cells. The power conversion efficiency (PCE) of the solar cells based on 1 and 2 are about 2.87% and 3.83%, respectively, when the active layers were processed from chlorobenzene (CB) solvent. The higher PCE of the solar cell based on 1 may be attributed to its low bandgap and broad absorption profile as compared to 2. The PCE of the solution processed BHJ solar cells was improved up to 3.88% and 5.81% for 1 and 2, respectively, when active layers were processed with 0.4% (v/v) 1-chloronaphthalene (CN) as additive in the CB solvent. The enhancement in the PCE was mainly due to the increase in Jsc and FF. The increase in the Jsc and FF may be attributed to the balance charge transport between the electron and hole transport and reduction in the bimolecular recombination, leading to an increase in the PCE.

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Blue Phosphorescent Iridium compounds based on bipyridine ligand

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강원대학교 과학교육과 [1]강원대학교 과학교육학부 [2]강원대학교 일반대학원 화학과 [3]강원대학교 화학과

Two blue phosphorescent Ir(III) compounds with a main fluorine-free bipyridine ligand have been synthesized. These molecules have the general formula of Ir(C?N)2(L?X), where C?N = 2',6'-dimethoxy-4-methyl-2,3'-bipyridine [(MeO)2pypy] and L?X = ancillary ligand, such as acetylacetonate (acac) (1) or 2-picolinate (pic) (2). Thermal, photophysical, and electrochemical properties for 1 and 2 have also been investigated systematically. The two compounds show high thermal stability with decomposition temperatures at ~ 350 °C due to strong and varied intermolecular interactions. A sky-blue emission with moderate phosphorescence quantum efficiency (ΦPL= 0.49~0.54) is observed in the spectral region of 460-470 nm for all compounds, which is attributed to both metal-to-ligand charge transfer (MLCT) and ligand-centered (LC) transition. Compounds 1 and 2 show only ~10 nm red-shifted emission in the fluid state, compared to similar fluorinated iridium counterparts. Multi-layered electroluminescent devices using compounds 1 and 2 as the dopant and 9-(3-(9H-carbazol-9-yl)phenyl)-9H-carbazol-3-yl)diphenylphosphine oxide as a host material have been fabricated. The electroluminescent device of 2 at the doping level of 5 wt% shows the best performance with an external quantum efficiency of 15.3% and the color coordinate of (0.16, 0.28) at a brightness of 100 cd/m2.

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Efficient Perovskite Solar Cells Based on Planar Triphenylamine Hole Conductors

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New type of hole transporting materials (HTMs) incorporated by a planar amine or triphenylamine as a core unit have been prepared. The two amine derivatives were demonstrated to be efficient hole transporting materials in fabricating solid-state organic-inorganic hybrid solar cells. Perovskite-based solar cells with a planar amine derivative gave a short circuit photocurrent density (J_{sc}) of 20.98 mAcm^{-2}, an open circuit voltage (V_{oc}) 0.972 V and a fill factor 0.67, corresponding to an overall conversion efficiency of 13.63%. The photovoltaic performance is comparable to that of the standard spiro-OMeTAD. Moreover, the device showed a good stability under light soaking for 500 h. The high efficiency, excellent stability, synthetically simple and inexpensive materials as the HTMs hold promise to replace the expensive spiro-OMeTAD.

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Solvothermal synthesis of magnesium based metal-organic frameworks and their synthetic time-based property

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울산과학기술대학교(UNIST) 화학과

Several isostructural MOFs, (cat)$[Mg_3(BTC)_3]^{3-}$ (where, cat = cationic species and H_3BTC = 1,3,5-benzenetricarboxylic acid) with different types of counter-cations were prepared via solvothermal method varying reaction time and counter-cations. The cations in the MOFs varied from partially occupied magnesium ion to alkylammonium ion. The existence of these cations altered the intrinsic pore structure and turned out to be distinct from its original structure. Their structural characteristics, PXRD patterns and sorption behaviors will be discussed in the presentation.

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Synthesis of monomeric and dimeric cadmium(II) complexes containing N’-substituted *N*,*N*-di(2-picolyl)amine

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경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The reaction of [$CdBr_2.4H_2O$] with *N*’-substituted N,N-di(2-picolyl)amine ligands such as 1-cyclohexyl-N,N-bis(pyridin-2-ylmethyl)methanamine (L_a), N,N-bis(pyridin-2-ylmethyl)aniline (L_b), 2-methoxy-N,N-bis(pyridin-2-ylmethyl)ethan-1-amine (L_c), and 3-methoxy-N,N-bis(pyridin-2-ylmethyl)propan-1-amine(L_d) has been synthesized and structurally characterized. X-ray crystallographic analysis determined that the 6-coordinate dimeric [$L_aCd(u\text{-}Br)Br]_2$ and [$L_dCd(u\text{-}Br)Br]_2$, and monomeric [$L_cCd(u\text{-}Br)Br]_2$ were distorted octahedral geometry. However, 5-coordinate monomeric [L_bCdBr_2] was square pyramidal geometry. The catalytic activity of [L_bCdBr_2] in the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) at 60°C was higher than that of comparable reference complex [$CdBr_2.4H_2O$].

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Methyl methacrylate polymerization by cobalt(II) complexes with *N*'-alkyl or *N*'-cycloalkyl amine substituted *N,N*-bispyrazole ligands

최성혜 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [L_nCoCl_2] (L_n = L_1 ─ L_5) were synthesized by the reaction between [$CoCl_2.6H_2O$] and the corresponding ligands, N-((1H-pyrazol-1-yl)methyl)-N-(cyclohexylmethyl)(1H-pyrazol-1-yl)methanamine (L_1), N,N-bis((1H-pyrazol-1-yl)methyl)-2,6-diethylbenzenamine (L_2), N,N-bis((1H-pyrazol-1-yl)methyl)cyclohexanamine (L_3), N-((1H-pyrazol-1-yl)methyl)-N-((furan-2-yl)methyl)(1H-pyrazol-1-yl)methanamine (L_4) and N,N-bis((1H-pyrazol-1-yl)methyl)-3-methoxypropan-1-amine (L_5), respectively. The molecular structure of [L_nCoCl_2] (L_n= L_1 and L_2) is best described as a distorted tetrahedral geometry involving non-coordination of the nitrogen atom of the N-cyclohexylmethylamine moiety and the Co(II) metal center, resulting in the formation of an eight-membered chelate ring. However, [L_nCoCl_2] (L_n = L_3 ─ L_5) showed distorted trigonal bipyramidal geometry around metal center, resulting from a coordination of the nitrogen atom of the N-cycloalkyamine moiety and the Co(II) metal center. Among Co(II) complexes, [L_3CoCl_2] showed the highest catalytic activity for the polymerisation of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 8.33 × 104 g PMMA/mol Co?h at 60°C and PMMA syndiotacticity (characterised using 1H NMR spectroscopy) of *ca*. 0.70.

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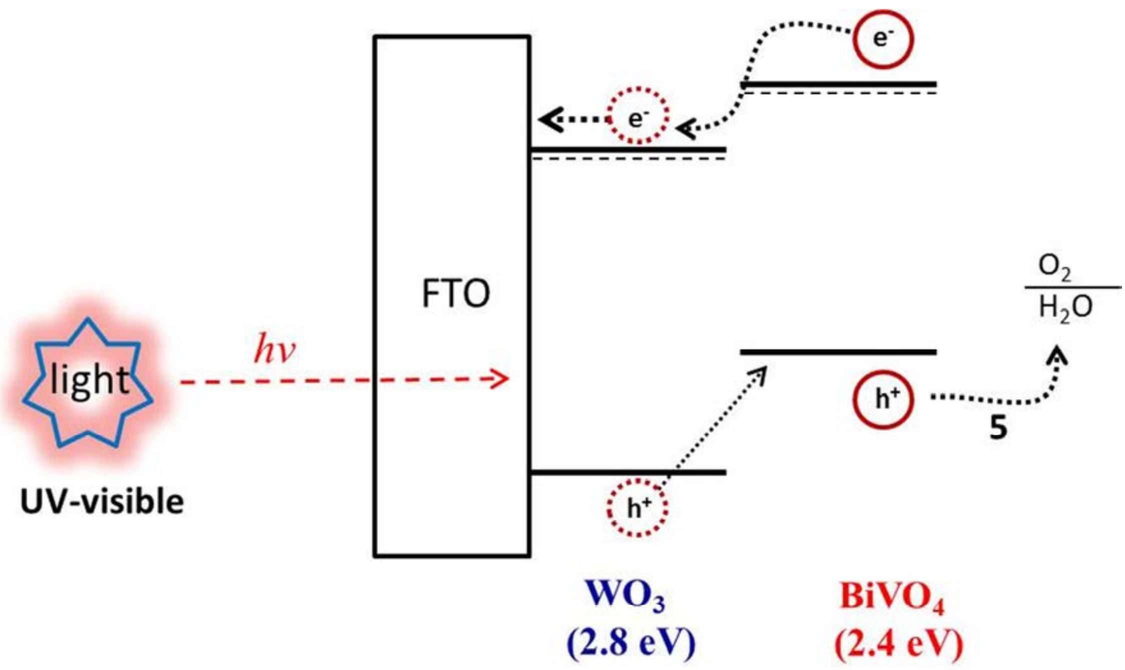
Photoelectrochemical Properties of WO3/BiVO4 Composites

남기민* 주은진

목포대학교 화학과

Photocatalysis is a light-driven chemical process over the surface of a semiconductor that can produce hydrogen from water. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary semiconductor that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through the composite. To investigate the effect of this composite structure, a layered structure was prepared using WO3 (band gap: 2.8 eV) and BiVO4 (band gap: 2.4 eV). The W and Mo co-doped BiVO43 was used instead of bare BiVO4 to exclude doping effect by WO3 bottom layer. This WO3/BiVO4 exhibits enhanced photocurrent beyond a simple additive behavior, which is attributed to enhanced charge separation of BiVO4 on the WO3 electrode.


e-
e-
FTO
O_2
H_2O
light
hv
h+
5
UV-visible
h+
WO_3
(2.8 eV)
$BiVO_4$
(2.4 eV)

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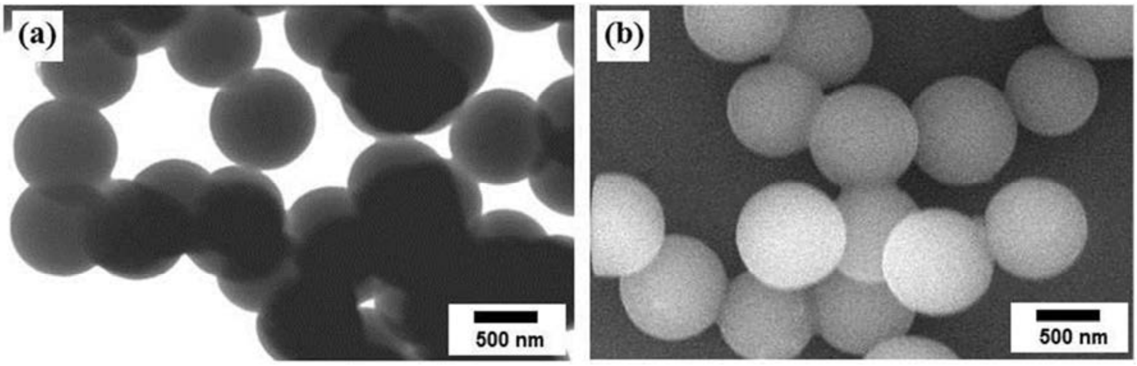
Preparation and Characterization of Colloidal Carbon Spheres and Their Composite Structures

남기민* 오경희

목포대학교 화학과

Hydrothermal carbonization of saccharides has been established with the aim of understanding the mechanism of coal formation. Recently, much attention has been focused on carbonization in the presence of inorganic salts, which gives rise to the formation of hybrid carbon/metal oxide materials. The objective of our investigations is to use these carbon spheres as templates for fabricating metal oxide nanomaterials. The oxygen functional groups at the surface of the carbon sphere improve the hydrophilicity, widening their application to the synthesis of carbon/metal oxide composite materials.The objective of our investigations is to use these carbon spheres as templates for fabricating metal oxide hollow nanomaterials. Carbon spheres with various sizes and shapes were prepared from glucose under hydrothermal conditions to facilitate the synthesis of hollow metal oxides.



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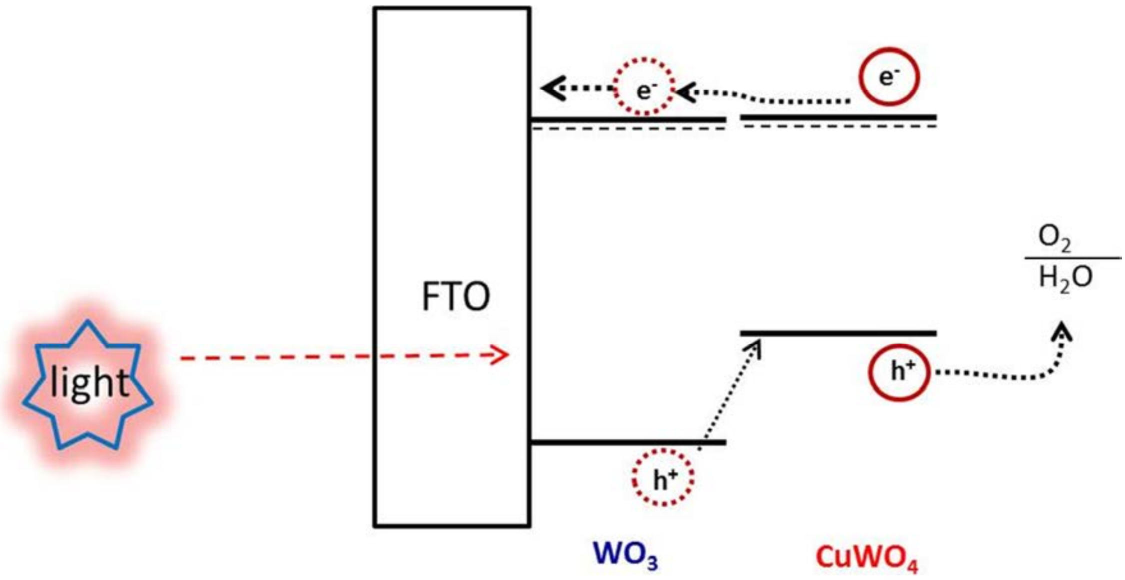
Photoelectrochemical Properties of $WO_3/CuWO_4$ Composites

남기민* <u>신원중</u>

목포대학교 화학과

Collecting and storing solar energy in chemical bonds, as nature accomplishes through photosynthesis, is a highly desirable approach to solving the energy challenge. The most popular strategy is photoelectrochemical (PEC) water splitting to produce hydrogen sustainably. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary semiconductor that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through the composite. A composite structure was prepared using $CuWO_4$ (2.4 eV band gap) and WO_3 (2.8 eV band gap). $CuWO_4$ and WO_3 have the same conduction band potential, but the valence band of WO_3 is more positive than that of $CuWO_4$. The composite shows enhanced photocurrent under full UV-visible illumination. The hole generation at the WO_3 plays an important role in the enhancement of the photocurrent.


FTO
e-
e-
O_2
H_2O
light
h+
h+
WO_3
$CuWO_4$

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Newly synthesized Metal-Organic Frameworks Using Europium and H3BTB

성준모 김동욱 나명수*

울산과학기술대학교(UNIST) 화학과

Lanthanide Metal-Organic Framework which is synthesized by using $Eu(CF_3CO_2)_3$ and 1,3,5-Tris(4-carpoxypenyl)benzene (H_3BTB) ligands has not been reported until now. This newly synthesized structure has $Eu_2(COO)_6$ as secondary building unit (SBU) with distorted octahedral geometry which is combined with six 3-c BTB ligands (four of BTB ligands are in-plane position and rest two of BTB ligands which are in outside of four BTB ligands' plane make structure be 3D network of an 3,6-c net topology). This structure has 1D solvent channels along the crystallographic b-axis direction, where the potential void volume is up to 39.4 % of the total framework. So, I'll introduce newly synthesized Europium MOFs' structure and its property.

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Synthesis of TiO_2 with different pore and particle size for study of diffusion-controlled photocatalytic activity

박우정 박찬호[1] 유원철*

한양대학교 응용화학과 [1]한양대학교 응용화학

TiO_2 is a semiconductor that shows photocatalytic activity. Hence, it has been lots of investigations for increase of photocatalytic efficiency of TiO_2, mainly influenced by crystallinity, portion of specific crystalline plane expose and surface area. However, a diffusion issue in liquid reaction in terms of sufficient interaction between a reactant and surface of a photocatalyst has less been studied. Therefore, a rationally designed photocatalytic material that can be controlled with pore and particle size, key factors for determining the diffusivity of reactant, could provide an insight for diffusion-driven photocatalytic reaction.Here, we has synthesized three-dimentionally ordered mesopore (3DOm) TiO_2 for realizing the aforementioned issue. The *fcc* packed silica spheres (10-40 nm) were used as a template for preparing 3DOm TiO_2. The size of mesopore can be controlled by choosing the size of silica particle and the size of 3DOm TiO_2 can be tuned by controlling reaction conditions. TiO_2 photocatalysts with mesopore sizes of 10-40 nm and particle sizes with 0.3-1 μm have been prepared to study the diffusion controlled photocatalytic decomposition of Methylene Blue.

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Postsynthetic Conversion of a Microporous Metal-Organic Framework to Micro/Meso-Biporous Structures

오민학 김혜현 나명수*

울산과학기술대학교(UNIST) 화학과

A Cu-MOF ($[Cu_{24}(mip)_{24}(dabco)_6(H_2O)_{12}]$ (2), (where H_2mip = 5-methylisophthalic acid; dabco = 1,4-diazabicyclo[2.2.2.]octane) was prepared via conventional one-pot solvothermal reaction using $Cu(II)(NO_3)_2$ and H_2mip as building blocks for the cuboctahedral MOP, $[(Cu_2)_{12}(mip)_{24}(S)_{24}]$ (where S is ligated solvent molecule), and dabco as a linker between the MOPs. Cu-MOF 2 is isostructural to the reported Zn-MOF, $[Zn_4(mip)_4(dabco)(H_2O)_2]$ (1), of a ubt net topology with 5-connected $[Zn_2(COO)_4(N_{dabco})S]$ (where, S is a ligated solvent molecule) cluster as a secondary building unit (SBU)).The structure of 2 was confirmed by powder X-ray diffraction (PXRD). 2 activated via vacuum-drying at ambient temperature shows type I N_2 sorption isotherms having three different sizes of micropores. The microporous 2 could be converted to a series of new micro/meso-biporous MOFs with different distributions of micro/meso-bipores simply controlling the activation temperature. The mesoporosity generation via the partial elimination of dabco linker between the MOPs was confirmed using PXRD, N2 sorption and the pore size analysis.

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Monitoring Fibrilization of Amyloid-β Peptide by EPR Spectroscopy

권송이 김선희*

한국기초과학지원연구원 서울서부센터

The formation of amyloid plaques is known to be a culprit for Alzheimer’s disease. However, the exact mechanism of amyloid fibrilization remains to be explored. Thus, we embark on monitoring the process of amyloid peptide fibrilization by using EPR spectroscopy along with spin probe methods. EPR spectroscopy is a powerful technique for investigating the local environment of paramagnetic species. We performed series of EPR experiments using stable nitroxide radicals such as TEMPO and TEMPOL to examine aggregation process of amyloid peptide (1-40). TEMPO is used for probing the hydrophobic environment and TEMPOL for the hydrophilic environment. During the fibrilization process these two probes behave differently. More detailed EPR data analysis will provide an insightful clue for illuminating the mechanism of amyloid peptide fibrilization at the molecular level.

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Catalytic property between monomeric, dimeric and polymeric copper(II) complexes

안승현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

Simple bidentate ligand L_n (L_1 =2,6-dimethyl-N-(pyridinyl-2-methyl)benzylamine, L_2 = 2,4,6-trimethyl-N-(pyridinyl-2-methyl)benzylamine, L_3 = N-(pyridinyl-2-methyl)benzylamine) have reacted with $[CuCl_2(H_2O)_2]$ to give complexes, $[L_1CuCl_2]$, $[L_2Cu(\mu\text{-}Cl)_2]_2$ and $[L_3CuCl_2]_n$. The copper(II) ion adopts a distorted square-planar geometry in monomeric $[L_1CuCl_2]$, dimeric $[L_2Cu(\mu\text{-}Cl)_2]_2$ and polymeric $[L_3CuCl_2]_n$. These complexes were employed as the catalyst for C-N bond coupling reaction, specifically N-arylation reaction.

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Pulsed EPR Study of Cu-Amyloid β Peptide Relevant to Alzheimer's Disease

김동훈 김선희*

한국기초과학지원연구원 서울서부센터

The amyloid β plaques seem to play a causative role in Alzheimer's disease. Copper ion has been proposed to play an important role in aggregation of the Aβ peptide. Thus, the elucidation of the structural details of Cu-amyloid β is essential in understanding the molecular of amyloid fibrillzation. In addition, a better understanding of the structural details of Cu-amyloid β requires investigations on Cu-hAβ (human-amyloid beta), Cu-mAβ (murine amyloid beta) and isotope labeling Cu-mAβ.we use multi-frequency, multi-technique pulsed EPR spectroscopy such as ENDOR (Electron Nuclear Double Resonance), ESEEM (Electron Spin Echo Envelope Modulation) and HYSCORE (Hyperfine Sublevel Correlation) to characterize Cu-Aβ complexes. These technique have advantage in understanding the mechanism of Cu-amyloid β

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Synthesis and Characterization of Ruthenium Compound for Semiconductor Device

정은애 정택모[1,*] 손성욱[2,*] 박보근 김창균

한국화학연구원 화학소재연구본부 [1]한국화학연구원 화학소재연구단 [2]성균관대학교 화학과

Elemental ruthenium (Ru) has been widely investigated in thin film technology for semiconductor microelectronic devices applications such as an electrode for the high-aspect-ration random access memory (e.g, dynamic RAM, ferroelectric RAM, or magnetic RAM), a gate for metal-oxide semiconductor transistors, and a seed layer for Cu metallization due to a low resistivity (7.1 μΩ?cm in the bulk) and a high work function of 4.7 eV even in the oxidized state.Ru films grown by ALD from a variety of precursors showed excellent properties such as low resistivity of 10-20 ?Ω-㎝ and ~100% step coverage in high-aspect ratio structures. However, previous results exhibited that Ru ALD processes had a relatively long incubation cycle with a lower film growth rate at the initial stages of film deposition. This results in a film with a rough morphology which is unsuitable for conformal film deposition on high aspect-ratio structures.In this presentation, we will talk the synthesis and characterization of novel ruthenium complexes. The ruthenium compounds were easily synthesized by the reaction of ruthenium halide with appropriate organic ligands in protic solvent, and characterized by NMR, elemental analysis, and thermogravimetric analysis. The molecular structures of the complexes were studied by single crystal diffraction.

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Study of Chromium Precursor in Ethylene Trimerization Catalyst

전종엽 박동식 이분열*

아주대학교 분자과학기술학과

The Phillips ethylene trimerization catalyst system prepared by reacting Cr(EH)3 (EH = 2-ethylhexanoate), 2,5-dimethylpyrrole (Me2C4H2NH), Et3Al, and Et2AlCl in an aromatic hydrocarbon solvent was rectified to a congener composed of a new chromium precursor (EH)2CrOH, (Me2C4H2N)AlEt2, and Et3Al?ClAlEt2. Reaction of CrCl3 with 3 equiv Na(EH) in water did not generate Cr(EH)3, but unexpectedly produced the new chromium precursor (EH)2CrOH. In comparison with the erratic catalytic performance of the original Phillips system due to ill-defined nature of the Cr(EH)3 source, the rectified system exhibited consistently high activity. Solution structure of (EH)2CrOH was inferred to be an adamantane skeleton composed of four (EH)2CrOH units and two water molecules (6) based on the cryoscopy measurement of the molecular weight and the revealed crystal structure of a side product obtained from the catalyst solution: a tetranuclear chromium(III) cluster (5) coordinated by three ?3-CH2 , one ?2-CH3, two ?2-OH, and three (?5-Me2C4H2N)AlMe2Cl ligands. Reaction of (EH)2CrOH with Me2AlCl in benzene afforded precipitates of MeCrCl2, the structure of which was revealed to be a THF adduct: MeCrCl2(THF)3. Reaction of (EH)2CrOH with (Me2C4H2N)AlMe2?OEt2 afforded the dimeric Cr(II)-complex (3) coordinated by (?5-Me2C4H2N)AlMe2(NC4H2Me2) and ?2-?1:?2-Me2C4H2N ligands, which provided highly active species when activated with Et3Al?ClAlEt2, indicating that 3 was a key intermediate in the Phillips catalyst preparation.

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Photocatalytic Hydrogen Production from Formate by Rh Complexes and Pt Nanoparticles: Mechanistic Study

김진홍* 김수진 이가예

이화여자대학교 화학·나노과학과

Carbon dioxide has been recently proposed as one of practical hydrogen storage materials. The selective photocatalytic reduction of CO2 to hydrogenated products containing a carbon has been the subject of considerable attention over the ages as a means for a carbon capture and light energy storage strategy. Various molecular metal complexes based on Ru, Rh, Ni, Fe, Mo, Ti, and Ir have demonstrated to hydrogenate carbon dioxide to formic acid. Most catalysts showing a high turnover frequency for CO2 reduction was used under supercritical conditions due to the solubility problem of carbon dioxide. Only a few molecular metal catalysts were used in water. Although most of transition metal hydride species proposed in their mechanisms were unstable, an isolated Ru-hydride species was reported for the reduction of CO2. In that study, the Ru-H bond was inserted by CO2 to produce formate. On the other hand, the decomposition of formic acid/formate in the presence of homogeneous metal catalysts has also been studied to produce hydrogen with carbon dioxide back. Although the decomposition of formic acid using molecular metal complexes has been poorly studied previously, several reports in this area have been published recently. Most studies with molecular metal catalysts reported the non-photochemical decomposition of formic acid, and often use thermal energy to achieve high conversion rates and yields. However, examples of photochemical systems with such metal complexes are rare in the decomposition studies of formic acid/formate. More studies of photochemical systems containing molecular metal catalysts for the HCOOH decomposition are required to understand their photocatalytic mechanisms and develop efficient catalytic systems utilizing one of the major sources of hydrogen.

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Mechanochemically induced structural transformation in [(3,6-dimethoxy-1,2,4,5-tetrazine)silver(I)]X (X= CF_3SO_3, ClO_4)

이준형 강필재 강혜지 최문근*

연세대학교 화학과

Silver(I) coordination polymers bearing 3,6-dimethoxy-1,2,4,5-tetrazine (dmotz), [Ag(dmotz)]X (X= CF_3SO_3, ClO_4), are synthesized via mechanochemical reaction. The structure of Ag(I) complexes were analyzed by single crystal X-ray diffraction and powder X-ray diffraction (PXRD) studies. When the counter anion is CF_3SO_3, the silver complex is one-dimensional linear structure. However the counter anion is ClO_4, the silver complex is two-dimensional network structure are shown below.The structural transformation of [Ag(dmotz)](CF_3SO_3) has been observed by mechanochemical anion exchange to [Ag(dmotz)](ClO_4). The reverse mechanochemical reaction has not been observed. The interesting mechanochemical structural transformation will be presented and discussed.

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Tailoring of the Physicochemical Properties of Graphene Nanosheet and Its Restacked Film via Controlled Reduction of Graphene Oxide Precursor

조윤경 김인영[1] 김수진 이영미 황성주[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

By controlled reduction of graphene oxide (G-O) precursor, we develop an efficient way of tailoring the physicochemical properties of reduced graphene oxide (rG-O) and its freestanding film. Tuning the reduction time is found remarkably effective in controlling the relative concentrations of epoxy, ether, and carboxylic acid groups, and the electrical conductivity of the rG-O. On the basis of a vacuum-assisted filtration method, the elastic freestanding rG-O films can be fabricated with all the present colloidal suspension of rG-O nanosheets having different degree of reduction. The surface morphology and crystal structures of the obtained films are tailorable with the change of reduction condition. Also, these rG-O films do not show a monotonous increase of electrical conductivity with elongation of reduction time. The electrical conductivity of the rG-O films becomes saturated after the reduction time of 30 min, demonstrating the rapid establishment of electron percolation paths. Of prime interest is that this rG-O film with the reduction time of 30 min displays a higher stability with respect to microwave heating than the other films, a result of the depression of microwave absorption by the increase of electrical conductivity and the reinforced dipolar interaction between restacked graphene by the presence of oxygenated functional groups. The control of reduction time is fairly effective in optimizing the functionality of rG-O nanosheets. The present work highlights the importance of controlled reduction condition not only in tuning the surface nature of rG-O but also in optimizing the transport property, surface morphology, and chemical stability of the rG-O freestanding films.

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Solvent controlled novel Cu+ and Cu+/2+ fluorescent Turn-ON probing

하용황 **D.G.Churchill***

한국과학기술원(KAIST) 화학과

A novel Schiff base probe, (carbamoyl salicylimine benzothiazole hydrazine) was prepared and measured for its probing ability. High sensitivity was shown for Cu+ and Cu2+. When solvent polarity was regulated by the combination of 100% H2O to 100% acetonitrile, selective sensing of Cu+ or total amount of Cu+ and Cu2+ was possible. In addition, a linear hypsochromic fluorescent shift of about 40 nm was shown. Binding stoichiometry of 1: 1 exists at low concentration. Time-dependent emission measurement showed exponential decay curve (τ1 = 2.99 x 103s, 10 equiv. of Cu+) and linear decay line (slope = -0.02159, 5 equiv of Cu+). Biothiols, L-cysteine, DL-homocysteine, Glutathione reduced, N-acetyl-L-cysteine showed almost complete reversibility of Cu+-induced emission in 50% acetonitrile in H2O, relative to partial reversibility of Cu2+ emission. Herein, by regulation of the ratio between acetonitrile and H2O, Cu+ and Cu+/2+can be probed selectively in this system.

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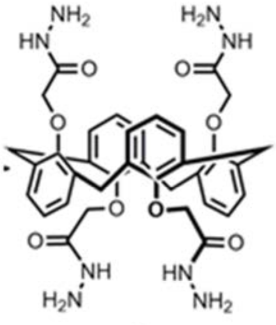
Calix[4]arene-based supramolecular gel and their mechanical properties

이지하 박재현 최희경 정종화*

경상대학교 화학과

We synthesized the calix[4]arene- based compound 1 and aldehyde compound 2. The compound 1 and 2 formed the supramolecular gels by hydrazone reaction in organic solvent. The supramolecular gels formed at different pH condition. Mixing clear DMSO solutions of compound 1 and compound 2 in a 1:2 ratio at pH 5, 6 and 7 at room resulted in the formation of viscous solution. Interestingly, at pH 7 mixing these solution resulted in the formation of stable transparent gels. On the other hands, at pH 5 and 6 mixing these solution resulted in the formation of stable opaque gels. Besides the properties of supramolecular gels observed in SEM , rheometer, DMA etc. by different pH conditions. In this symposium, I will present the properties of supramolecular gels.



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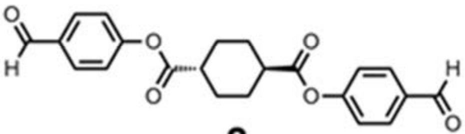

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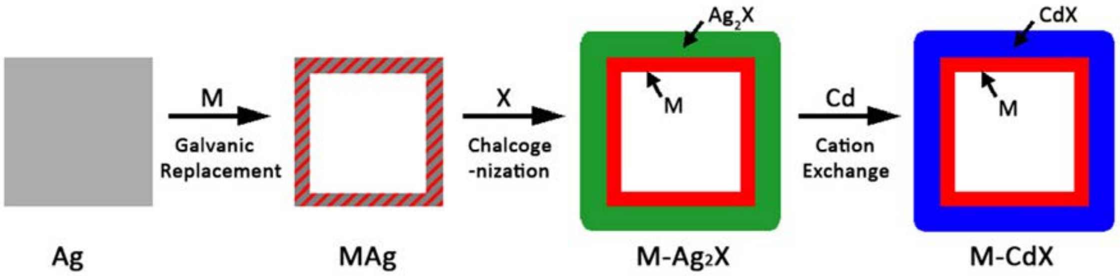
Synthesis of Metal-Semiconductor Double Shell Hollow Nanocubes via Sequential Nanoscale Reactions

최웅 송현준*

한국과학기술원(KAIST) 화학과

Hybrid nanostructures comprising noble metals and semiconductors have become significant for various applications such as photocatalysts. In this study, we demonstrate a general synthetic protocol of double shell hollow nanostructures, where the hollow cubes contain double shells with metal and semiconductor layers separately. The double hollow shells were synthesized through three steps from Ag nanocubes. For the first step, hollow structures were synthesized via a partial galvanic replacement reaction by noble metals, including Pt, Au, and Pd. Outer shells were formed by chalcogenization of Ag components to Ag2X (X = S, Se) via the kirkendall effect. Cationic exchange of Ag cations with Cd2+ generated hybrid structures of metals and CdX. TEM images with elemental mapping show a clear separation between metal inner shells and semiconductor outer shells in the hollow cubes. The thickness of each shell can be controlled by tuning a degree of the Galvanic replacement reaction.



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Artesunate-layered zinc hydroxide nanohybrid with enhanced dissolution property

김지영 양재훈 최진호*

이화여자대학교 화학.나노과학과

Artesunate (AS) is generally used for the treatment of malaria. And it also shows anticancer activity, but bioavailability is low. In order to overcome this low bioavailability, it is necessary to develop the novel drug delivery vehicle system with sustained release property. Recently, we have successfully accomplished this delivery system by intercalating AS into layered zinc hydroxides (ZBS) via co-precipitation for enhanced bioavailability. And, The AS loaded ZBS nanovehicle was coated with an anionic polymer, Eudragit L100, for enhanced dissolution property. According to the powder x-ray diffraction analysis, the basal spacing of the nanohybrids were determined to be 2.88nm for ZBS, indicating that AS was successfully incorporated in those layered zinc hydroxides. The fourier transformed infrared spectra reveal that AS molecules were deprotonated and electrostatically interacted with cationic zinc hydroxide layers without any structural change. Through CHNS analysis, TG analysis and HPLC analysis, the content of AS in ZBS nanohybrids was determined to be 45.8 wt%. Furthermore we would systematically discuss on the AS release property in the simulated body fluid solution.

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Magnesium aluminum Yttrium layered double hydroxide for radiotherapy

엄새란 양재훈 백승민[1] 최진호*

이화여자대학교 화학.나노과학과 [1]경북대학교 화학과

Yttrium-90 is one of the radiotherapeutic species for treating cancer. In the case of Y-90 microspheres, after they are inserted into the blood vessel linked the cancer and used for radioactive cancer treatment, the used Y-90 microspheres are not eliminated from the body, but remain in the body. Therefore it is necessary to develope the novel radiotherapeutic materials containing Y-90, which should be eliminated from body after cancer treatment. Layered double hydroxides (LDHs) containing Y is a good candiate material due to the bio-compatiblity, that is, LDH is non-toxic material and slowly dissolved in the body fluid condition. In the present study, we prepared Mg/Al LDH containing Y (Mg2Al1-xYx-CO3-LDH) via coprecipitation and hydrothermal treatment, in which the Y content (x) was varied from 0.0 to 1.0. The local structure of Y in LDH would be confirmed with the X-ray absorption spectroscopic analysis. According to X-ray diffraction analysis, the basal spacings of (003) peak were determined to be ~ 7.6 ?, indicating that LDHs were successfully synthesized. However, with increasing x value, the crystallinity of LDHs became poorer and the (hkl) peaks slightly shifted to lower angle, indicating the unit cell expansion because Y3+ ions with larger ionic radius were substituted to some octahedral Al3+ sites. The cell parameter, a, of Mg2Al1-xYx-CO3-LDH gradually increased 3.041 ? to 3.071 ? with increasing x value from 0 to x = 0.4, and then was saturated at more than x= 4. Based on this data, the solid solution limit of Mg2Al1-xYx-CO3-LDHs is x = 0.4.

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Synthesis of a metal-organic framework with an unprecedented net topology

신선영 정석 김동욱 나명수*

울산과학기술대학교(UNIST) 화학과

The solvothermal reaction of $Ni(NO_3)_2$ with 1,3,5-benzenedicarboxylic acid (H_3BTC) and pyrazine (pz) in mixed solvent, DMF and methanol, produced a 3D metal-organic framework (MOF), $((CH_3)_2NH_2)_2[Ni_3O(BTC)_2(pz)(MeOH)]$. A $Ni_3O(COO)_6$ secondary building unit (SBU) in the MOF is combined with six 3-c BTC ligands and the SBUs are further interlinked by a ditopic pz linker to form a 3D network of an unprecedented 3,8-c net topology. The MOF has two different diameters of 1D solvent channels along the crystallographic c-axis direction, where the potential void volume corresponds to 20% of the total framework. The various properties of this MOF including gas sorption behaviors will be discussed.

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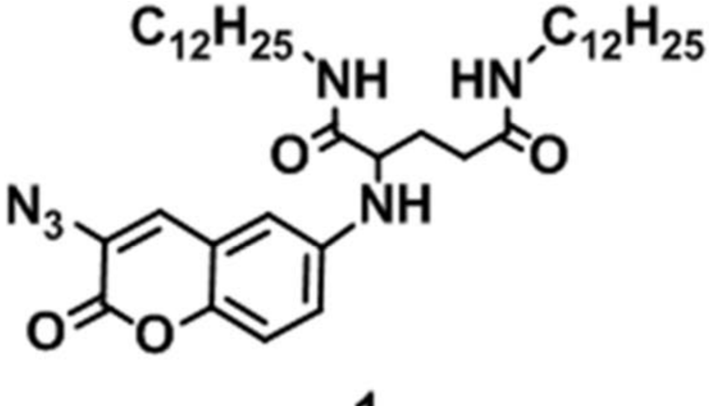
Coumarin-Based Organogels Formed at Different Solvent Compositions and Their Luminescent Properties

정진환 이지하 박재현 최희경 정종화* 최명룡*

경상대학교 화학과

The curmarine-based gelator 1 was synthesized by several steps, and the gelation ability was evaluated in pure and a mixture of organic solvents. The gelator 1 could be gelate a pure ethanol, toluene, dichrolomethane. In addition 1 formed a gel in different composite of ethanol/DMSO (10:1 ~ 5:5 v/v%). SEM images of organogels prepared at different composite solvents exhibited a typical fiber structure with 70-100 nm diameters. The luminescence properties of organogels prepared at different composite of ethanol/DMSO by fluorometry and time resolved fluorescence lifetimes. Interestingly, the organogel showed dramatic luminescence enhancement, which was dependent on the ethanol/DMSO ratio of the solvent. The luminescence lifetimes of the organogel were particularly long, on the order of several nanoseconds. The luminescence lifetimes were also slightly dependent on the solvent composition.



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Fluorescent "crowdoxidation" probes

D.G.Churchill

한국과학기술원(KAIST) 화학과

Chalcogen and organochalcogen chemistry is extremely rich. Chalcogenides provide sites of metal coordination and chemical oxidation. The chalcogens, as individual atoms, can be incorporated into the design of fluorescent (fluorogenic) molecules. This may enable novel classes of fluorophores to be produced and exploited for sensing, therapeutics and theranostics (e.g., GPx systems). The rudimentary chemistry of the chalcogens (oxides, etc) can be considered in larger or more complicated molecules, or arrays with chalcogens bearing unique positions. So far, we have produced molecules where chalcogens make up four different motifs. A simple photoinduced electron transfer (PET) donor-acceptor design can serve as the basis for rationally-designed next generation probing systems. The rotation of the “electron donor” group is critical in fluorescence properties in these systems. Our laboratory reported the first well-defined molecular probe involving chalcogen chemical oxidation as the chemical switch for fluorescence / optical changes. The benzothienyl-BODIPY serves as the PET “electron donor”. Since our original reports, other recent literature fluorophore / chromophore examples of chalcogen chemical oxidation have emerged. Our laboratory first reported a probe in which there are multiple sites of oxidation (multi-input) where a total of four oxidation sites are possible. Our laboratory first synthesized a BODIPY diselenide probe (BODIPY-*o*-Phenylene-Se-Se-*o*-Phenylene-BODIPY). Generally, it is the second diselenide probe known, but the first one that reacts with ROS. It is the second one to behave as a reversible superoxide probe. Here, the sensitivity, selectivity, time response, cell studies, stability of this sterical probe are all affirmative and decent, or excellent. An unexpected annulation product was also obtained (first chalcogen annulation product known for dipyrrins, or aryl-meso porphyrins, etc). The discovery of this molecule is an important development because the entire fluorogenic skeleton can be kept small, and the donor-acceptor moieties become blended. Synthetic molecules less than 500 Da are said to have appropriate "drug likeness." The probe exhibits “off-on” fluorescent probing at the Se or Te center, and is reversible.

The structure shows large mean planarity and rigidity; the chalcogen atom is saddled halfway between the aryl ring and chromophore resulting in a red-shifted emission band relative to the parent chromophore.

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Novel and Selective Fluorescent Probe for the Detection of Tabun Nerve Agent Tabun Mimics[1]

장윤정 정정아 **D.G.Churchill***

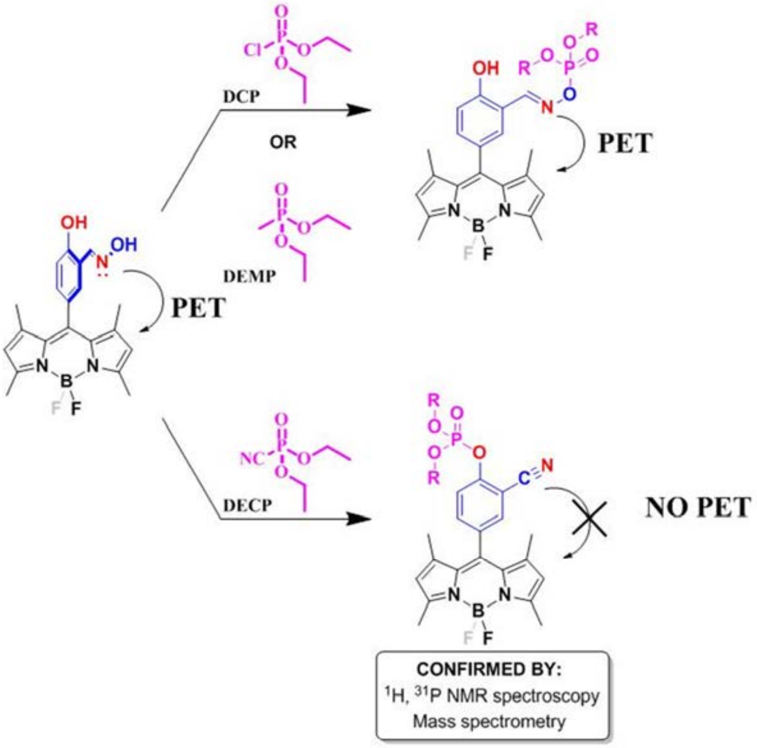
한국과학기술원(KAIST) 화학과

Among nerve agents, Tabun (GA) is very unique since it includes a P-CN bond whereas others include a P-F bond. The use of fluorescent molecules in sensing agents specifically is an ongoing aim.[1-3] The selective detection of Tabun is very important. In this study, a salicylaldehyde oxime based on a BODIPY system was introduced and developed for the detection of nerve agent-related molecules. The fluorescence intensity of the B-SAL-OXIME species increases in the presence of DECP, whereas it decreases in the presence of DCP and DEMP (limit of detection = 997 nM). Benzonitrile formation in the novel fluorescent B-SAL-OXIME system was elucidated using model substrates.

Key words: Nerve agent, Tabun, BODIPY, Salicylaldehyde oxime

References

1. Y. J. Jang, O. G. Tsay, D. P. Murale, J. A. Jeong, A. Segev and D. G. Churchill Chem. Commun., 2014, 50, 7531-75342. K. Kim, O. G. Tsay, D. A. Atwood and D. G. Churchill, Chem. Rev., 2011, 111, 5345-5403.3. Y. J. Jang, D. P. Murale and D. G. Churchill Analyst, 2014, 139, 1614-1617


DCP
OR
DEMP
DECP
PET
PET
NO PET
CONFIRMED BY:
^{1}H, ^{31}P NMR spectroscopy
Mass spectrometry

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Novel fluorescent probes for the detection of hypochlorite

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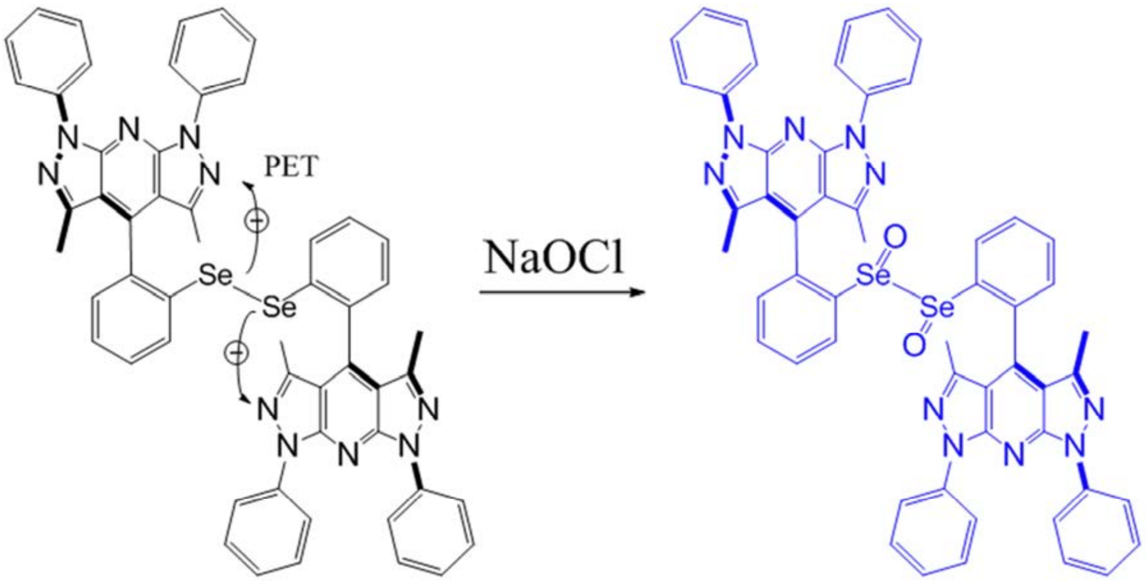
한국과학기술원(KAIST) 화학과 [1]기초과학연구원(IBS) 분자활성 촉매반응 연구단 [2]한국과학기술원(KAIST) 생명과학과

Molecular fluorescence continues to be one of major techniques for probing biology. Selective and sensitive small molecule probes continue to develop for biologically important analytes. Well-defined molecular probes are powerful tools in starting to unravel the roles of molecules, proteins and endogenous ions in biology to help further understanding these species with respect to aspects of health and disease. Selective fluorescent probe, for the detection of reactive oxygen species (ROS), has been developed. Probe (see below) was designed to have an oxidazible selenium with a non-traditional dipyrazolopyridine system. Probe gave a selective ~180-fold “turn-on” response to hypochlorite over the other ROS. Probe showed cell membrane permeability and ability of the detection analytes in the cells.



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The Research of “Molecular Aggregation PL Model” for Graphene Oxide Solution by using Integrated Time-Resolved Spectroscopy and Photoreduction

김창호[*] 정세채[1,*] 이홍순[2]

엘투케이플러스 기업부설연구소 [1]한국표준과학연구원(KRISS) 양자연구부 분광그룹 [2]한국표준과학연구원 미래융합기술부 의료융합측정표준센터

We found the fluorescence properties of Graphene Oxide(GO) to be dependent on concentration in aqueous solution via fluorescence spectroscopy and time-resolved spectroscopy by femtosecond laser. So, we proposed that the molecular aggregation is the origin of variable fluorescence from Graphene Oxide (GO) via “Molecular Aggregation PL model”. Herein, we deeper have characterized about “Molecular Aggregation PL model” for Graphene Oxide(GO) in water through Integrated Time-Resolved Spectroscopy performed with TCSPC & Pump-Probe by utilizing 100 kHz ultrashort pulse generated from Pharos. Also, we have done research for the conversion of reduced Graphene Oxide (rGO) from Graphene Oxide (GO) via photoreduction method by using UV ultrashort pulse.

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

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-fluoro-5-chlorotoluene 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-fluoro-5-chlorobenzyl as well as 2-fluorobenzyl radicals. A possible pathway for the formation of these benzyl-type radicals is proposed. Also, the electronic energy in the $D_1 \rightarrow D_0$ transition and the vibrational mode frequencies of the 2-fluoro-5-chlorobenzyl radical in the D_0 state were accurately determined, for the first time, by comparison with ab initio calculations and the known vibrational data of the precursor. In addition, substituent effect on electronic transition energy was discussed for substituents on the benzene ring.

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Radicals generated from 2-chloro-5-fluorotoluene by corona discharge

이은혜 윤영욱 이상국*

부산대학교 화학과

To observe production of benzyl-type radical from precursors, several techniques have been developed. Of several techniques, the corona excited supersonic expansion (CESE) technique, originally invented by Engelking and further developed by Lee, has been recognized as a powerful spectroscopic technique for observing molecular spectra in the gas phase. In this work, we report the benzyl-type radicals generated in a corona discharge from 2-chloro-5-fluorobenzen at different voltages and provide the first spectroscopic evidence of the $D_1 \rightarrow D_0$ electronic transition of 2-chloro-5-fluorobenzyl radical and their vibrational mode frequencies in the ground electronic state have been determined by comparison with an ab initio calculation and the known vibrational mode frequencies of the precursor. In addition we propose a possible pathway for the generation of benzyl-type radicals which can explain the results of the spectroscopic observation.

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Mechanistic Studies of Solvolytic Displacement of Chloride Ion from Sulfur

__고한중__

전주교육대학교 과학교육과

The solvolysis rate constants of 5-dimethylamino-naphthalene-1-sulfonyl chloride (DNSC) in 31 different solvents are well correlated with the extended Grunwald-Winstein equation, using the N solvent nucleophilicity scale and Y solvent ionizing scale with sensitivity values of 0.96±0.09 and 0.53±0.03 for l and m, respectively. These l and m values can be considered to support a SN2 reaction pathway having similar transition state (TS) structure with that of the benzenesulfonyl chloride reaction. This interpretation is further supported by the activation parameters, i.e., relatively small positive $\Delta H\neq$ and large negative $\Delta S\neq$ values, and the solvent kinetic isotope effects. Also, the selectivity values obtained in binary solvents were consistent with the proposed mechanism.

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Nonadiabatic molecular dynamics with the Tully's surface hopping method in the framework of TDDFT

이승훈 최철호[1,*]

서울대학교 화학부 [1]경북대학교 화학과

In some real chemical systems, electronic transitions occur when energies of different states are closer. In order to study the systems, nonadiabatic molecular dynamics is needed. I will introduce basic theory of nonadiabatic molecular dynamics with the Tully's surface hopping method. and I will announce recent studies using the MD simulation. The MD simulations were performed by a modified version of ab initio quantum chemistry package GAMESS.

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Theoretical study for the structures and binding energies of HOOO-(H2O)n (n=1～5) radicals and anions

김종민 김승준*

한남대학교 화학과

본 연구는 HOOO-(H2O)n (n=1～5) 라디칼과 음이온에 대해서 다양한 기저집합(basis set)과 범밀도 함수이론(DFT)을 사용하여 구조를 최적화하고 결합에너지와 조화진동수를 계산하였다. 라디칼의 경우 HOOO 라디칼의 H-O 를 중심으로 둘러싼 물(H2O) 분자들이 링(ring)구조를 이루며 안정화되는 경향을 보이는 반면, 음이온의 경우에는 말단 산소를 중심으로 H2O 분자들이 케이지(cage)구조를 이룰 때 안정화 되는 경향을 보였다. 결과적으로 라디칼 보다 음이온이 모체의 말단 산소와 물 분자 사이의 거리가 더 짧아 더 강한 수소 결합을 하고 있으며, 물 분자의 O-H 스트레칭이 적색 전이(red shift)됨을 확인하였다. 결국 음이온의 경우 말단 산소의 음전하와 물 분자 사이에 전하-쌍극자 인력이 라디칼의 일반적인 수소결합보다 더 강한 분자 간 인력으로 작용함을 확인하였다.

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Unfolding of the Azide-bound Ferric Hemoglobin by Guanidine HCl

이명현 임만호*

부산대학교 화학과

Unfolding of azide-bound ferric hemoglobin (HbN_3) was investigated as a function of guanidine HCl (GdnHCl) concentration by probing two absorption bands of azide in HbN_3, one minor band (5%) at 2046 $cm^{?1}$ with a full width at half maximum (fwhm) of 6 $cm^{?1}$ and the other major one (95%) at 2023 $cm^{?1}$ with a fwhm of 10 $cm^{?1}$. These two bands are narrower than that of the antisymmetric stretching mode of free azide ion in water solution, centered at 2042 $cm^{?1}$ with fwhm of 24 $cm^{?1}$. As concentration of the GdnHCl increases, the band at 2042 $cm^{?1}$ of free azide ion in water shifts toward the higher frequency, its absorption extinction coefficient decreases monotonically, and its fwhm broadens. As Hb unfolds, the band intensity of the free azide increases and shows a folding curve-like behavior, suggesting that the binding constant of the azide ion to the unfolded ferric Hb is negligible. On the assumption that the unfolded ferric Hb does not bind azide ion, unfolding curve of the HbN_3 as a concentration of GdnHCl was recovered. The unfolding curve showed the midpoint at 1.9 M with transition width of 0.3 M. It is very similar to the unfolding of CO bound ferrous Hb (HbCO), where the midpoint is at 1.7 M with transition width of 0.3 M. It appears that the HbN_3 is slightly more stable than HbCO in the GdnHCl denaturation. The similarity and the difference of the unfolding between anion bound ferric Hb and neutral molecule bound ferrous Hb will be discussed.

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Concentration effects on the rates of irreversible diffusion-influenced reactions

김민정 이상엽* 김지현[1,*]

서울대학교 화학부 [1]중앙대학교 화학과

We formulate a new theory of the effects of like-particle interactions on the irreversible diffusion-influenced bimolecular reactions of the type A + B → P + B by considering the evolution equation of the triplet ABB number density field explicitly. The solution to the evolution equation is aided by a recently proposed method for solving the Fredholm integral equation of the second kind. We evaluate the theory by comparing its predictions with the results of extensive computer simulations. The new theory provides a reasonable explanation of the simulation results.

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Complex refractive index change measurement of photoactive yellow protein (PYP) upon light irradiation using ssFTLS

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기초과학연구원 나노물질및 화학반응 연구단 [1]한국과학기술원(KAIST) 화학과

Complex refractive index (RI), related to the electric permittivity, is the value that describes the overall light-interacting property of materials. Although either the real or imaginary part of complex RI is used in various practical fields: biology, chemistry, food industry, agriculture, pharmaceutical industry, and even gemology, the whole information of complex RI as a function of wavelength, has not been fully utilized.We present the measurements of complex RI of photoactive yellow protein (PYP) in various wavelengths using swept-source Fourier transform light scattering (ssFTLS) technique [1]. PYP is one of the small bacterial photo-receptor. When PYP molecules absorb blue light, they become excited state, and about 0.2 seconds later, they relax down to the original ground state [2].We found significant RI difference between ground and excited state of PYP upon excitation with blue light. Interestingly, it is not only imaginary, but also real part of the complex RI changes significantly. Since the two states are composed of exactly same compounds, this difference should be originated by the structural change of the protein. This result cannot be explained by the theory that the real RI of protein can be solely determined by their amino acid compositions [3]. Applying Kramer-Kronig relations, we also found the causality of our results, and discussed the origin of real RI of proteins.

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Computational Prediction of Molecular Partition Coefficients Based on Solvent-Contact Model

김태호

세종대학교 생명공학과 신약디자인

We propose an extended solvent contact model to estimate the partition coefficient of organic molecules from individual atomic contributions. In this model, the partition coefficient is assumed to be the ratio of molecular solvation free energy in water to that in octanol. The calculation of solvation free energy involves the optimization of three kinds of parameters in the solvation free energy function: atomic fragmental volume, maximum atomic occupancy, and atomic solvation parameters. All of these atomic parameters for varying atom types are optimized by the operation of a standard genetic algorithm in such a way as to minimize the difference between experimental and calculated solvation free energies. Linear regressions with the optimized atomic parameters yield fits with the squared correlation coefficient larger than 0.8 for the training set and the test set. Overall, the results indicate that the extended solvent contact model with the newly developed atomic parameters would be a useful tool for rapid calculation of the partition coefficients of organic molecules.

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Theoretical examinations for different CO photolabilities of Ru geometrical isomer complexes controlled by ancillary 2-phenylazopyridine ligand

장효원[*] 허경식

순천대학교 화학과

Carrington et al synthesized two geometrical isomers of dicarbonyl octahedral Ru complexes and reported that the trans isomer of CO to azo group of ancillary ligand releases CO more easily than the cis isomer upon illumination. Such properties could have therapeutic applications in heart attacks. They suggested that the competing back-donation effect for metal electrons toward azo groups weakens binding of CO which occupies trans position, resulting strong photolability than otherwise. We try to examine the released CO contributions originated from various coodination sites by simulating binding energies for CO ligands using DFT method.

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Theoretical studies of preferential hydrogen exchange reaction pathways with ammonia in amido hydride coordinated pincer type complex of iridium

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순천대학교 화학과 [1]순천대학교 기초의화학부

Morgan et al experimentally observed that ammonia undergoes oxidative addition to an unsaturated Ir pincer complex to form amido hydride complex. Such reaction may be useful for functionalization of amine in synthetic applications. They also suggested that the reaction pathway might involve agostic interaction of ammonia's N-H bond with Ir, which was examined by Cho et al by DFT calculations reporting about 29kcal/mol activation free energy barrier for forming amido hydride complex. The resulting amido hydride product undergoes hydrogen exchanges in amido hydrogens exclusively with atmospheric ammonia, excluding hydride position in the further experimental treatments. We suggest the plausible pathways for such hydrogen exchange reactions in this work. The major aspect of the pathway is the participation of the second ammonia molecule binding weakly to complex and providing hydrogens to amide positions preferentially.

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A Computational Approach for UV-vis Spectrum in Liquid Phase by Using QM/MM Molecular Dynamics Simulation

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중앙대학교 화학과 [1]군산대학교 화학과 [2]한국과학기술원(KAIST) 화학과

In the field of organic photovoltaics, light absorption is crucial to determine the performance of photovoltaics. Thus, the excited-state calculations (CIS, TDDFT, etc.) are commonly used to predict or describe UV-vis spectrum. Usually, the full quantum mechanical method for excited state has been conducted considering only one conformation followed by ground state geometry optimization calculation. However, there should be distributions of molecular structures within the given finite temperature. For example, backbone structure of highly conjugated organic molecules often determines the HOMO/LUMO electronic structures and UV-Vis spectrum. Then, the distribution of backbone structures can produce the distribution of UV-Vis spectrum which often appears as asymmetric line shape or shoulder peaks. Therefore, Molecular Dynamics Simulation is required to consider more than one conformation to get the simulated UV-vis spectrum in liquid phase properly. In this study, we will introduce the method of getting the simulated UV-vis spectrum with high resolution by using QM/MM MD simulation.

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Spectroscopic Studies on the Interaction between Morin and various Metal ions

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Flavonols are a class of flavonoid compounds with a potential use as chemical markers for cultivar authentication of grapes and their wines, like anthocyanin do in the case of red grape and wine. Flavonols have the advantage of occurring in both red and white grapes and wines. Morin (3, 5, 7, 2’, 4’-pentahydroxyflavone) containing many hydroxyl group is one of the flavonol compounds and it is important bioactive compound by interacting with nucleic acids, enzymes and protein. There are some metal ions in the human body such as Fe^{2+}, Cu^{2+}, Co^{2+}, Mn^{2+}, Zn^{2+}, and Ca^{2+} ions. These are vital for biological functions, such as gene expression, apoptosis, enzyme regulation, and neurotransmission. It is, therefore, interesting to investigate the interaction between morin and metal ions. 50 μM morin added the various concentration metal ions from 200 μM to 0 μM. The absorption spectra maximum peaks of 50 μM morin added with metal ions are increased and shifted to longer wavelength according to the metal ion concentration. Moreover, the fluorescence emission spectra maximum peaks decreased. These spectroscopic results show that most of metal ions might be participated mainly in the redox reaction in the aqueous morin solutions.

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Analysis of magnetic properties in Maricite and Triphylite $NaFePO_4$ polymorphs on the Basis of Electronic Structure Calculations

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The spin exchange interactions of maricite(m-) and triphylite(t-) $NaFePO_4$ Polymorphs were examined by performing the spin dimer analysis based on the extended Hueckel tight binding method. Crystal structures of both polymorphs consist of slightly distorted octahedron of FeO_6 and tetrahedron of PO_4 units. Spin exchange interactions in $NaFePO_4$ occur through both superexchange(SE) and super-superexchange(SSE) paths. Although m- and t-$NaFePO_4$ polymorphs have FeO_6 units, their condensed structures made up of FeO_6 units are different, i.e., t-$NaFePO_4$ has corner-sharing FeO_6 chain and m-$NaFePO_4$ has edge-sharing FeO_6 chain. Our spin dimer analysis for $NaFePO_4$ shows that SE interaction in t-$NaFePO_4$ is much stronger than SSE interaction, but in m-$NaFePO_4$, SSE interaction is stronger than SE interaction.

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Measurements of the Rebinding Dynamics of O_2 to Myoglobin

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Time-resolved vibrational spectroscopy was used to probe the rebinding dynamics of O_2 to myoglobin (Mb) in the time range from femtosecond to microsecond after excitation of oxymyoglobin (MbO_2) in D_2O with a 575-nm pulse at 293K. Since the weak O-O stretch band is overlapped with the strong absorption bands in the 1200 ~ 1000 cm^{-1} region by water solvent, protein, and buffer molecule, difference time-resolved spectra ($Mb^{16}O_2$ - $Mb^{18}O_2$) were obtained to delineate O_2-related bands from the absorption changes due to conformational and thermal relaxation. The O-O stretch mode in MbO_2 is known to exhibit two conformational bands but one conformation band in $Mb^{16}O_2$ is split due to a perturbing vibration, resulting in three absorption bands for $Mb^{16}O_2$ (1147, 1123, and 1104 cm^{-1}) and two absorption bands for $Mb^{18}O_2$ (1086 and 1067 cm^{-1}). Therefore, after the Q-band excitation the difference transient spectra exhibit three photo-bleaching bands for $Mb^{16}O_2$ and two transient absorptions for $Mb^{18}O_2$. All the transient signals decay with the same kinetics and were described by two exponential function plus an equation describing bimolecular reaction. The recovered time constants for the exponential function were 4.4 ps (77%) and 34 ns (11%) and the bimolecular rate constant was 21×10^6 $M^{-1}s^{-1}$. The 4.4-ps and 34-ns decays were attributed to thermal relaxation of six-coordinate heme subsequent to fast electronic relaxation without photodeligation and geminate recombination (GR) of O_2 after photodeligation, respectively. The cooling process for the six-coordinate heme group can be observed due to anharmonic coupling of low frequency modes with the O_2 stretching mode. When photoexcited in the Q-band, about 23% of MbO_2 undergoes photodeligation (quantum yield, QY = 0.23), about 50% of the deligated O_2 geminately rebinds in a time constant of 34 ns, and the remaining O_2 escapes into solvent and bimolecularly rebinds with the rate constant of 21×10^6 $M^{-1}s^{-1}$. Fast and efficient GR of O_2 indicates that the heme pocket is efficient in trapping the deligated O_2. Conformation-independent dynamics of photoexcited MbO_2 suggests that the O_2 binding characteristics is independent of conformatiomnal substates of MbO_2 or transition between conformational substates is faster than 34 ns.

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Effects of Laser Wavelength and Power in the Production of NiNanoparticles by Pulsed Laser Ablation in Deionized Water

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Size dependent properties of metal and metal oxide nanoparticles in the liquid phase havebeen great interest due to their wide variety of potential applications in the biomedical,optical and electronic field. Among various synthesis methods, pulsed laser ablation in liquid(PLAL) has been demonstrated to be an effective, simple, and versatile method forsynthesizing nanoparticles from appropriate liquid and solid precursors. The PLAL methodallows a versatile design of nanoparticles by adjusting experimental parameters such as thelaser wavelength, fluence, and the presence of surfactants.In this study, a nickel plate was ablated by a pulsed Nd:YAF laser to produce nano-structuredNiO in deionized water in the presence of surfactant of sodium dodecyl sulfate (SDS). In thisstudy, the mean diameter and the width of size distribution of the nanoparticles wasinfluenced by the laser power and wavelength, resulting in the production of smaller andlarger sizes of nanoparticles with higher wavelength and lower laser power, respectively. Theinfluence of laser wavelength and power on the mean diameter and the width of sizedistribution of as-prepared nanoparticles generated by the laser ablation process wasexplained by the space homogeneity of the plasma plume, where the nucleation ofnanoparticles has occurred. In addition, catalytic, structural and morphologicalcharacterizations of synthesized NiO nanoparticles were conducted by cyclic voltammetry(CV) using multi-walled carbon nanotube (MWCNT), X-ray diffraction (XRD) and highresolution transmission electron microscope (HR-TEM).

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The Effects of Dimensionality and Flexibility of Conductive fillers on their Percolation network

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Polymer composites incorporated with conductive fillers are one of the most widely used materials in modern industrial field due to their excellent electrical and mechanical properties. The electrical conductivity of polymer composites can be understood in terms of the percolation theory. The percolation threshold concentration, φc, is a critical factor that determines the conductivity of polymer composites, and is affected by the dimensionality and flexibility of conductive fillers. We perform Langevin dynamics (LD) simulations to explore how the dimensionality and flexibility of conductive fillers influence the percolation threshold concentration φc. Three kinds of model for conductive fillers are used : sphere (0D), rod (1D), and plate (2D). We find that the percolation threshold for non-spherical conductive fillers increases with an increase in their flexibility and that the 1D conductive fillers percolate at the lowest concentration compared to 0D and 1D. The electrical conductivity also shows the same trend as the percolation threshold. The conductivity is the highest with the 1D fillers and lowest in case of 0D . These results give an physical insight in the effects of shape of conductive fillers on their percolation threshold and conductivity.

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A study on Single Polymer in Solution Confined between walls using Molecular Dynamics and Langevin Dynamics Simulations

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The static and dynamic properties of a flexible polymer chain confined between two walls are investigated using computersimulation. In order to investigate the effect of hydrodynamic interaction, we perform two different simulations: (a) Molecular dynamics simulation for explicit solvent model with hydrodynamic interaction and (b) Langevin dynamics simulation for implicit solvent model. The confinement effect is studied by changing the height H between walls. We observe that the radius of gyration of the polymer chain Rg scales as Rg~ N2/3 (where N is degree of polymerization) for H ≥ Rg,bulk.(where Rg,bulk is polymer radius gyration in bulk), which changes to Rg ~N3/4 for H < Rg,bulk in both two methods. The transitional diffusion coefficient,D, behaves like a Zimm model with D~N -2/3 for H ≥ Rg,bulk and a Rouse model with D~N -1 for H < Rg,bulk in Langevin dynamics simulations. The shape parameter S = 2Rg,z/(Rg,x+Rg,y) , measured in order to characterize quantitatively the chain anisotropy, gradually decreases with a decrease in the height between walls in both two cases. It is found that density profile of monomers between walls is different between MD and LD simulations. In case of LD, there is a peak in the center between walls, while in case of MD, there is a large peak near the wall, which corresponds to effect of solvent.

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Terahertz spectrum of Melamine: experiment and computation

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The terahertz (THz) spectrum of melamine was obtained from 0.1 THz to 3 THz at room temperature. THz spectroscopy can be used to identify the lattice vibrational modes since it is sensitive to the intermolecular interactions in the solid state. In this study, we measured the THz images and spectra of melamine by using a TPS spectra 3000 spectrometer (TeraView Ltd.). We used the signals transmitted by the pure HDPE pellets as the reference signal and by the center of the melamine pellets as the sample signals. It is hard to analyze the lattice vibrational modes through THz spectra from experiments, but computational methods can help to understand such vibrational motions in THz region. The structural analysis and vibrational assignment of the melamine were performed by solid-state density functional theory (DFT) using DMol3 (version 6.1) software package. All calculations employed the DNP (double numerical with d and p polarization) basis set with PW91 functional which is one of the GGA (generalized gradient approximation) density functionals. The THz spectrum contains three characteristic absorption peaks (2, 2.26, and 2.6 THz) and there are 4 infrared-active vibrational modes at the PW91/DNP level providing the well-reproduced experimental spectrum. All peaks are related to the intermolecular vibrational motions. This result suggests that solid-state DFT calculation of THz spectrum can be useful method to analyze the lattice vibrational motions.

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Conformational and vibrational analysis of Glucopyranose in aqueous solution: A combined study of quantum mechanical calculation and QM/MM-MD Simulations

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The standard agent glucose has been the subject of numerous experimental and theoretical studies, especially in the aqueous environments which are present in most biochem-ical processes. The impact of the solvation process on the vibrational spectra of glucose in the mid-infrared region is investigated in this work. The association process of glucose in aqueous solution was studied by a combination of quantum mechanical calculations and QM/MM-MD simulations for glucose with 290 TIP5P water molecules. Con?gurations in which the water molecules created a favorable network completely around and under glucose were found to have low energy for both α and β anomers. Quantum mechanical calculation of the α/β anomeric ratio using MP2/cc-pVTZ level provides, ~32/68%, highly favoring the β anomer in good agreement with the experimental ~36/64% value. An appro-ximate hydroxymethyl population was obtained by noting average relative energies among the three conformational states, gg, gt, and tg. MD simulation shows that in both α (gg : gt : tg = 54 : 41 : 5) and β (gg : gt : tg = 52 : 40 : 8) (%) rotamer complexes the gg conformation was favored over the gt state, with the tg conformations all being of higher energy making little or no contri-bution to the rotamer population is in good agreement with Experimental homo nuclear J-coupling data. Our simulation shows experimental vibrational spectrum is closely related with the gg (ω=-60) structure of both α & β conformer.

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Real-time observation of endosome escape of nanoparticles using FRET in live cells

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Upconverting nanoparticles (UCNPs) have recently attracted enormous attention owing to their unique optical properties. In particular, they are extremely photostable (non- photoblinking and non-photobleaching) and have been proved to be ideal for continuous, long-term observation of dynamic system such as endocytic pathway in live cells. We used FRET imaging to monitor the encapsulation of UCNPs by endosomes and subsequent release into the cytosol. In such FRET system, UCNPs acted as the donor and the endosome staining dye as the acceptor. We believe that, with optical probes other than UCNPs, it would have been hard to guarantee that the on-off signal switching is due to the genuine cellular process or the artifact (photoblinking or photobleaching) by the probes.

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A New Computational Approach for Protein Folding Thermodynamics

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Folding free energy is the fundamental thermodynamic quantity characterizing the stability of a protein. Yet, its accurate determination based on computational techniques remains a challenge in physical chemistry. A straightforward brute-force approach would be to conduct molecular dynamics simulations and to estimate the folding free energy from the equilibrium population ratio of the unfolded and folded states. However, this approach is not sensible at physiological conditions where the equilibrium population ratio is vanishingly small: it is extremely difficult to reliably obtain such a small equilibrium population ratio due to the low rate of folding/unfolding transitions. It is therefore desirable to have a computational method that solely relies on simulations independently carried out for the folded and unfolded states. Here, we present such an approach that focuses on the probability distributions of the effective energy (solvent-averaged protein potential energy) in the folded and unfolded states. We construct these probability distributions for the protein villin headpiece subdomain by performing extensive molecular dynamics simulations and carrying out solvation free energy calculations. We find that the probability distributions of the effective energy are well described by the Gaussian distributions for both the folded and unfolded states thanks to the central limit theorem, which enables us to calculate the protein folding free energy in terms of the mean and the width of the distributions. The computed protein folding free energy (?2.5 kcal/mol) is in accord with the experimental result (ranging from ?2.3 to ?3.2 kcal/mol depending on the experimental methods).

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Finite Size Effects on the Dynamic Heterogeneity of Single Component Lipid Membranes

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Cellular membranes are composed of various different types of molecules such as phospholipids, cholesterol and membrane proteins. And the composition of lipids membrane is heterogeneous in cellular membranes. Not only its component but also its dynamics becomes spatially heterogeneous when temperature is sufficiently low. At low temperature, when the dynamics of lipids in cell membranes becomes spatially heterogeneous, there are regions of fast and slow lipids. The heterogeneous dynamics plays an important role in cellular functions such as signal transduction. However, the physical origin of the heterogeneous dynamics of lipid membranes is poorly understood. Recent simulations suggested that the dynamic heterogeneity was intrinsic nature of lipids membrane because one could observe the dynamic heterogeneity even in single component lipid membranes. (Soft Matter, 2014, 10, 3036) However, it is difficult to systematically investigate such dynamic heterogeneity in molecular simulations because the size and lifetime of slow regions of lipid are not well known in a quantitative fashion. If simulation cell size is too small compared to the size of slow regions, molecular simulations would fail to describe the lipid dynamics and its heterogeneity. Therefore, investigating the finite size effects on heterogeneous dynamic region is an issue of fundamental importance. In this work, we systematically investigate how the lipid heterogeneous dynamics is affected by finite system sizes. Single component lipid bilayers are constructed using MARTINI force field and three different simulation cell sizes (L = 5nm, 10nm and 20nm). We show that fast and slow dynamic regions can be observed for single component lipid bilayers and the size of region is dependent on the system size significantly.

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Light-induced, ring-shaped fluorescent agglomeration for in-situ fluorescence marker

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We discovered a novel phenomenon for the formation of a ring-shaped fluorescent agglomeration under a few milliwatt of light irradiation upon a light-absorbing medium. This ring-shaped agglomeration was solid and fluorescent which showed completely different characteristics in comparison with the one before light irradiation. These phenomena were dependent on the intensity and the polarization of the laser light, types of the mounting media, and irradiation time. Based on microscopic and spectroscopic control experiments, we reached sufficient conditions for the occurrence of fluorescent agglomeration. Furthermore, because the agglomeration formed on the surface of cover glass is fixed in position, we propose a novel application of this phenomenon for in-situ fluorescent marking during the microscopic observation of moving objects such as living cells.

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Construction of bacteriochlorophyll a (BChl a) molecular potential energy surfaces with quantum chemical calculations

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Photosynthesis is one of the most important and widely studied biological processes. In the light reaction, which is the former part of photosynthesis, the absorbed solar energy is transferred to the reaction center in the form of exciton. The exciton transfer pathway involves a number of energetically coupled chromophore molecules that form an 'energy funnel' directed to the reaction center. The overall transfer process can exhibit near-unity efficiency in some situations, and recent studies suggest that such a high efficiency may result from quantum interactions between nearby chromophores. Theoretical studies of the energy transfer between chromophores in the condensed phase can be conducted with various levels of models, and there have been many studies based on abstract models of chromophores. There have also been reports where the researchers have tried to simulate exciton dynamics in an atomistic level, with the help of molecular dynamics (MD) simulations. To perform MD simulation, a molecular model that can accurately describe actual behavior of the chromophore is definitely needed. This study focuses on the modeling of the bacteriochlorophyll a (BChl-a) molecule in the Fenna-Matthews-Olson complex, a prototypical system for photosynthesis research. We have constructed the force field parameters for BChl-a ground and excited states by using the Hessian matching protocol, where the parameters are fitted to provide accurate vibrational description of the chromophore in reference to quantum chemical calculations. The model validation is performed based on the frequency-dependent system-bath coupling (spectral density) and the absorption reorganization energy, both of which can be obtained using classical MD simulations.

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Structural and Thermodynamic Properties of Amyloid beta and Tau Proteins associated Alzheimer's disease

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The accumulation of amyloid beta (Aβ) into senile plaques and abnormal hyperphosphorylated tau into neurofibrillary tangles are the classical hallmarks of Alzheimer's disease (AD). Here, we characterized structures and thermodynamics of physiological 42-residue Aβ peptide (Aβ42), one of the major components of amyloid plaques, and paired helical filaments comprising 43 residues (termed PHF43), the minimal sequence to obtain aggregation in tau pathology by performing the fully atomistic, explicit-water molecular dynamics simulations as well as the solvation thermodynamic analysis based on the integral-equation theory of liquids. Based on the structural investigations of Aβ42 and PHF43 conformations, we find that Aβ42 displays higher β-sheet propensity than PHF43. Based on the solvation free energy analysis, we observe that PHF43 is more hydrophobic than Aβ42. We suggest that PHF43 is more prone to aggregate than Aβ42 in aqueous environment.

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Temperature-Dependent IR Spectroscopy of Ion Solvation of $LiPF_6$ in Electrolyte : Thermodynamic study

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Despite that the carbonate-based solvent have been used as the electrolyte of Li-ion secondary battery over the past two decades, Li^+ ion solvation energy in the electrolyte system have not been revealed. In order to obtain thermodynamic functions of Li^+ ion solvation, we carried out temperature-dependent IR experiments of $LiPF_6$ in dimethyl carbonate (DMC), diethyl carbonate (DEC) and ethyl methyl carbonate (EMC). The carbonyl stretching vibrational mode in carbonate-based solvent is used as a probe to monitor whether the Li^+ is solvated by base solvent. Due to the strong absorbance of solvent molecule, the sample solution was contained in the newly built IR cell having the ultrathin path length. The proper amount of SiO_2 was deposited on the CaF_2 window by the sputtering technique to adjust the IR absorbance of the target band to be below the upper detection limit of FR-IR spectrometer. In measured spectrum, the frequency of solvent which does not solvate Li^+ is about 1755 cm^{-1}, while one of molecule solvating Li ion is red-shifted by about 30 cm^{-1}. Singular value decomposition of temperature-dependent IR spectra was performed to obtain the equilibrium constant of Li ion solvation reaction as a function of temperature. We can determine the thermodynamics properties by plotting van't hoff equation.

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Solvent-Dependent Structure of Molecular Iodine Probed by Picosecond X-ray Solution Scattering

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The effect of solute-solvent interaction on the molecular structure and the reaction dynamics of the solute molecules has been a target of intense studies in solution phase, but it is often challenging to characterize the subtle effect of solute-solvent interaction, even for the simplest diatomic molecules. Since I2 molecule has only one structural parameter and exhibits solvatochromism, it can be used as a good model system for investigating the effect of solute-solvent interaction. By using X-ray as a probe, time-resolved X-ray liquidography (TRXL) can directly elucidate the structures of reacting molecules in the solution and thus can determine the solvent-dependent structural change with atomic resolution. Here, by applying TRXL, we characterized the molecular structure of I2 in methanol and cyclohexane with sub-angstrom accuracy. Specifically, we found that the I?I bond length of I2 is longer in polar solvent (methanol) by ~0.2 ? than in nonpolar solvents (cyclohexane and CCl4). The elongated bond distance of I2 in methanol is well reproduced by density functional theory (DFT) calculation using 22 explicit methanol molecules, confirming that the origin of the bond elongation is the partial negative charge filled in antibonding orbital through the solvent-to-solute charge transfer.

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Viscosity-dependent Rebinding Dynamics of NO to Ferrous Iron in Viscous Solution

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부산대학교 화학과

Femtosecond vibrational spectroscopy was used to probe rebinding dynamics of NO in $Fe^{II}(D_2O)_5NO$ dissolved in D_2O and 90 % glycerol/D_2O mixture. The NO-bound ferrous Fe complex was prepared by bubbling NO gas to $Fe^{II}Cl_2$ in the corresponding solution. The stretching mode of NO in the complex was peaked near 1808 $cm^{?1}$ with a full width at half maximum of 21 $cm^{?1}$, red-shifted from that in the gas phase value of 1876 $cm^{?1}$. The red-shift indicates that the bound NO in the complex has $NO^{?}$ character upon binding to the ferrous Fe. When $Fe^{II}(D_2O)_5NO$ in D_2O was photoexcited by 266 nm, about 52 % of the deligated NO geminately rebinds in time constant of 15 ps and the remaining deligated NO survives beyond 100 ps. When $Fe^{II}(D_2O)_5NO$ in 90 % glycerol/D_2O mixture was photoexcited by 266 nm, about 12 % of the deligated NO geminately rebinds in time constant of 10 ps. Higher geminate rebinding yield in more viscous solution indicates that the solvent viscosity hinders the diffusion away of the deligated NO and thus facilitates more efficient geminate rebinding.

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Time-resolved X-ray absorption spectroscopy of Ruthenium L3-edge as a Probe of the Metal-to-Ligand Charge-Transfer Process in Solution Phase

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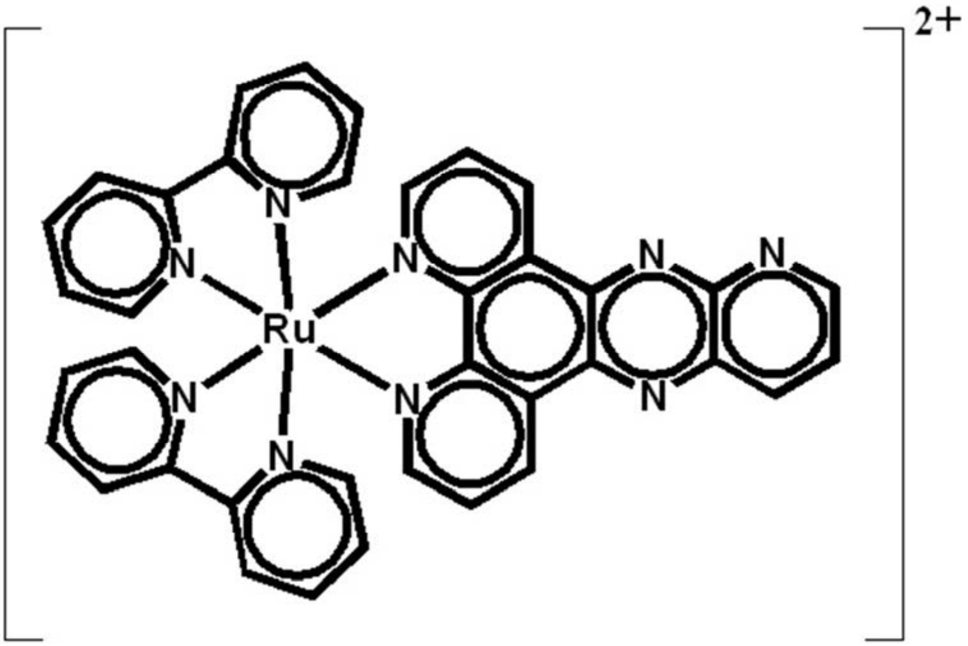
부산대학교 화학과

Time-resolved X-ray absorption spectroscopy (TR-XAS) is a useful technique to probe thestructural and electronic changes of ultrafast charge-transfer processes during photochemicalreaction. Specially, Ru(II) complexes have been widely investigated for use in the various area as solar energy conversion, luminescence sensing and photodynamic therapyapplications. We directly observed the transient triplet metal-to-ligand charge-transfer (3MLCT) state of ruthenium based dye molecule, [Ru(bpy)2(dppp2)]2+ (bpy = 2,2′-bipyridine, dppp2 = pyrido[2′,3′:5,6]pyrazino[2,3-f][1,10]phenanthroline) in various solvent by means of ultrafast transient XAS at Ru L3-edge region. To interpret transient x-ray spectra, we performed the time-dependent density functional theory (TD-DFT) calculations of Ru 2pcore-level excitations to visualize the movement of charge densities between Ru center and surrounding ligands upon an ultrafast MLCT process. We find that the stabilization of Ru 2p core and 4d valence orbitals by 1.9 and 1.5 eV, respectively, in the 3MLCT state of [Ru(bpy)2(dppp2)]2+. This study provides the detailed understanding of the electronic structure for the ultrafast transient 3MLCT state of transition Ru complex.


2+
Ru
N

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Synthesis and characterization of fluorescent sensor for carbonate ions in mixed aqueous organic media

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The design and development of reliable optical sensors for inorganic anions with auspicious selectivity, reassuring sensitivity and low detection-limit have recently been intensively explored as conscientious mean for potential applications in real sample analysis. Herein, a novel fluorogenic signaling probe 6 for the selective detection of carbonate ions in mixed aqueous organic media has been developed through microwave assisted Schiff base formation by reacting 4-amino-3-(4-methoxyphenyl)-1H-1,2,4-triazole-5(4H)-thione (5) with 4-nitrobenzaldehyde in methanol. The anion recognition occurs through hydrogen bonding assessed by ^{1}H NMR titration experiment. The photophysical results of (E)-3-(4-methoxyphenyl)-4-[(4-nitrobenzylidene)amino]-1H-1,2,4-triazole-5(4H)-thione (6) corroborates its applicability as optical sensing platform for selective carbonate ion detection in mixed aqueous organic media. The fluorescence emission signal enhancement at 424 nm and appearance of unique red shifted signal only on carbonate ion addition in case of absorption spectral recording suggest the selective affinity of probe 6 with only carbonate ions in comparison to a variety of competitive ions (F^-, Cl^-, Br^-, I^-, NO_2^-, ClO_2^-, ClO_3^-, ClO_4^-, SO_4^{2-}, SiO_3^{2-}, NO_3^{2-}, CH_3COO^- and HCO_3^-) in aqueous/ethanol (7:3, v/v) under neutral pH at ambient temperature. Due to simplicity, low cost, wide scope, fast response time, appreciable sensitivity of 1×10^{-7} mol/L and robustness, the proposed sensing method might be a practical tool for environmental samples analysis and biological studies.

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High spatial-resolution mapping of nanomagnetic fields using a radical pair reaction

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Magnetic micro- and nano-structures haven developed with various potential applications spanning from high density data storage devices to cancer therapeutic practices. However, it is still not a simple task to characterize magnetic field distribution of those synthesized magnetic structures ironically because of their small dimensions. Magnetosensitive fluorophores are promising candidates that allow us to directly visualize magnetic flux density (B) around the small scale magnetic structures using relatively simple fluorescence-based microscopic techniques. We synthesized one of the magnetosensitive fluorophores, phenanthrene-(CH2)12-O-(CH2)2-N,N-dimethyaniline by a two-step reaction and investigated its properties regarding magnetic field sensitivity: the fluorescence intensity was measured as swiping external magnetic field up to 0.1 T and as changing temperature. A spectrally resolved fluorescence lifetime was also studied. Here we also demonstrate our pursuit for high spatial-resolution images of field distributions around various shapes of micro- and nano-magnetic structures using epifluorescence microscopy, two-photon microscopy and super-resolution microscopy.

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Development of optical chemosensor for selective Fe^{3+} detection

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공주대학교 화학과

Recently, there has been significant interest in the design and development of optical chemosensors for recognition of biologically and environmentally important analytes with high selectivity, sensitivity and low detection-limit because of their fundamental role in medical, environmental and biological applications. Herein, a novel fluorogenic signaling probe 6 for the selective detection of ferric ion in mixed aqueous organic media has been developed through microwave assisted Schiff base formation by reacting 4-amino-3-(2-fluorobenzyl)-1H-1,2,4-triazole-5(4H)-thione 5 with thiophene-2-carbaldehyde. The formation of probe 6 was characterized by FT-IR, ^{1}H NMR, ^{13}C NMR and single crystal X-ray diffraction analysis. The photophysical results of (Z)-3-(2-fluorobenzyl)-4-[(thiophen-2-ylmethylene) amino]-1H-1,2,4-triazole-5(4H)-thione (6) corroborates its applicability as optical sensing platform for selective Fe^{3+} detection in pure organic as well as mixed organic-aqueous media. Through fluorescence titration at 478 nm, we were confirmed that the ligand 6 exhibited remarkable decline in the fluorescence intensity by complexation between 6 and Fe^{3+} while it appeared negligible fluorescent quenching in case of the competitive ions (Fe^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Ag^{+}, Zn^{2+}, Cd^{2+} and Hg^{2+}) in MeOH/water (8:2, v/v, pH 7) at ambient temperature. Meanwhile, the emergence of a new characteristic red shifted signal at 357 nm with gradual increment in the absorption intensity on gentle increase in the ferric ion concentration and continuous shifting in the ligand absorption bands after Fe^{3+} addition ascribed the conformational changes in the ligand structure upon Fe^{3+} binding. Due to simplicity, low cost, fast response time, considerable sensitivity of 2×10^{-7} mol/L and robustness, the proposed sensing method might be a practical tool for environmental samples analysis and biological studies.

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Two-dimensional chiral honeycomb structures of unnatural amino acids on Au(111)

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Crystallization has become the most popular technique for the separation of enantiomers since the Pasteur's discovery. To investigate mechanism of crystallization of chiral molecules, it is necessary to study self-assembled structures on two-dimensional surface. Here, we have studied two-dimensional self-assembled structures of an unnatural amino acid, (S)-β-methyl naphthalen-1-γ-aminobutyric acid (γ2-1-naphthylalanine) on the Au(111) surface at 150 K using scanning tunneling microscopy (STM) and high resolution photoemission spectroscopy (HRPES). According to our STM images, at initial stage, we found two chiral honeycomb structures which are counter-clockwise and clockwise configurations in one domain. The molecules are arranged around molecular vacancies, dark hole. By further increasing the amounts of adsorbed γ2-1-naphthylalanine, a well-ordered square packed structure was observed. In addition, we found the other structure that molecules were trapped in the pore of the hexagonal molecular assembly. In addition, the HRPES analysis results indicates that there are no bonding between γ2-1-naphthylalanine and Au(111). Therefore, γ2-1-naphthylalanine can form self-assembled structures by intermolecular interactions.

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Synthesis, characterization, biological and photophysical properties of novel 3,6-disubstituted 1,2,4-triazolo[3,4-b]1,3,4-thiadiazole derivatives

강충호 **Muhammad Saleem*** 이기환*

공주대학교 화학과

Fused heterocyclic compounds have established considerable attention for the development of organic light emitting diodes, electroluminescent material, dye sensitized solar cells, bioimaging, fluorescent labelling of biomolecules and cells due to their facile synthetic strategy, fascinating tunable optical characteristics and friendly nature toward biomolecules. This paper concerns the design, synthesis, structural characterization, thermal stability evaluation, biological and fluorescence properties of novel triazolothiadiazole derivatives. The target compounds were synthesized by condensing 4-amino-3-(4-methoxybenzyl)-1H-1,2,4-triazole-5(4H)-thione with various substituted carboxylic acid in the presence of phosphorous oxychloride. The structures of newly synthesized compounds were characterized by IR, ^{1}H NMR and ^{13}C NMR analysis. Photophysical properties including UV-visible absorption spectra, fluorescence emission spectra, molar absorption co-efficient, Stokes shift and the relative fluorescence quantum yield were measured in a variety of organic solvents of variable polarities. Spectral properties of the compounds were highly dependent on the nature of the substituent and coupling components attached to the triazolothiadiazole skeleton as well as slightly affected by the solvent polarities. Correlation of the absorption spectra and fluorescence emission response of 3,6-disubstituted 1,2,4-triazolo[3,4-b]1,3,4-thiadiazole derivatives with the substituent effect revealed that the fluorescent properties can easily be tuned by varying conjugation length of attached substituent. The newly synthesized derivatives represent a new type of fluorescent materials which could be a promising candidate for bioimaging, photonic applications, such as organic light emitting diodes and dye sensitized solar cells, which possess efficient visible absorption, higher quantum yields and surpassing brightness.

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A theoretical study on enhancement of CO_2 absorption in various blended amine solvents

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성균관대학교 화학과

Carbon dioxide is one of the greenhouse gases that cause the global warming. During last few decades, there were many efforts to remove CO_2 from the fossil fuel combustion fumes and control the CO_2 concentration in air. Nowadays, the interest in the solvents of blended amines is increased in order to find best blending combination for the CO_2 solubility and regeneration performance. In spite of many studies about the effect of blended amine solvent, there have been no appropriate literature data for understanding about the reaction mechanism and the reason of performance enhancement. Herein, a mechanism for the carbamic acid formation from the reaction of carbon dioxide and various amines which is a rate determining step during CO_2 capturing process was investigated by DFT calculations (B3LYP / 6-31G*). The reactants were CO_2 and amines (MEA, DEA, PZ, AMP, AEEA and DETA) and the reactions were designated without or with catalyst (water or amine). These catalysts play a role as proton donor and accepter, namely, they transfer proton form amino group of amine to oxygen of CO_2 moiety. Moreover, amine catalyzed process can be applied to understand the enhancement effect of CO_2 absorption in blended amine solvents. Among various blended amine solvents, the enhancement effect on the CO_2 absorption by additive amines was in the order of PZ > AEEA > DETA > DEA > AMP based on the activation energy, which is in excellent agreement with experiment. Our work should be useful in choosing a proper blended amine solvent for better CO_2 absorption.

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Mechanistic study of the interaction between Chiral ligand and substrate on Pd(111) for enantioselective hydrogenation

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The new efficient chiral ligand and α-β-unsaturated acid substrate were synthesized from (R) -1, 1’-bi(2-naphthol) and cinnamaldehyde. Asymmetric reaction with heterogeneous catalyst exhibited reasonably high activity for hydrogenation of α-β-unsaturated acid substrate. However, the interaction between ligand and substrate on Pd(111) has not been clearly revealed before. Thus, we report here the detailed phenomena of ligand and substrate using high resolution photoemission spectroscopy (HRPES) and nuclear magnetic resonance spectroscopy (NMR). The results of HRPES spectra and NMR spectrum clearly showed that interaction between chiral ligand and substrate on Pd(111) surface.

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IR-dip Spectroscopic Studies of Jet-cooled Acetaminophen-Water Clusters in the Gas Phase

민아름 안아름 문철주 이지훈 김성근[1] 최명룡[*]

경상대학교 화학과 [1]서울대학교 화학부

The conformational structures of jet-cooled acetaminophen (AAP) were investigated by resonant 2-photon ionization (R2PI) and UV-UV hole-burning (UVHB) spectroscopy. [*Phys.Chen.Chem.Phys.,2011,13,16537-16541*]. Recent investigation with IR-dip spectroscopy revealed that each conformer of AAP gives two independent transitions starting from the most stable $0a_1$ and the hot 1e internal rotational level. Further spectroscopic investigation of AAP-water clusters with an aid of IR-dip spectroscopy will be presented and discussed.

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Conformationally resolved structures of jet-cooled phenacetin and its hydrogen-bondedwater complex

<u>문철주</u> 민아름 안아름 이지훈 김경구 김성근[1] 최명룡[*]

경상대학교 화학과 [1]서울대학교 화학부

Phenacetin (PA) is one of the typical synthetic fever reducers as similar to acetaminophen (AAP), a major ingredient of Tylenol. PA and AAP are both derivatives of acetanilide (AA), substituted by ethoxyl group and hydroxyl group in the para position of AA, respectively. In this work, we present the conformational investigations and photochemistry of jet-cooled PA and its 1:1 hydrates using resonance enhanced multi photon ionization (REMPI), UV-UV hole-burning and IR-dip spectroscopy. Moreover we calculated the optimized structures of PA and its 1:1 hydrates by density functional theory (DFT). Here, we report the structural information of PA and its 1:1 hydrates with an aid of the experimental data and the ab initio calculations.

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Conformational structures of 3-cyanoindole-(H2O)n(n=0-2): Franck-Condon simulations

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경상대학교 화학과

Franck-Condon (FC) simulation was applied to 3-cyanoindole (3CI) and its water clusters (3CI-Wn, n = 1, 2) for the first time to determine their molecular structures using mass-selected resonant two-photon ionization (R2PI) and UV-UV hole-burning (UVHB) spectroscopy. R2PI and UVHB spectra were compared with the results of Franck-Condon (FC) simulation that can determine the change in a molecular geometry of 3CI-Wn (n = 0 - 2) on electronic excitation. It was found that the most stable structure for each 3CI-Wn (n = 0 - 2) was identified and their excited state geometries were little influenced upon excitation. For the 3CI-W2a cluster, we speculate that the S1 potential energy surface is significantly affected by anharmonicity.

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REMPI, UV-UV Hole-burning and IR-dip spectroscopic Studies of Jet-cooled 3-Acetaminophen

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경상대학교 화학과

We measured the excitation spectra of jet-cooled 3-AAP using resonance-enhanced multiphoton ionization (REMPI) in the gas phase. As a result, we obtained sharply congested REMPI spectrum of 3-AAP. Then, we identified that 3-AAP has two conformers via UV-UV hole-burning (0?0 bands of the cis and trans isomers were found at 35316.3 and 35237.3 cm$^{?1}$) and IR dip spectroscopy. Moreover, we also calculated the optimized structure of 3-AAP by density functional theory (DFT) with a 6-311++ G(d,p) basis set. Here, we report the structural information of 3-AAP by comparing the each experimental data and from the theory.

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Proton coupled electron transfer in an end-to-end loop forming peptide

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An electronically excited dye experiences fluorescence quenching by nearby tyrosine (Tyr), due to photoinduced electron transfer (PET). However, in case of intermolecular PET, it is difficult to observe fluorescence quenching because the water solubility of Tyr is not high enough. Therefore, we prepared a model peptide with which we can observe intramolecular PET involving Tyr. We used a dye-labelled tetrapeptide, fluorophore-Ala-Gly-Gln-Tyr where the electron transfer is expected to occur between photoexcited fluorophore and Tyr when the peptide forms an end-to-end loop. The fluorescence lifetimes of the model peptide were measured as a function of pH by using a time-correlated single photon counting (TCSPC) system and the PET rate constants were obtained from the measured fluorescence lifetimes as a function of pH. Dependence of the fluorescence lifetime of our model peptide on pH showed that the PET only occurs between dye and deprotonated tyrosine (YO-), strongly indicating that the process is proton coupled electron transfer.

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The effect of VC and FEC on the SEI film of the cathode in Li-ion battery at high voltage

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Li-ion battery has become a important power source of electric vehicles (EVs) and hybrid electric vehicles (HEVs) as well as portable devices due to its high voltage, high cyclablility and high energy density. However Li-ion battery has stability problems at high voltage owing to distortion of cathode structure, the formation of insulating film and generation of gas and heat. To improve the stability of cathode at high voltage, we used organic additives such as vinylene carbonate (VC) and fluoroethylene carbonate (FEC) in the electrolyte. In this study we analyzed the surface-electrolyte interface (SEI) film on the cathode with organic additives at high voltage by using charge-discharge testing, electrochemical impedance spectroscopy (EIS), cyclic voltammetry and spectroscopies. We also performed 2-dimensonal correlation spectroscopy to understand the mechanism of reaction on the surface of the cathode. The results show that the additives delay the formation of carbonates on the surface and enhance the performance of the cathode. The effect of additives on Li-ion battery will be discussed in detail.

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Optical and biological properties of some novel 4,5-disubstituted 1,3,4-oxadiazole derivatives

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공주대학교 화학과

A series of four 4,5-disubstituted 1,3,4-oxadiazole derivatives with various length of conjugation have been synthesized by treating the substituted aromatic acid hydrazides with substituted aromatic acids in the presence of phosphorus oxychloride under reflux conditions. All the synthesized compounds were characterized by FT-IR, ^{1}H NMR and ^{13}C NMR analysis. Optical properties including UV-visible absorption spectra, fluorescence emission spectra, molar absorption co-efficient, Stokes shift and the relative fluorescence quantum yield were measured in a variety of organic solvents. Solvatochromism studied was done in a varieties of organic solvent of different polarities and spectral properties of the compounds were found to be affected by the nature of substituent and coupling components attached to the oxadiazole skeleton as well as slightly affected by the solvent polarities. The synthesized compounds were further employed for enzyme inhibition activities through spectrophotometric bioassay, interestingly some of the derivatives exhibited admirable enzyme inhibition activities against the tested bioassay.

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Aggregation Kinetics of Ferric Hemoglobin Probed by Infrared Spectroscopy

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부산대학교 화학과

Protein aggregation is an important phenomenon that alternatively is part of the normal functioning. Nature has negative consequences via its suggested central role in neurodegenerative diseases. A key to controlling protein aggregation is the knowledge on the kinetics of protein aggregation. We have measured aggregation kinetics of ferric hemoglobin at various temperatures by probing the changes of the amide bands and the background absorption near 4000 cm^{-1}. We assumed that the background absorption increases due to scattering by the aggregated protein and the change in the amide band arise from unfolding as well as the aggregation of the unfolded protein. For the sake of the simplicity, we also assumed that the aggregation proceeds via the addition of the unfolded protein to the aggregated one and the aggregation rate is independent of the size of the aggregated protein. The recovered rate constants for folding, unfolding, and aggregation are 0.025 ~ 0.054, 0.011 ~ 0.025, and 0.003 ~ 0.007 min^{-1}, respectively at the temperature range of 55 ~ 64℃. The activation energy for the folding, unfolding, and aggregation was found to be about the same, 81 ± 1 kJ/mol. Implication of these findings will be presented.

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Influence of double D-π-A configurations on the efficiencies of dye-sensitized solar cells

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군산대학교 화학과

Two double D-π-A branched organic dye linked at the thiophene bridge were designed and synthesized for dye-sensitized solar cells. Their photophysical, electrochemical, and photovoltaic properties were investigated. As compared to the reference dye isomer containing a single D-π-A branch, the double D-π-A branched dye isomer consisting of two separated light-harvesting moieties in one molecule are beneficial to photocurrent generation provided that they are properly separated not to introduced exciton annihilation, as shown with the results. A 17 % increase in conversion efficiency was achieved in double D-π-A branched organic dye as compared to the reference dye under simalated AM1.5G solar irradiation.

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XY-H---X'(X, X'=F, Cl, Br, CN; Y=O, S) 저-준위 전자 상태들의 전하 분포 특성과 해리-동역학 경로의 에너지 특성과 비-단열 짝지음 특성에 대한 양자화학 계산연구

문자연 안희선 백경구*

강릉원주대학교 화학과

비-공유 상호작용을 가지는 간단한 실제 화합물인 XY-H---X' (X, X'=F, Cl, Br, CN; Y=O, S) 음이온의 분자구조와 진동 특성을 여러 ab initio 방법과 DFT 방법으로 계산한 후, 해당 중성 분자의 저-준위(Low-lying) 들뜬 전자상태들의 수직-들뜸 에너지를 IP-EOMCC 및 TD-DFT 방법으로 구하고, 각 전자 상태의 전하분포 특성을 분석하였다. 중성분자들의 여러 가능한 해리 경로들의 해리 한계와 전이상태(TS) 구조의 에너지 특성을 탐색하고, 해리 과정에 대한 엄밀한 양자 동역학 연구에서 요구되는 비-단열 짝지음 특성을 조사하였다. 치환기(X, Y, X')가 이들 특성에 미치는 영향의 경향성을 중심으로 분석하였다. 본 연구는 양성자-짝진 전자-이동(PCET)[1]에 엄밀한 양자 동역학을 적용한 최근의 연구 성과[2]를 한 단계 더 확장하려는 탐색 과정에 해당한다.

[1] R. I. Cukier, D. G. Nocera, Annu. Rev. Phys. Chem. 1998, 49, 337; S. Hammes-Schiffer, A. A. Stuchenbrukhov, Chem. Rev., 2010, 110, 6939.

[2] H. An, K. K. Baeck, J. Phys. Chem. Lett., 2014, 5, 1307.

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The reaction of hydrogen bromide with hydroxyl radical on temperature between 20 and 2000 K

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The main theme of the present research is to study the temperature dependence of the reaction H' Br + OH → Br + H'OH using analytic forms of the interaction potential energies in quasi-classical trajectory calculations over the range of room temperature down to 20 K. The overall potential energy is formulated in terms of two-, three-, four-body and long-range interactions. The potential energy yields well behaving potential energy surfaces and a potential well with the depth of -4 kcal mol^{-1} forming strong hydrogen bonds in the entrance channel. Below 300 K, the reaction is attraction-driven and occurs through the formation of a collision-complex BrH ... OH, which is sufficiently long-lived to enhance H-atom tunneling. A strong negative temperature dependence of the complex mode rate is found between 20 and 300 K consistent with the experimental data reported by various authors. Above 300 K, the reaction occurs primarily through a direct-reaction mechanism. The sum of the complex- and direct-mode rates is shown to describe the reaction over the wide range of 20 - 2000 K. The primary kinetic isotope effect is nearly constant with the normal H reaction faster by ~1.8 over the entire temperature range. The product energy distribution in vibration, rotation and translation at 300 K is found to be 40, 9 and 51 %, respectively. More than 90 % of the H_2O vibrational energy is distributed in the symmetric and asymmetric modes and the rest in the bending mode.

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Analysis of pH-dependent IR and Raman spectra for alpha-lactalbumin

박연주 김예슬 **Boguska Czarnik-Matusewicz**[1] 정영미[*]

강원대학교 화학과 [1]Faculty of Chemistry, University of Wroclaw

alpha-lactalbumin (α-LA) is one of the globular proteins, which can be converted to the intermediate state from both the apo-form (calcium-depleted) and the holo-form (calcium-containing) by various physical or chemical agents. The study of the intermediate state is currently important to enhance our understanding of the structures of these proteins. Despite some common features, a coherent picture of the intermediate state is still subject of debate and independent investigations are necessary for each case. In this study, pH-induced transition of holo-form of bovine α-LA from the native to the intermediate state was analyzed by IR and Raman spectroscopy. The results of two-dimensional correlation spectroscopy (2DCOS) combined with principal component analysis (PCA) of α-LA with decreasing pH will be discussed more details.

Acknowledgments This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (No. NRF-2012R1A1A3011844).

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Structure and Residual Hydrophobicity of Zn^{2+} Bound Amyloid β-Peptide (1-40/42)

SHIHU Kang baotao 김선경 문종훈 박영근 조대흠 이진용*

성균관대학교 화학과

The aggregation of amyloid β-peptide (Aβ peptide) has been associated with the pathogenesis of Alzheimer's disease (AD). In present study, we aimed to disclose how Zn^{2+} affects the Aβ aggregation in detail. Thus, molecular dynamics simulation was implemented to elucidate the changes of structure and residual hydrophobicity upon Zn^{2+} coordination. Our results show that Zn^{2+} can strongly influence the structural properties of Aβ40 and Aβ42 by reducing helical formation and increasing turn formation to expose the hydrophobic regions. Furthermore, hydrophobicity of Zn^{2+}-Aβ40 and Zn^{2+}-Aβ42 was much higher than that of each monomer, since Zn^{2+} binding can significantly influence the hydrophilic domains of Aβ. The further analyses indicate that not only four residues (H6, E11, H13, and H14) but also R5, D7, K16, K28, and terminal residues influence hydrophobicity upon Zn^{2+} coordination. Importantly, R5, K16, and K28 play a crucial role to regulate solvation free energies. This work is helpful to understand the fundamental role of Zn^{2+} in aggregation, which could be useful for further development of new drugs to inhibit Zn^{2+}-Aβ aggregation.

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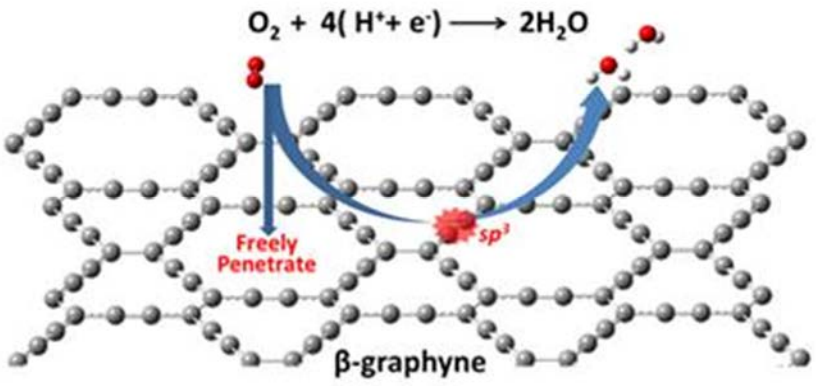
Graphynes as Promising Cathode Material of Fuel Cell: Improvement of Oxygen Reduction Efficiency

Kang baotao **SHIHU** 문종훈 박영근 김선경 조대흠 이진용*

성균관대학교 화학과

The sluggish kinetics of oxygen reduction reaction (ORR) on cathode is an invariable bottleneck in fuel cell industry. Recently, a rising 2D carbon allotrope, graphyne with fascinating properties, appears to be a potential candidate to promote fuel cell performance. We investigated ORR process on three different graphyne models by density functional theory calculations. Due to the acetylenic linkage (-C≡C-) insertion, some carbon atoms in graphyne are positively charged to facilitate O_2 dissociation. It was found that the first two-hydrogen addition produces a water molecule, then next two hydrogens furnish another water formation accompanying with the recovery of graphyne planarity. The ORR process on three graphyne models exhibits an efficient four-electron process. Moreover, the 18-membered rings in α- and β-graphyne allow O_2 penetration nearly barrierlessly, hence to improve ORR efficiency. Our results imply that α- and β-graphyne systems are promising cathode materials to promote the performance of fuel cell.



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The reaction of cyanoethyl radical(C_3N) with ethylene including H elimination: Theorical investigation

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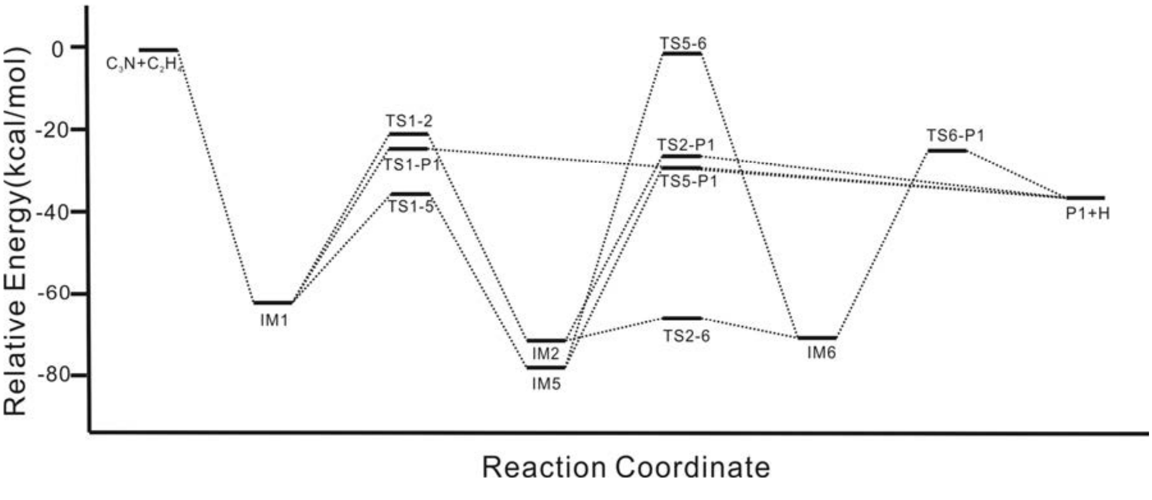
가톨릭대학교 화학과 [1]한국표준과학연구원(KRISS) 대기환경표준센터

The reaction mechanisms of the cyanoethyl radical (C_3N) with ethylene (C_2H_4) to form C_5H_3N and H are investigated using the density functional theory and high-level ab initio method such as CCSD(T). In addition, the natural population analysis (NPA) was also performed to characterize the electronic structure. We categorize the complicate reaction pathways into two types. One type proceeds through only the chain intermediates without any ring components. Another type contains ring intermediates. According to the calculated results, the most favorable reaction pathway is the first types; H elimination from the initial chain adduct of C_3N with C_2H_4. Since cyanoethyl radical is isoelectronic to butadiynyl radical (C_4H), we compare the reaction mechanisms of C_3N with C_2H_4 with those of C_4H with C_2H_4.



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Diabatic potential-energy-surfaces constructed by using an analytic function for the non-adiabatic coupling terms, and there use in quantum wave-packet propagations for a non-adiabatic chemical dynamics

안희선 백경구*

강릉원주대학교 화학과

The quantitative aspects of quantum dynamical study for non-adiabatic processes heavily depend on the reliability of the potential-energy-surfaces (PESs) of the work, especially the coupling term between them. To be more rigorous then the previous work,[1,2] the non-adiabatic coupling (NAC) terms between the ground and the excited charge-transfer (CT) states are calculated rigorously by using the multi-reference configuration interaction plus Davidson correction (MRCI+Q) method. An analytic function is used to overcome the singularity problem in the computation of the NAC near the conical intersections between electronic states. A constraint is also applied in the path integral for the mixing angle to ensure the correct behavior of the angle. Then, the diabatic PESs and their coupling term are determined by using the adiabatic PESs and the mixing angle. The results of quantum wave-packet propagations with our new PESs are compared with the corresponding ones of our earlier works for FH--Cl[1] and H_2NH--Cl [2].

[1] H. An, K. K. Baeck, J. Phys. Chem. Lett. 5, 1307 (2014).
[2] Y. C. Park, H. An, H. Choi, Y. S. Lee, K. K. Baeck, Theor. Chem. Acc. 131, 1212 (2012).

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Aggregation effect of silver nanoparticles to the energy conversion efficiency of the surface plasmon-enhanced dye-sensitized solar cells

김현영 서정쌍*

서울대학교 화학부

We have fabricated Ag nanoplates that have two broad extinction bands in visible region, which are found in similar spectral regions of two visible absorption bands of N719 dye. The efficiency of the dye-sensitized solar cells (DSSCs) based on composite films consisting of TiO2 and Ag nanoplates was affected by the degree of the spectral overlap between these bands and weight percent of Ag nanoplates to TiO2 nanoparticles (NPs). By optimizing the size and geometry of Ag nanoplates to match to the absorption of N719 dye and the weight percent of Ag nanoplates to TiO2 NPs, the energy conversion efficiency was improved from 8.7% to 10.3%. The energy conversion efficiency was significantly enhanced by including Ag nanoplates. The efficiency increased up to 0.35 wt% of Ag nanoplates but then decreased as the weight percent was increased further. The cause of the efficiency decrease was studied. The extinction of the TiO2 NP/Ag nanoplate composite films adsorbed N719 dye was the highest when the weight percent of Ag nanoplates was 0.35 w%, while that adsorbed black dye increased with increasing the weight percent up to 0.7 w%. N719 dye has two strong absorption bands centred at 393 and 533 nm, while black dye centred near at 410 and 610 nm. Since the in-plane mode of the localized surface plasmon of Ag nanoplates is red-shifted when Ag nanoplates are aggregated, an enhanced absorption of black dye is expected on or near the surface of the aggregated Ag nanoplates. This means that aggregation of Ag nanoplates took place significantly when the percent was higher than 0.35 w%. By aggregation, the efficiency of the plasmon enhanced absorption of N719 dye would be decreased, and the energy conversion efficiency was decreased.?

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Surface Plasmon-Enhanced Dye-Sensitized Solar Cells Based on Double-Layered Composite Films Consisting of TiO2/Ag and TiO2/Au Nanoparticles

송다현 서정쌍* 김현영

서울대학교 화학부

We have fabricated silver and gold colloid particles, and used them to fabricate surface plasmon-enhanced dye-sensitized solar cells (DSSCs) based on N719 dye. N719 dye, which is the most heavily used dye in DSSCs, has two strong visible absorption bands centered at 393 and 533 nm. The localized surface plasmon absorption band of Ag nanoparticles (NPs) was well matched with the higher energy band of N719 dye, while that of Au NPs with the lower one. The energy conversion efficiency was significantly improved from the DSSCs based on double-layered composite films; the bottom layer consisted of TiO2 and Ag NPs, while the top one consisted of TiO2 and Au NPs. The efficiency was 10.0%, which was almost the same as the highest value reported on the surface plasmon-enhanced DSSCs. The high efficiency might be due to a good energy matching between the extinction bands of Ag and Au NPs and absorption bands of N719 dye.

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"Comparison of CH3CH2OH and CH3CH2SH in the reaction with atomic hydrogen on ZnO(0001 ?)"

MOTINABDUL 김창민*

경북대학교 화학과

The thermal reaction of ethanol and ethanethiol on a ZnO(0001 ?) surface was studied with and without the presence of co-adsorbed atomic hydrogen using a Temperature Programmed Desorption (TPD) technique. Ethanol decomposes on clean ZnO(0001 ?) to produce acetaldehyde at ~ 506 K, molecular hydrogen at ~ 525 K, ethylene at ~ 540 K, and carbon monoxide at ~730 K. In the case of thermal decomposition of ethanethiol on clean ZnO(0001 ?), the decomposition products are ethylene at ~ 510 K, water at ~ 520 K and carbon dioxide at ~ 570 K. When ethanol co-adsorbed atomic hydrogen, a new ethylene desorption feature at ~ 485 appears, and desorption peak at ~ 540 K is attenuated as the coverage of H increased. In contrast, when ethanethiol is co-adsorbed with hydrogen a new desorption feature appears at 665 K, the peak has been identified as ethylene. The difference of ethanol and ethanethiol in the surface reaction is attributed to the acidity of two compounds.

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Computational Modeling of the Initial Steps in Copper Oxide-Catalyzed Formation of Poly-Chlorinated Dibenzo Dioxins and Furans

배균택

충북대학교 사범대학 화학교육과

Metal oxide nanoparticles catalyze the formation of hazardous materials including polychlorinated dibenzo dioxins and furans. These nanoparticles are widespread in the environment. A proposed mechanism for the catalysis involves the presence of a metal oxide bound free radical formed by a reaction of phenol or a chlorinated phenol with the hydroxylated surface of the metal oxide. Density functional theory calculations were used to study the reactions of phenol and chlorinated phenols with hydroxylated neutral copper oxide clusters, $(CuO)_n$ with n=1-8. Reaction energetics used to determine the most probable reaction sites on the clusters and the molecular orbitals of the products and the change of Bader charges during the reactions were used to assess the proposed mechanism. Molecular orbitals show the presence of a radical localized on the phenolic species and the Bader charges show a small degree of electron transfer from the phenolic species to the metal oxide cluster. Both results are consistent with the proposed mechanism.

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Theoretical Study on Chemical Reactions of Fluorine-Containing Plasma Molecules

최희철

국가핵융합연구소 플라즈마기술연구센터

Chemical and physical properties of fluorine-containing plasma molecules (C_4F_6, C_4F_8 and NF_3) were elucidated with the aid of DFT and CC methods. The geometries and activation barriers of intermediates and transition states in a variety of isomerization and dissociation channels were presented at the level of ωB97X-D/aug-cc-pVTZ for a deep insight into their mechanisms. Especially, the geometry, energy, and spectroscopic properties of low-lying electronic states of NF_3 were calculated at CCSD(T)/aug-cc-pVTZ and the Lennard-Jones parameters of NF_3 dimers were obtained by constructing BSSE-corrected potential energy surfaces at ωB97X-D/aug-cc-pVTZ. Our theoretical values in this work can be provided to further plasma process simulations as initial parameters and would be used as key information for analysis and prediction of F-containing plasma process.

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Ultraclean, Ultraflat and Perfect-Crystal Gold Nanoplate : Premier Protein-immobilizing Surface

이미연 이효반 김봉수*

한국과학기술원(KAIST) 화학과

Self-assembled monolayers (SAMs) is one of the most important issues of the 21st century. SAMs is readily formed by attaching thiolated molecules on a gold film, but there exist numerous defects on the gold surface. We can synthesize Au nanoplate having perfect crystallinity without defects and atomically smooth surface by heating a lump of gold and then transporting the metal vapor onto the substrate at low temperatures in downstream. Highly ordered molecular arrangement could be constructed by attaching thiolated molecules via covalent bond on the Au substrate without a domain boundary or irregular steps on the surface. We research depending on several variables (e.g. substrate, concentration, and buffer) that can affect the structure of IgG on the binding protein layer using cysteine-tagged protein G. In order to compare the topologies of variety variable, roughness was estimated from the AFM images. Adsorption of cysteine-tagged protein G on Au nanoplate surface is highly ordered. This result reveals that our Perfect-Crystal Au nanoplate can better orientation of immobilized antibodies.

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Fast Read-out System for Chip-based Immunoassay Using SERS nanoprobes

장혜진 고은별 이윤식[1] 정대홍[*]

서울대학교 화학교육과 [1]서울대학교 화학생물공학부

Surface-enhanced Raman scattering (SERS)-based techniques are widely used for bioassay because of its high sensitivity and multiplex capacity. However, the conventional micro-Raman system has disadvantages for measurement of chip-based immunoassay owing to the limited field of view (~ 1 μm^2 of beam diameter). SERS imaging techniques are the possible alternatives, however, still suffer from long mapping times required for detection of large area. To resolve this problem, we designed the methodology for quantitative measurement of large area (maximum of 200 μm x 200 μm) by confocal scanning. The developed read-out system, referred to fast Raman scanning system, generated a single spectrum which contains averaged characteristic of 2-dimensional area in a single scanning with short duration. Compared with the case of point-based mapping, signal to noise ratio (SNR) increased by 4-fold, while acquisition time decreased by one-eighth. And also, measurement of SERS dot distributed on the substrate by fast Raman scanning system indicated the feasibility of Raman based quantification for 2-dimensional area. The system was applied to immunoassay of prostate specific antigen (PSA) with SERS nanoprobes. The sandwich-type immunoassay based on glass substrates exhibited detectable dynamic range of 0.001 - 1000 ng/ml, and the limit of detection was 0.13 pg/ml.

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Theoretical models for predicting the oxidation potentials of organic additives in Carbonates solvent

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중앙대학교 화학과 [1]군산대학교 화학과

Lithium-Ion Batteries (LIBs) technology has been developed for many years. It had been emphasized that the oxidation potentials of LIBs were experimentally evaluated in terms of the efficiency of batteries industries. By the use of computational modelling last decades, it is well known that oxidation potentials on the results of experiments of cyclic voltammetry are consistent with those of quantum calculations.In this study, we suggest that quantum chemical calculations are performed in implicit solvation models with gaussian09 program for predicting the oxidation potentials by using the thermodynamic cycles. We apply the implicit solvent models to calculate the oxidation potentials in carbonates solvent, which is evaluated and predictable for several additives. In thermodynamic cycles, the ionization potentials and solvation energy of the neutral additives are well explained. On the other hand, it has a shortcoming that the solvation energy of the charged additives with the implicit solvation model is not correct.

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Formation and Structure of Self-Assembled Monolayers by Adsorption of Otaneselenocyanates on Au(111)

한슬기 노재근* 한진욱 강훈구 박희건

한양대학교 화학과

Alkanethiol self-assembled monolayers (SAMs) on metal surfaces have been frequently used for various practical applications. However, one of the drawbacks encountered during the formation of organosulfur SAMs is that the thiol group can be oxidized to disulfides and/or other oxidized compounds during SAM formation in solution. To overcome this problem, SAMs prepared using organic selenocyanates having high chemical oxidation stability were fabricated and characterized by cyclic voltammetry (CV) and scanning tunneling microscopy (STM) in this work. Octaneselenocyanate (OSC) on Au(111) was prepared by using both solution and ambient-pressure vapor deposition methods. STM observation showed that the adsorption of OSC SAMs on Au(111) by solution deposition had relatively long-range ordered domains and few vacancy islands, whereas the OSC SAMs by ambient-pressure vapor deposition had relatively smaller ordered domains, multiple small bright spots (due to aggregation), and irregular shaped vacancy islands. CV measurements showed that reductive desorption potential for OSC SAMs was higher than that for OT SAMs, which means that the Se-Au interaction for OSC SAMs is stronger than the S-Au interaction for OT SAMs.

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Displacement of Cyclohexanethiolate and Cyclohaxaneselenolate Self-Assembled Monolayers on Au(111) by Alkanethiols: Headgroup-Gold Interactions

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Selenol (Se)-based self-assembled monolayers (SAMs) have drawn much interest in nanoscience and technology due to their superior structural and long-range order properties compared to thiol (S)-based SAMs. We have investigated the difference in bond strength between S-Au and Se-Au using displacement method. In this study, dicyclohexyl disulfide (DCDS) and dicyclohexyl diselenide (DCDSe) with an identical cyclohexyl ring as a tail group were used for obtaining pre-covered SAMs. We found that the packing structure of these SAMs on Au(111) surface is remarkably different from each other due to a difference in headgroup-gold interactions. Pre-covered cylcohexanethiolate (CH-S) SAMs or cyclohexaneselenolate (CH-Se) SAMs were replaced by octanethiol (or decanethiol) for 20 min, 1, and 2 hr. It was found that structural change of CH-Se SAMs is minimal as a function of displacement, while structure of CH-S SAMs were totally changed due to displacement of these molecules by alkanethiols. Therefore, we conclude that the bond strength of Se-Au is much stronger than that of S-Au.

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Alkyl Spacer Effect on the Formation and Stability of Self-Assembled Monolayers of Benzenethiol and Benzenemethanethiol on Au(111)

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한양대학교 화학과

The surface structure, adsorption condition, and thermal desorption behaviors of benzenethiol (BT) and benzenemethanethiol (BMT) self-assembled monolayers (SAMs) on Au(111) were examined by means of scanning tunneling microscopy (STM), X-ray photoelectron microscopy (XPS), and thermal desorption spectroscopy to understand the effects of the alkyl spacer between the phenyl group and sulfur atom. Although XPS spectra for both SAMs are nearly the same, the surface structures and thermal desorption behaviors significantly differ from each other. BT SAMs on Au(111) were composed of disordered phases, whereas BMT SAMs have well-ordered phases containing vacancy islands. It was found that the strong desorption peak for parent mass species (m/z = 110, $C6H5SH+$) was observed from BT SAMs at about 500 K, whereas no desorption peak for them (m/z = 124, $C6H5CH2SH+$) was observed from BMT SAMs. Interestingly, the dominant TD peak for the benzyl fragments (m/z = 91, $C6H5CH2+$) formed via the cleavage of C?S bond was observed from BMT SAMs at around 400 K. From this study, we clearly revealed that the small modification of chemical structure of molecules by inserting of a methylene spacer between the phenyl group and sulfur atom affects 2D SAM structures, adsorption conditions, and thermal desorption behaviors and stability.

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Surface morphology control and enhanced scattering properties of Silver nanoshell

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Controlled synthesis of the metal nanoparticles (NPs) is an important issue due to distinct optical properties of its metal NPs depend on their size, shape and surface morphology. Especially, nanoshell structure have gained much attention for their tunable surface plasmon resonance bands just by varying the ratio of core size to metallic shell thickness or controlling surface morphology of metallic shell. In that sense, a controlling surface morphology of metal nanoshell is one of the key factors to regulate surface plasmon resonance and scattering properties of such NPs. In previous reported papers, surface morphology control of gold nanoshell has been studied by changing surfactant such as cetyltrimethylammonium bromide (CTAB) or their halide derivatives. However, they have several problems such as a using of an excessive amount of bulky surfactant and time-consuming multi-step processes.In this poster, we present one-step and a surfactant free synthesis for controlling morphology and thickness of silver nanoshells using alkylamines as a reductant and capping agent. As alkylamines, the butylamine, 3-amino-1-propanol, ethanolamine, octylamine, dodecylamine, hexadecylamine and tributylamine were used for studying on effects of an alkyl chain length, an existence of hydroxyl group, and the number of alkyl chain in silver shell formation, which result in a change on surface morphology and thickness of silver shell. And, optical properties of silver nanoshells were investigated by observing near-field and far-field scattering at the single particle levels.

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Infrared near-field mapping of twisted bilayer graphene

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We have investigated by infrared and visible scattering-type scanning near-field optical microscopy (Vis- and IR- s-SNOM) in the linearly polarized lights from wavelengths of 633 nm and 3.391um. The bilayer graphene prepared by chemical vapor deposition (CVD) is twisted bilayer graphenes and then relocated onto silicon substrates covered with a 300 nm thermal oxide layer. Twisted Bilayer graphenes (tBLG) are composite of two single layer graphenes with variable twisted angles between top and bottom layers. The typical dimensions of tBG randomly growth by CVD method are ~20 um. We experimentally display that localized optical conductivity maps of tBLGs a demonstrated with the Beranal (AB) stacking and the non-AB stacking order domains in tBLGs. It also demonstrates that near infrared microscopy technique is a great tool to observe high resolution localized conductivity maps different in tBLGs.

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Preparation of a Zn/Ag complex superhydrophobic surface

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Superhydrophobic is a ubiquitous phenomenon in the natural world that is very interesting and of great value for research and applications.[1] A surface is generally defined as superhydrophobic if it possesses a large contact angle (>150°) and a very small sliding angle ($^{-3}$ mol/L $AgNO_3$ solution for a period of time. The substrate exhibited excellent superhydrophobic properties, with a contact angle 167° and a sliding angle less than 2°.

References

[1]J. Wang, Y. Zhang, S. Wang, Y. Song and L. Jiang, *Acc. Chem. Res.*, **2011**, *44*, 405-415.
[2]Y. Xiu, L. Zhu, D. W. Hess and C. P. Wong, *Nano Lett.*, **2007**, *7*, 3388-3393.

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Prediction of Heat of Formation of Nitro derivatives of Azoles using G4MP2-SFM scheme

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The nitrogen containing heterocycles, Azoles, are of high interest as the basis for a new generation of high energy density materials for use as propellants and explosives. The heats of formation of Pyrrole, Imidazole, Pyrazole, Triazole, Tetrazole and Pentazole with their nitro derivatives have been studied. A fast and highly accurate prediction procedure has been established to predict the heat of formation, using the parameterization scheme, G4MP2-SFM, combining SFM (Systematic Fragmentation Method) and high accuracy G4MP2 theories for these compounds. We suggest the parameterization scheme of groups (fragment) of SFM whose heats of formation are predicted by G4MP2. In the applications to 48 NO2 derivatives of azoles, our G4MP2-SFM (opt) yielded an overall MAD (mean absolute deviation) of 2.2 kcal/mol and RMSD (root mean square deviation) of 2.9 kcal/mol, as compared to full G4MP2 values, which determines its high prediction accuracy and statistical stability replacing the further quantum mechanical calculations with a set of simple calculation. This reliable method confirms that accuracy is not necessarily enhanced by greater complexity as well as gives the simplest and easiest pathway for the calculation of gas phase heat of formation of energetic compounds.

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Kinetic Isotope Effect as a Probe of Spin-Crossover in the C-H Activation of Methane by FeO^+ Cation: A Theoretical Study

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Two-state reactivity (TSR) or multi-state reactivity models are usually used to explain the reaction of high-valent transition metal-oxo reagents in the bare form or in complex with heme or non-heme ligand. The evidences for TSR model usually come from theoretical calculation, which shows a spin-crossover in the rate-determining step, but not in experimental data. In order to demonstrate the validation of TSR, the gas phase methane hydroxylation by bare FeO^+ cation, which can happens at quartet or sextet spin state, is explored. Direct reaction dynamics approach was used to calculate rate constants and KIEs using variational transition state theory including multidimensional tunneling based on the potential energy surfaces of the sextet and quartet H-transfers generated at the B3LYP/def2-TZVPP level. The minimum energy crossing point is very close to the minimum energy paths of the sextet and quartet H-transfer. We demonstrated that the interplay of experimental and theoretical studies for the H/D KIEs could be used to uncover the spin crossover in the H-transfer reaction involving transition metal complexes.

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Adsorption and Various Reaction Mechanisms of SO2 on Ice Surface

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Theoretical calculations have been carried out regarding the adsorption and reaction mechanism of SO2 on ice surface with the help of DFT/6-311++G(d,p) basis set using our QM/EFP scheme. At first SO2 physically adsorbed on ice surface and then H2SO3 formed by chemical adsorption. It was found that reaction barrier depends on surface heterogeneity as well as ice surface model and the net barrier of H2SO3 can be as low as 0.2 Kcal/mol. Reaction barrier found in this study is 18.8 kcal/mol, which is about 3 kcal/mol lower than previous studies indicating that H2SO3 can be easily formed. Further, using large ice cluster model various reaction mechanisms of SO2 is observed.

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Self-Assembly of Polyethylenimine-Capped Au Nanoparticle Films with Controlled Interparticle Distances and Their Application as SERS Substrates

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Accurate control over interparticle distance between nanoparticles while creating effective and homogeneous surface-enhanced Raman scattering (SERS) substrates is crucial to exploit an enhanced electromagnetic field. In this study, we investigated the self-assembly of large-area 2-dimensional (2D) films of polyethylenimine (PEI)-capped Au nanoparticles on a glass substrate with varying interparticle distances, which can be controlled by the alkyl chain lengths, ranging from C2 (ethanethiolate) to C10 (1-decanethiolate) at the hexane-water interface. These 2D films show strong collective localized surface plasmon resonance (LSPR) extinction bands which are tunable via near-field coupling of adjacent Au nanoparticles. Pronounced chain-length-dependent red shifts of LSPR bands have been observed for the PEI-capped Au films. The obtained PEI-capped Au nanoparticle films exhibit distinct interparticle-distance-dependent SERS characteristics and are useful in the development of plasmon-based analytical devices, specifically SERS-based biosensors.

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Fabrication of Au Nanoparticles Grown on Polyelectrolyte Multilayered Films for Efficient Surface-Enhanced Raman Scattering

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숭실대학교 화학과

We report a facile method for the fabrication of Au nanoparticles grown on polyelectrolyte multilayered films and application as surface-enhanced Raman scattering (SERS) substrates. The multilayered films were constructed via a layer-by-layer deposition method of aliphatic polyelectrolytes, such as anionic poly(acrylic acid) and cationic poly(ethylenimine), on the glass surface. Then, Au nanoparticles are readily prepared using butylamine as the reductant of $HAuCl_4$ on top of the polyelectrolyte multilayered films. Our method not only alleviates the costly and time-consuming amino-silanization process of glass substrates but also is suitable for the preparation of highly dispersed Au nanoparticles on any solid substrates possibly coated with polyelectrolytes. These Au films have been shown to possess very homogeneous morphology and high SERS activity, suggesting that the present fabrication protocol must be invaluable in the development of plasmonics and SERS-based analytical devices.

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Tip-Enhanced Fluorescence with nanoparticle attached scanning probe

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서울대학교 화학과 [1]포항공과대학교(POSTECH) 화학과

We carried out tip-enhanced fluorescence(TEF) by using a specialized tip to which Au nanostar hybrid(NS) is attached. We combine a confocal microscope with a radially polarized light at 532 nm wavelength and a non-contact mode atomic force microscope(AFM) fitted with the NS probe. The spatial resolution and signal enhancement is evaluated with 20 nm dyed polystyrene bead. We find an improved optical resolution below 50 nm with sufficient signal enhancement.

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Fabrication and Luminescence Properties of Silica Nano spheresIncorporated with $[Eu(ethylN_2O_2)_2]^-$ and $[Eu(propylN_2O_2)_2]^-$

함아리 강준길*

충남대학교 화학과

Two Schiff bases, $EthylN_2O_2H_2$ (2,2'-(1E,1'E)-(ethane-1,2-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol) and $PropylN_2O_2H_2$ (2,2'-(1E,1'E)-(propane-1,3-diylbis(azan-1-yl-1-ylidene))bis(methan-1-yl-1-ylidene)diphenol) were synthesized by necleophilic addition of ethylenediamine or 1,3-diaminopropane and salicylaldehyde. The synthesized Schiff bases were characterized by EA, IR, NMR, UV. Eu(III) complexes with $[EthylN_2O_2]^{2-}$ and $[PropylN_2O_2]^{2-}$ were synthesized, and their crystal structure and luminescence properties were characterized. Furthermore, the complexes were incorporated to SiO_2 nanospheres (NSs) as outer-shell and core-shell. The morphology of Eu(III) complex-incorporated SiO_2 NSs were confirmed by FE-SEM and TEM. Luminescence properties of the SiO_2 NSs were investigated as a function of temperature. The Eu(III) complexes excited at UV and emitted sensitized luminescence via the energy transfer from Schiff base ligands to Eu(III). The efficiency of the sensitized luminescence was markedly enhanced by incorporating as outer-shell. The luminescence enhancement could be associated with the surface extension of the complex, resulting in the reduction of non radiative transitions.

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The interaction of Copper (I) hexafluoro-2,4-pentanedionate-cyclooctadiene with atomic hydrogen: UHV study of the CVD process on Si(100)

SAHASUVASREE* 김창민*

경북대학교 화학과

The interaction of Copper complex, Copper(I) hexafluoro-2,4-pentanedionate-cyclooctadiene (COD-Cu-hfac) on Si(100) in the presence/absence of atomic hydrogen has been studied by using Temperature programmed Desorption(TPD) technique, Auger Electron Spectroscopy and LEED. We carried out this experiment to elucidate the surface reaction mechanism of COD-Cu-hfac in the CVD process of Cu on Si. We will present the detailed reaction mechanism of the CVD process on Si.

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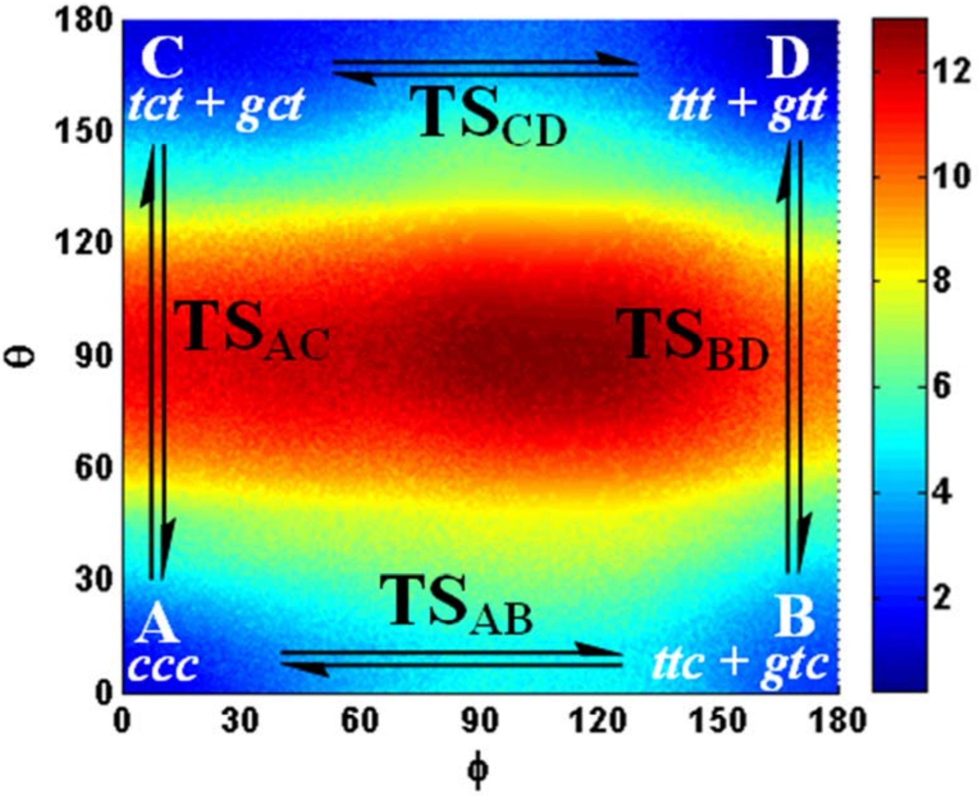
Torsional Isomers of Non-ionized Glycine in Water Solution by QM/EFP-MD

Manik Kumer Ghosh 최철호*

경북대학교 화학과

As building blocks of proteins, amino acids have been the subject of a variety of experimental and theoretical studies. Although glycine is the smallest amino acid, it is nevertheless sufficiently large and has enough conformational flexibility such that its complete description poses a formidable challenge to computational chemists. The conformational potential energy surface of non-ionized glycine has been studied by using high level ab initio electronic structure calculations in gas phase and QM/EFP-MD simulations in water solution. According to gas phase studies, it appears that the relative populations of various conformers depend not only on the relative energies but also on the kinetic isomerization barriers. Energetically, ttt, ccc, gtt, tct, and gct conformers are stable. However, a large spread of isomerization barrier heights makes it difficult to determine the conformational populations. Furthermore, the relative energetics is sensitive to the number of water molecules. To overcome this challenge and to obtain the free energy landscape of various conformers of glycine in solution, QM/EFP-MD simulation has been performed. Four district major minima are predominantly seen at $(\varphi=0^\circ, \theta=0^\circ)$, $(\varphi=0^\circ, \theta=180^\circ)$, $(\varphi=180^\circ, \theta=0^\circ)$, and $(\varphi=180^\circ, \theta=180^\circ)$. The most probable and stable conformers at those regions are ccc, (tct and gct), (ttc and gtc), and (ttt and gtt), respectively. The relative free energies among the four minima are nearly identical, which is in contrast to the gas phase relative energies, where large differences exist depending on the conformations. This indicates that hydrogen bonding between glycine and water molecules by solvation reduce the free energy differences among various conformers of glycine.


180
150
120
90
60
30
0
θ
0
30
60
90
120
150
180
ϕ
C
tct + gct
D
ttt + gtt
TS$_{CD}$
TS$_{AC}$
TS$_{BD}$
TS$_{AB}$
A
ccc
B
ttc + gtc
12
10
8
6
4
2

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Role of central base in the stabilization of the telomere quadruplex and their interaction with cationic porphyrin

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Telomere takes important role in protecting chromosome, cell aging and development of cancer and consists of several continuous G bases. This G-rich oligonucleotide forms well-known G quadruplex in the presence of mono-cation such as K^+ or Na^+ ion. In the quadruplex, four G bases connected via the Hoogsteen type base pairing. Role of the central purine base in stabilization of the quadruplex was investigated in this work using conventional melting profile and theoretical calculations. the sequence investigated is GGTTGGTXTGGTTGG (where X=A, I or G). When the central G was replaced by A, the quadruplex significantly destabilized; the melting temperature decreased by 5.4 °C. On the other hand, replacement of G by I resulted in a 1.2 °C decrease in melting profile. The detailed structure calculated by Charm reveals that the carbonyl group of the central G and I was close to G1:H21, G1:H22, G1:H1 and G6:H8 residues, suggesting the possibility of the hydrogen bond formation, while A base lacks this carbonyl group. This observation suggested that the nature of the central base was important in stabilizing the quadruplex. The binding mode of *meso*-tetrakis(*N*-methylpyridium-4-yl)porphyrin (TMPyP) to these quadruplex was probed by induced circular dichroism spectrum. In all three oligonucleotide cases, CD spectrum in the Soret region consisted of a positive band, which suggested that the central base of the quadruplex did not affect the binding mode of TMPyP. Therefore, it is conclusive that TMPyP bind side of the quadruplexes. and Furthermore, T and bind exterior of the quadruplexes.

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Effect of replacement of guanine base of quadruplex by inosine on the interaction with metallo- and nonmetallo cationic porphyrins

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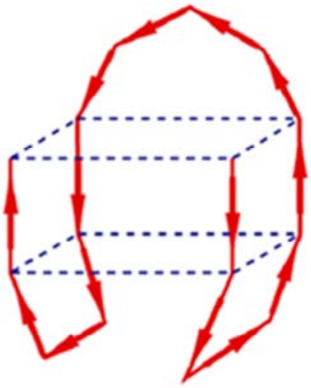
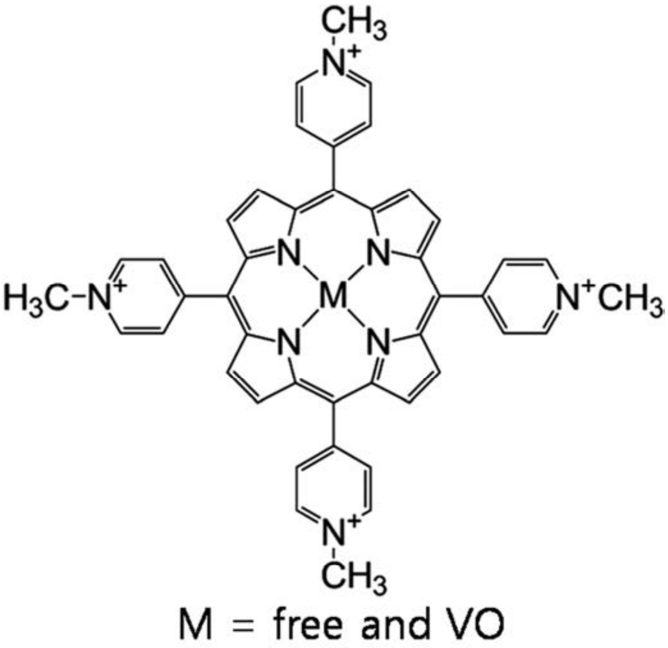
영남대학교 화학과

Telomeric oligonucleotide, 5´-GGTTGGTGTGGTTGG, forms a quadruplex, in which four G bases are connected via the Hoogsteen-type hydrogen bonds. This quadruplex has been well-known to interact with various cationic porphyrins. A variety of binding modes for planar *meso*-tetrakis(*N*-methylpyridium-4-yl)porphyrin(TMPyP) have been reported when form a complex with the quadruplex. In this study, G bases were systematically replaced by I and their stability and binding mode to porphyrins were compared. When any of G was replaced by I, the melting temperature decreased as it was expected from the number of the hydrogen bond that I can forms. Destabilization was particularly pronounced when G1 was replaced by I, suggesting the importance of the G1 base in the quadruplex stabilization. Induced circular dichroism (CD) showed that the binding mode of TMPyP is similar even when one of the G was replaced by I, except for G2. When G2 was replaced by I, a bisignate CD spectrum was produced. Therefore, it can be suggested that the interaction of G2 with TMPyP is the strongest when they form a complex. VOTMPyP exhibited similar positive CD spectrum, suggesting that, similarly with TMPyP, VOTMPyP bind exterior of the quadruplex. The Raman spectrum of VOTMPyP in the absence of the quadruplex was similar to those of the VOTMPyP-quadruplex complex, further supporting the external binding mode. Replacement of G at any position by I did not affect the appearance of CD and Raman spectrum of VOTMPyP.




CH3
N+
H3C-N+
N
M
N+CH3
M = free and VO

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Ligand Effect and Cooperative Role of Metal Ions on the DNA Cleavage Efficiency of Mono and Binuclear Cu(II) Macrocyclic Ligands Complexes

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영남대학교 기초교육대학 [1]영남대학교 화학과 [2]선문대학교 화학과

Two binuclear Cu(II) complexes of N-functionalized macrocycle ligands, namely 1,3-bis(1,4,7-triaza-1-cyclonomyl)propane and 1-(3-(1,4,7-triazonan-1-yl)propyl-1,4,7,10-tetraazacyclo-dodecane, were synthesized and their ability to hydrolyze the cleavage of supercoiled plasmid DNA (pBR322) was compared with that of structurally related non-functionalized mononuclear Cu(II) complexes. The former, binuclear Cu(II) complex with the symmetrical ligand exhibited enhanced double-strand cleavage activity compared to the other three complexes at the same [Cu^{2+}] concentration. In contrast, the latter binuclear complex with unsymmetrical macrocylic ligand did not give rise to double-strand DNA cleavage. The linear DNA formation induced by the mononuclear Cu(II) 1,4,7,10-tetraazacyclo-dodecane complex was realized via a non-random double-stranded scission process. The differential cleavage activity is discussed in relation to dimer formation, effective cooperation and coordination environment of the metal center. The hydrolytic cleavage by the copper complexes without H_2O_2 is supported by evidence from an anaerobic reaction, free radical quenching, and nitro blue tetrazolium assay. In contrast, both the binuclear complexes cleaved supercoiled DNA efficiently to form III (linearized DNA) in the presence of the hydrogen peroxide, indicating that nuclearity is a crucial parameter in oxidative cleavage. The radical scavenger inhibition study and nitro blue tetrazolium assay suggested the involvement of hydrogen peroxide and superoxide ions in the oxidative cleavage of DNA by the binuclear complexes.

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Interaction of V(=O)meso-tetrakis(N-methylpyridinium-4-yl)porphyrin with duplex and triplex DNAs

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영남대학교 화학과 [1]영남대학교 기초교육대학

Binding mode of V(=O)meso-tetrakis(N-methylpyridinium-4-yl)porphyrin (VOTMPyP) to various duplex and triplex synthetic polynucleotides were investigated using polarized light spectroscopy and Raman spectrum. The poly(dT) and poly(dC)$^+$ strand run in the major groove of the poly(dA)·poly(dT) and poly(dG)·poly(dC) duplex when form the poly(dA)·[poly(dT)]$_2$ and poly(dC)·poly(dG)·poly(dC)$^+$ triplex, respectively. As a results, the third strand in the major groove blocks or interferes with any drug that binds at the major groove of the duplexes, resulting in a large alteration in the spectroscopic properties of the major groove binding drugs. Positive circular dichroism spectrum (CD) of the VOTMPyP- poly(dA)·poly(dT) remained when bound to the triplex poly(dA)·[poly(dT)]$_2$. Observed positive CD spectrum suggested that VOTMPyP bind exterior of AT polynucleotides near the minor groove of both duplex and triplex case. On the other hand, similar negative CD in the Soret region was appeared in the presence of poly(dG)·poly(dC) duplex and poly(dC)·poly(dG)·poly(dC)$^+$ triplex. Although negative CD spectrum has been considered as a diagnostic for intercalative binding mode, VOTMPyP was suggested to bind at the minor groove of poly(dG)·poly(dC) duplex based on Raman and linear dichroism study (Biochim. Biophys. Acta (2006) 1760, 388). Thus, VOTMPyP probably bind at the minor groove of the poly(dC)·poly(dG)·poly(dC)$^+$ triplex.

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Binding Mode of Proflavine to DNA Probed by Polarized Light Spectroscopy

성기웅 김래영 김석규*

영남대학교 화학과

Proflavine has been known to binds to DNA. The binding mode of proflavine to native DNA was investigated using linear dichroism (LD) and fluorescence techniques. Observed change of proflavine upon formation of a complex with DNA can be summarized as red-shift and hypochromism in the absorption spectrum, negative LD^r in the proflavine absorption region with its magnitude comparable or larger than that in the DNA absorption region confirm the intercalative binding mode of proflavine to DNA. Saturation of LD spectrum in the proflavine absorption region at $R = 0.25$ and decrease in the fluorescence intensity provide further evidence for intercalation. From this study, coupling of electric transition of intercalated proflavine is newly observed. Although proflavine has been reported to stack along the DNA stem at a high [proflavine]/[DNA base] ratio, the spectral characteristics including a clear isosbestic point in absorption spectrum and proportionality in the LD magnitude in the proflavine absorption region do not showed any possibility for the outside binding.

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Binding Geometry of Free Base and Mn(III)*meso-Tetrakis*(*N*-methylpyridium-4-yl)porphyrin to Various Duplex and Triplex DNAs

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영남대학교 화학과 [1]경운대학교 환경공학과 [2]경일대학교 화학공학과

The binding mode of free base and Mn(III)*meso*-tetrakis(*N*-methylpyridium-4-yl)porphyrin (TMPyP and MnTMPyP) to various duplex and triplex synthetic polynucleotides was investigated by circular and linear dichroism spectroscopy (CD and LD). Both TMPyP and MnTMPyP produced a similar positive CD spectrum in the Soret absorption region when bound to poly(dA)·poly(dT) duplex and poly(dA)·$[\text{poly(dT)}]_2$ triplex. Considering that the third poly(dT) strand blocks the major groove, this result suggested that both porphyrins bound near the minor groove where the axial ligands of the central Mn(III) ion did not affect the binding mode. In contrast, TMPyP intercalated and MnTMPyP bound the exterior of poly(dG)·poly(dC) and poly(dI)·poly(dC) duplexes, as judged from the negative and positive CD signals. The CD signals for both intercalated TMPyP and externally bound MnTMPyP were greatly altered when bound to poly(dG)·poly(dC)·poly(dC)^+ and poly(dI)·poly(dC)·poly(dC)^+ triplexes, indicating that the binding modes of both porphyrins were affected by the presence of the third strand, which contrasted with the AT polynucleotides. This observation supported the conclusion that the external binding site of MnTMPyP at GC and IC duplexes is the major groove. The reduced LD spectrum indicated that the angles of the two electric transition moments of both TMPyP and MnTMPyP in the Soret absorption region were 57° and 65° with respect to the local DNA helix axis when bound to poly(dA)·$[\text{poly(dT)}]_2$ triplex. On the other hand, strong wavelength-dependent reduced LD observed for the CGC triplex prevented any calculation of the reasonable angles.

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A theoretical study on electric permittivities of noble metal alloys

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조선대학교 화학과

We calculated the electronic band structures of ordered binary-component noble-metal alloys, i.e., intermetallic compounds such as $CuAg_3$, $CuAu_3$, CuAu, and Cu_3Au, using density functional theory methods with plane-wave basis sets. Based on the band structures, electric permittivities of the intermetallics were calculated in the linear response regime, and changes in permittivity with alloy composition were analyzed in detail with band structures and density of electronic states for both alloys and pure metals. Considering that the intrinsic plasmonic optical properties of metal nanoparticles are determined solely by the permittivity of the metal, we estimated the extent to which optical properties of the noble-metal alloy nanoparticles could be modulated.

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Enhancing Photoconversion Efficiency by Using Up-conversion Phosphors in Dye-Sensitized Solar Cell

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서강대학교 화학과

Up-conversion is a process where low-energy photon is converted into a high-energy photon[1]. Up-conversion phosphor can convert infrared light into visible light. β-NaYF4:Yb3+,Er3+ up-converting microparticles (UCMPs) were synthesized by a facile hydrothermal method. Sodium citrate was used as a chelating agent in the hydrothermal reaction, the initial pH value of the solution critically affected on the morphology and the up-conversion efficiency of the prepared β-NaYF4:Yb3+,Er3+ UCMPs. At pH 3.13, β-NaYF4:Yb3+,Er3+ UCMPs with hexagonal-tube morphology were synthesized. As the pH was changed to basic conditions, UCMPs with increased diameter and decreased length were produced. At pH 11.20, β-NaYF4:Yb3+,Er3+ UCMPs with hexagonal-plate morphology were synthesized. Different morphologies of the prepared β-NaYF4:Yb3+,Er3+ UCMPs showed different up-conversion efficiency. β-NaYF4:Yb3+,Er3+ UCMPs prepared at pH 3.13 showed the highest upward wavelength conversion efficiency due to their high single crystalline quality. For the application as the up-converting reflection film of dye-sensitized solar cell (DSSC), hexagonal-tube β-NaYF4:Yb3+,Er3+ UCMPs were evenly dispersed on the surface of a glass substrate. The prepared film was placed on the back side of the Pt-counter electrode as a reflecting plate to increase the efficiency of the DSSC. Thickness of the film also critically affected on the efficiency increase of DSSC. And then hexagonal-tube UCMPs used as dispersing into electrolyte solution and on the TiO2 scattering layer. Finally, three locations of UCMPs in the DSSC system will be placed simultaneously.References[1] M. Haase, H. Schafer, Upconverting Nanoparticles, Angew. Chem. Int. Ed., 50, 5805-5829 (2011).

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Annealing Temperature Dependence on Photocatalytic Activity of Hematite Thin Film on Fluorine Doped Tin Oxide Substrate

조은수 강명종 강영수*

서강대학교 화학과

Among various candidate materials, hematite has been emerged as a promising photo-electrode due to many advantages for photoelectrochemical water splitting. It has narrow band gap about 2.2 eV and it can absorb almost 15% of the sunlight. Also, it is inexpensive, abundant in nature, and very stable in electrolytes over pH 3. In this research, deposition and annealing method was used to synthesize hematite thin film. Hematite was deposited by spin-coating on the fluorine tin oxide (FTO) as a substrate, and the drying and annealing procedures were followed. Then, the hematite thin film was annealed at various temperature conditions. As the annealing temperature was varied from 550℃ to 700℃, the photocurrent density was increased. The film annealed at 700℃ has the maximum photocurrent of 0.6 mA/cm2 at 1.23 V vs. RHE under 1 sun illumination. This work deals on the optimum temperature for synthesizing the hematite film and the reason why the photocurrent density increased.

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Exchange-coupled Nd2Fe14B /α-Fe Nanocomposites Magnetic Materials

정지훈 강영수*

서강대학교 화학과

One of the important permanent magnetic materials offering a high coercivity and an energy product is Nd2Fe14B. The magnetic energy product is defined as the area enclosed in the second quadrant of the B-H loop. Hence, the large energy product can be obtained from the combination of a high coercivity and a large remanence value. Exchange-coupled nanocomposites are composed of a combination of hard and soft phase magnets for the achievement of a higher energy product. Nd2Fe14B-based nanocomposites, containing exchange-coupled magnetic hard and soft phases, are considered to be desirable permanent magnets for their large coercivity, high magnetization, and enhanced maximum energy product. However, the major difficulties of these conventional methods are to maintain alloy composition and particles size control due to the high negative reduction potential of Nd3+/Nd and easy oxidation of Nd2Fe14B powders. For the complete exchange-coupled nanocomposites, hard and soft magnetic materials need to be nano-size particles. So, we focused on the fabricating of Nd2Fe14B magnets to downsize by wet chemical methods.

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Synthesis of Layer by Layers Composed of Y2O3:Er3+ and Gold nanoparticles and its Application of Dye Sensitized Solar Cell

엄태영 강영수*

서강대학교 화학과

Lanthanide-doped upconversion nanocrystals which can convert near-IR lights to visible lights have attracted growing interest because of their great potentials in fields of advanced materials. However, it remains a challenge to maneuver the intensity ratio between different emission lines and enable tunable upconversion functions. Herein, we present a facile method to enhance property of Y2O3:Er3+ upconversion nanocrystals with gold nanoparticles for fabricating Y2O3:Er3+@Au hybrid nanostructures by using MPTMS((3-mercaptopropyl)trimethoxy silane) as adhesive materials between phosphor and gold NPs. Each material was fabricated by sol-gel process and citrate reduction. Fabricated double layers have both property, wavelength converting and amplification, and it will be applied very useful in DSSC or other solar devices.

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Change in Photoelectrochemical Activity of α-Fe2O3 Nanocrystal Thin Film by Cu Doping

안나현 강영수*

서강대학교 화학과

α-Fe2O3 has so many advantages such as visible light absorption, which corresponds to low band gap energy, and stability. It was deposited on the FTO substrate changing the amount of Cu dopant(1, 2, 3, 5 mol% of Fe precursor). Fe3+ ions in α-Fe2O3 nanocrystal structure are substituted by Cu2+ ions causing lattice distortion and increase of hole trapping sites. XRD pattern shows that nanocrystal is crystallized well and there is no significant difference in crystal structure depending on the amount of Cu doping. Also, crystal structure was confirmed by TEM diffraction pattern. D-spacing values increased as dopants increased, but the specificity to the planes was not found. The morphology was a cubic with round edges. Due to charge imbalance, when Cu2+ ions occupied Fe3+ sites, hole trapping occurred leading to the decrease in PEC value. Furthermore, electrochemical impedance value was increased as Cu doping increased, which was consistent with PEC data.

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Synthesis of Co/SmCo5 Hard Magnets by Core/Shell Nanoparticles for Exchange- coupled Nanocomposite

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Exchange-coupled nanocomposite can be synthesized by alternative arrangement of hard magnet and soft magnet in 3-dimension for better magnetic properties. Perfect assembly of the hard/soft phase magnetic nanoparticles shows large coercivity value, higher magnetization, enhancement of maximum energy product due to magnetic spin exchange interaction. However, for better magnetic spin exchange interaction, hard and soft magnetic materials should be synthesized as nanoparticles. Among the hard magnet materials, SmCo5 has advantages of high working temperature while it has still good coercivity and remanence value. To fabricate hard phase magnet in nano-size particles, the core/shell nanoparticles are used. After synthesis of Co nanoparticles by thermal decomposition, the core part is covered with Sm2O3 as shell. Finally, SmCo5 nanoparticle can be fabricated by reductive annealing process of core/shell-structured Co/Sm2O3.

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A study on adsorption of Li from aqueous solution using various adsorbents

유건상* 홍용표

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The aim of the present study is to explore the possibility of utilizing fly ash, loess and activated charcoal for the adsorption of Li in aqueous solution. Batch adsorption experiments were performed to evaluate the influences of various factors like initial concentration, contact time and temperature. The adsorption data showed that fly ash and activated charcoal are not effective for the adsorption of Li. On the contrary, loess showed much higher adsorption capacity for Li. The adsorption of Li on loess was highly concentration dependent. It was found that the adsorption capacity of loess is favored at a lower Li concentration. At equilibrium, approximately 95 % of adsorption was achieved by loess. The equilibrium data were fitted well to the Freundlich isotherm model. The pseudo-second-order kinetic model appeared to be the better-fitting model because it has higher R2 compared to the pseudo-first-order and intra-particle diffusion kinetic models. The thermodynamic parameters such as free energy ΔG, the enthalpy ΔH and the entropy ΔS were calculated. The values of ΔG were negative at the studied temperatures. It indicates that the adsorption of Li on loess is a favorable and spontaneous process. The positive values of ΔH and ΔS suggest that the adsorption process of Li by loess is endothermic in nature and aided by increased randomness at the solid/solution surface.

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Evaluation of loess capability for adsorption of total nitrogen (T-N) and total phosphorous (T-P) in aqueous solution

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The aim of the present study is to explore the possibility of utilizing loess for the adsorption of total phosphorous (T-P) and total nitrogen (T-N) in water. Batch adsorption studies were performed to evaluate the influences of various factors like initial concentration, contact time and temperature on the adsorption of T-P and T-N. The adsorption data showed that loess is not effective for the adsorption of T-N. However, loess exhibited much higher adsorption capacity for T-P. The adsorption of T-P on loess was highly concentration dependent. It was found that the/ adsorption capacity of loess is favored at a lower T-P concentration. At concentration of 1.0 mg L-1, approximately 97 % of T-P adsorption was achieved by loess. The equilibrium data were fitted well to the Langmuir isotherm model. The pseudo-second-order kinetic model appeared to be the better-fitting model because it has higher R2 compared with the pseudo-first-order and intra-particle kinetic model. The theoretical adsorption equilibrium qe,cal from pseudo-second-order kinetic model was relatively similar to the experimental adsorption equilibrium qe,exp. The thermodynamic parameters such as free energy ΔG, the enthalpy ΔH and the entropy ΔS were calculated. The ΔG values of loess were all negative at the studied temperatures. It indicates that the adsorption of T-P on loess is of a fairly favorable and spontaneous process. The positive ΔH values of loess suggest that the T-P adsorption process is endothermic in nature. In addition, the positive ΔS value shows that increased randomness occurs at the adsorbent-solution surface.

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Twinned GaAsP Ternary Nanowires and band gap tunning

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$GaAs_{1-x}P_x$ ternary alloy nanowires have drawn much interest because their tunable band gaps, which range from the nearinfrared to visible region, are promising for advanced and integrated nanoscale optoelectronic devices. In this study, we synthesized compositionally tuned $GaAs_{1-x}P_x$ ($0 \le x \le 1$) alloy nanowires with two average diameters of 60 and 120 nm by vapor transport method. The nanowires exhibit exclusively twinned superlattice structures, consisting of zinc blende phase twinned octahedral slice segments between wurtzite phase planes. Smaller diameter and higher P content (x) result in shorter periodic superlattice structures. The band gap of the smaller diameter nanowires is larger than that of the larger diameter nanowires by about 90 meV, suggesting that the twinned superlattice structure increases the band gap. The increase in band gap is ascribed to the higher band gap of the wurtzite phase than that of the zinc blende phase.

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Controlled growth of one dimensional GaS_xSe_{1-x} nanobelts and there color tunable photoluminescence properties

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Layer structured GaSe and GaS are composed of isomorphic, 4-fold atomic layers, each monolayer contains two gallium and two chalcogen closed-packed sublayers in the stacking sequence of S(Se)-Ga-Ga-S(Se) along c-axis. We controlled synthesis and characterization of one dimensional GaS_xSe_{1-x} nanobelts via a catalyst-assisted vapor-liquid-solid (VLS) growth mechanism during Ga_2S_3 or Ga_2Se_3 powder evaporation. The chemical composition and crystal structure of GaS_xSe_{1-x} nanobelts were investigated by X-ray diffraction, Raman spectroscopy and energy dispersive X-ray spectroscopy. These results confirmed that there composition tuned completely over the whole range ($0 \leq x \leq 1$).The luminescence properties of GaS_xSe_{1-x} series has been measured at 8 K. There PL emission peak energy monotonically increase with S concentration. The spectral range of the PL emissions covering from 2.0 eV (GaSe) to 2.51 eV (GaS) which corresponding to the full range visible irradiations. This result provides the potential usage for these nanobelts to be fabricated in fullcolor displays.

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Highly Efficient Electrocatalytic Oxygen Evolution of Transition Metal-Doped ZnO and TiO_2 Nanocrystals

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Catalysts for oxygen reduction and evolution reactions are at the heart of key renewable-energy technologies including fuel cells and water splitting. Despite tremendous efforts, developing oxygen electrode catalysts with high activity at low cost remains a great challenge. In this study, we synthesized a series of transition metal (e.g., Mn, Fe, Co, Ni, Ru, and Ir)-doped ZnO and TiO_2 nanocrystals, and compared their electrocatalytic performance for oxygen evolution reaction (OER). Although oxide alone has little activity, the transition metal-doped oxide exhibits the higher OER activity that is mostly enhanced by the Ru. The overpotential of the metal doped ZnO or TiO_2 shows the sequence of Ru < Ir < Co < Ni = Mn = Fe, which follows the same trend as the catalytic activity of (pure) metal oxides such as RuO_2, IrO_2, Co_2O_3, etc. It indicates that the ZnO and TiO_2 matrix guard the catalytically active doped metal oxide sites. X-ray photoelectron spectroscopy revealed the high oxidation state of the metal ions that would be responsible for the high-efficiency OER by stabilizing the intermediate hydroperoxo or peroxo species.

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Composition-Tuned $Sn_xGe_{1-x}S$ Nanocrystals for Enhanced-Performance Lithium Ion Batteries

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Germanium- or tin-based nanostructures have recently demonstrated outstanding lithium ion storage ability and are considered to be the most promising candidates to substitute current carbonaceous anodes in lithium ion batteries. Tin germanium sulfide ($Sn_xGe_{1-x}S$) ternary alloy nanocrystals (NCs) were synthesized by a gas-phase laser photolysis reaction with complete composition control ($0 \leq x \leq 1$). All of these composition-tuned nanocrystals showed excellent cycling performances in lithium ion batteries. Reversible capacities were in the range 800?1200 mAh/g after 70 cycles, which is close to the theoretical capacities of each composition. As the tin composition (x) was increased, the rate capability greatly enhanced, reaching a maximum at x = 0.8 ? 0.9. This unique composition dependence of the electrochemical properties was explained by the lower charge transfer resistance due to the high conductivity of $Sn_xGe_{1-x}S$ NCs as well as Sn_xGe_{1-x} alloy NCs produced upon lithiation. Sn-rich $Sn_xGe_{1-x}S$ NCs are, therefore, promising candidates for applications in high-performance energy conversion systems.

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Synthesis of rhodium-doped $SrTiO_3$ nanocrystals by hydrothermal reaction and the efficiency of photocatalytic water splitting

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TiO_2 (band gap = 3.2 eV) exhibit promising photoelectric and photocatalytic performances in solar cells, water splitting and photocatalytic systems. However, their poor visible light utilization as well as the high recombination rate of photoexcited electron-hole pairs greatly limit their practical applications. Thereby, much effort has been devoted to the design and construction of novel composite nanostructures to address these issues. $SrTiO_3$ (band gap=2.4 eV), whose conduction band edge is 200 mV more negative than TiO_2, have been considered as an alternate candidate for improving photoelectrochemical and photocatalytic performances. Simultaneously, doping transition metals with $SrTiO_3$ for narrowing its band gap and enhancing absorption of visible light have attracted considerable attention. In particular, rhodium (Rh) doping is of great interest because of the partial overlap of Rh $4d^6$ (Rh^{3+}) and O 2p orbitals to form the valence band, resulting in a negative-potential shift of the valence top. Herein, we demonstrate a facile synthetic strategy for fabricating uniform metal (including Rh)-doped $SrTiO_3$ nanocrystals by in situ hydrothermal method using metal-doped TiO_2 nanocrystals as both template and precursor, and their structure and composition can be rationally tailored by simply adjusting the reaction time. Furthermore, it has been found that the metal-doped $SrTiO_3$ nanocrystals exhibit much higher photoelectrochemical as well as photocatalytic performances than pure $SrTiO_3$ under visible light irradiation.

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Composition and Phase Tuned GaP-ZnS Pseudobinary Nanowires

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Multicomponent nanowires (NWs) are of great interest for integrated nanoscale optoelectronic devices owing to their widely tunable band gaps. In this study, we synthesize a series of $(GaP)_{1-x}(ZnS)_x$ ($0 \le x \le 1$) pseudobinary alloy NWs using the vapor transport method. Compositional tuning results in the phase evolution from the zinc blende (ZB) ($x < 0.4$) to the wurtzite (WZ) phase ($x > 0.7$). A coexistence of ZB and WZ phases ($x = 0.4$-0.7) is also observed. The phase evolution leads to enhanced photoluminescence emission. Strikingly, the photoluminescence spectrum shows a blue-shift with increasing excitation power, and a wavelength-dependent decay time. Based on the photoluminescence data, we propose a type-II pseudobinary heterojunction band structure for the single-crystalline WZ phase ZnS-host NWs. The slight incorporation of GaP into the ZnS induces a higher photocurrent and excellent photocurrent stability, which opens up a new strategy for enhancing the performance of photodetectors.

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Time-resolved X-ray absorption spectroscopy for photoisomerization in photochromic Ru complex: experimental and theoretical studies

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부산대학교 화학과

Efficient convertibility of photochromic Ru complexes for transduction of photonic energy to potential energy has attracted interest over the past decade. Since the attractive their nature of photochromic Ru complexes is produced by bond breaking and forming of long-live metastable state, it is imperative that fundamental understanding of photophysicochemical property relating to electronic and structural changes during photochemical reaction is investigated. For this purpose, we have investigated photoisomerization of solvated $[Ru(bpy)_2(pyESO)]^{2+}$ complex by means of time-resolved X-ray absorption spectroscopy (TR-XAS) combine with time-dependent density functional theory (TDDFT) at Ru L_3-edge region. Transient X-ray absorption spectra at specific delays provide evidence for isomerization of sulfoxide occurs within 640 ps following laser excitation of 400 nm. Moreover alterations in differential spectral features show that the isomerization process takes place through certain metastable state, such as triplet metal-to-ligand charge-transfer (MLCT) state and metal-centered (MC) state. In order to visualize the electronic structures and local geometries for reaction intermediates (^{1}S = singlet S-bonded isomer; ^{3}MLCT$_S$ = triplet S-bonded MLCT state; ^{3}MC$_O$ = triplet O-bonded MC state; ^{3}MLCT$_O$ = triplet O-bonded MLCT state; ^{1}O = singlet O-bonded isomer), we performed TDDFT calculations using ORCA program. The Ru L_3-edge XAS spectra for all reaction intermediates, which get from TDDFT calculations, were employed to carry out the global fits to determine lifetime of each intermediate state. The fit results demonstrate that S→O isomerization is most likely to proceed via not only ^{3}MLCT states but also ^{3}MC state.

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Enhanced Photocatalytic activity of Ta_2O_5, TaON, and Ta_3N_5 Nanocrystals

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Photocatalysis of the degradation of organic pollutants by using light absorbing semiconductors such as TiO_2 has been widely investigated due to not only its scientific interest, but also its relevance in environmental protection. Unfortunately, TiO_2 has a wide band gap (Eg= 3.2 eV), so it can only be excited by ultraviolet light. In order to fully utilize the sunlight, significant effort has been made to develop visible light sensitive photocatalysts. Tantalum nitride (Ta_3N_5) and tantalum oxynitrides (TaON) as the current example, introducing N atoms into tantalum oxide (Ta_2O_5) brings a remarkably tunable band-gap energy, as such, TaON and Ta_3N_5 with band gaps of 2.5 and 2.1 eV are both smaller than that of Ta_2O_5 (3.9 eV). Therefore, the controllable synthesis of TaON nanoparticles(NPs) with tailored chemical composition is an attractive goal. However, which is difficult to achieve by current strategies because of easy over reactions due to the high rate of nitridation. For example, by-products of Ta_3N_5, Ta_4N_5, and TaN will be easily generated from during calcination.Herein, we focused on the tailored chemical composition relative photocatalyticabilities of Ta_2O_5, TaON, and Ta_3N_5 NCs toward the degradation of Methyleneblue (MB) dye under visible light irradiation

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Metal and Nitrogen-doped Graphitized Nanodiamond Hybrid Nanostructures for Electrochemical Carbon Dioxide Reduction

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The development of an efficient catalyst for electrochemical reduction of carbon dioxide into useful hydrocarbon products is a major research topic. Here we report the catalytic ability of metal nanocrystal-N-doped graphitized onion-like nanodiamond (NC-NGND) hybrid nanostructures for carbon dioxide reduction into carbon monoxide. Metal NC-NGND hybrid nanostructures were prepared by laser induced reaction of metal precursor (CoO, MnO, CuO, $RuCl_3$ etc.) and nanodiamonds in ethanol. The graphitized NDs were easily doped with the N and metal oxide nanocrystals reduced into metal nanocrystals by the thermal annealing under NH3 gas. The metal NC-NGND hybrid nanostructures exhibits low overpotential and selectivity for carbon dioxide reduction into carbon monoxide. Faradaic efficiencies for carbon monoxide production of > 90 % have been reached. The efficient performance is credited to electronic structures of NGND and selectivity of metal nanocrystals. The finding may lead to a new strategy to develop cost-effective electrocatalysts with superior efficiency for carbon dioxide conversion.

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Photocatalytic Activity of Tungsten Oxide : Dependence on the Morphology and Metal Doping

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We report synthesis of tungsten oxide (WO_3) nanocrystals with three different morphologies such as thin nanowires (diameter = 5-10 nm), hollow nanospheres (diameter = 30 nm), and 10-nm-thick nanosheets (avg, Length = 200 nm), via various synthetic routes. The photoreaction of nanocrystal colloidal solution produces the nanospheres and nanosheets, respectively, under 1064 and 355 nm pulsed laser irradiation. Furthermore, the rhodium and iridium metal doping was successfully achieved for each nanocrystals. Detailed structure evolution was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM), and UV-vis-NIR spectroscopy. We investigated visible-light-driven photocatalytic activity of water splitting for these WO_3 nanostructures (band gap = ~2.8 eV) to find the most effective crystal planes of monoclinic phase.

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Density functional theory reactivity studies on Molecular Oxygen with Aluminum Cluster

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부산대학교 화학과

In this study, density functional theory (DFT) reactivity studies on Molecular Oxygen (O_2) with Aluminum cluster have been performed. The calculations were carried out on Al_7^- cluster reaction with O_2 using M06-2X, TPSSh and N12-SX functionals with 6-311+G(d) basis set. The molecular geometries of isolated Al_7^-, O_2 and reacted species that are structures with smaller O-O distance, and O and O dissociated structures were optimized. The atomic and molecular properties such as bond distances, HOMO-LUMO gap, Vertical and adiabatic spin excitation energy, of isolated and reacted species have been calculated using above functionals. Further, we have also performed atom-centered density matrix propagation (ADMP) molecular dynamics simulations on Al_7^- reaction with O_2, in both singlet and triplet frameworks. To calculate the barrier energy, potential energy surfaces have been generated on O_2 approach with Al_7^- in singlet and triplet states. Our calculations have shown that the M06-2X and TPSSh functionals could be useful for the studies on larger systems containing Al and O. In addition, the barrier energy calculated by TPSSh functional coincides very well with experimental value.

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Release of bending energy in dsDNA by fast dynamics between sharp kink and local end-melting

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

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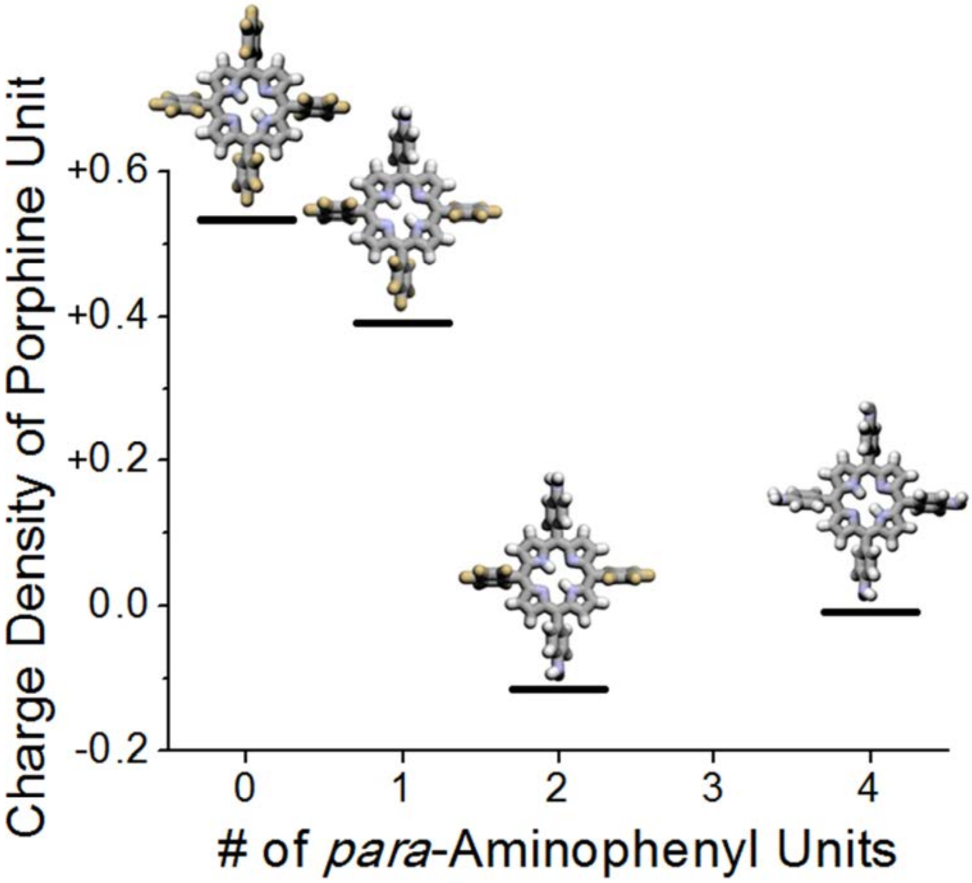
Characteristic Electronic Perturbation by Asymmetric Arrangements of *para*-Aminophenyl Substituents in Free-Base Porphyrins

조성

전남대학교 화학과

We have investigated the perturbed electronic properties of *meso*-substituted free-base porphyrins with symmetric and asymmetric arrangements of substituents using time-resolved spectroscopic measurements and theoretical calculations. The extent of electronic perturbation by substituents in *meso*-substituted porphyrins is mainly affected by the isoenergetic condition of frontier MOs of porphine and substituent units, nonorthogonal geometry, and geometrical arrangement of substituents. By using the asymmetric arrangements of *para*-aminophenyl and pentafluorophenyl substituents, we can induce the electron-rich condition on the porphine unit and the intramolecular charge transfer character in the excited state.


Charge Density of Porphine Unit
+0.6
+0.4
+0.2
0.0
-0.2
0
1
2
3
4
of *para*-Aminophenyl Units

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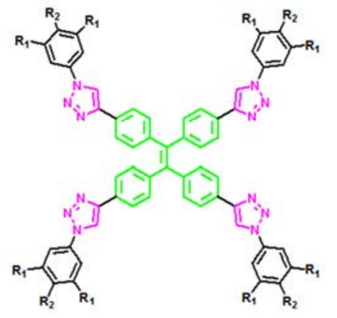
Temperature-induced Core Ordering of TPE Derivatives at Liquid Crystal Phase

조성

전남대학교 화학과

We have investigated the temperature-dependent aggregation-induced photophysical properties of TPE (tetraphenylethene) derivatives at liquid crystal phase using time-resolved spectroscopic measurements. There are two parts in the TPE derivatives; an inner rigid core and several external flexible chains (Figure 1). The emission intensities and spectra shapes of TPE derivatives exhibit characteristic temperature dependence depending on the externally substituted chains (Figure 2). On the basis of the experimental results, we revealed that the interunit interaction strength between externally substituted chains is the main factor of the packing structures of the TPE derivatives and their temperature-induced core ordering.



1: $R_1=R_2=O(CH_2)_{11}CH_3$
2: $R_1=O(CH_2)_{11}CH_3$, $R_2=H$
3: $R_1=O(CH_2)_2O(CH_2)_2OCH_3$, $R_2=H$

Figure 1

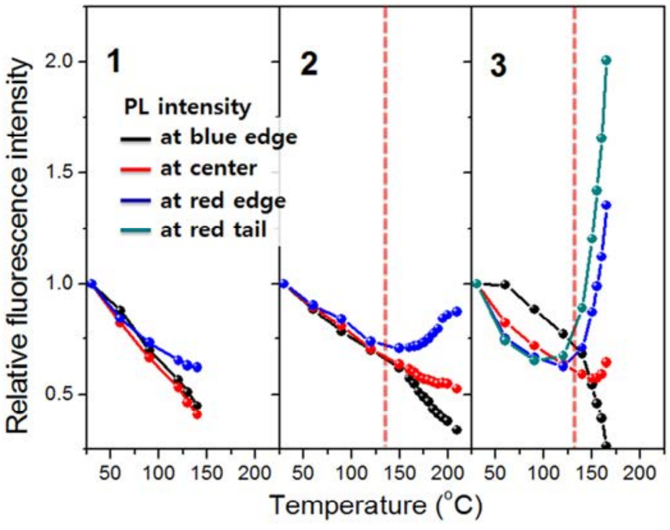


Figure 2

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Electrochemical Sensing Platform Based on Large-Area Gold Nanostructures with Ultraclean and Ultraflat Surface

성유리 강미정 양시영 김봉수*

한국과학기술원(KAIST) 화학과

DNA detection has become a critical issue in diagnosis, since it is one of the powerful tools to predict the existence and progress of various diseases. Although numerous approaches for DNA detection have been suggested, challenges to overcome still remain, for example, cumbersome procedures, dedicated instrumentation and expert knowledge required for analysis. Electrochemical sensing method has attracted great attention because of its simplicity, cost-effectiveness, and great potential for point-of-care applications. In order to fabricate DNA biosensor with a large area and enhanced sensitivity, we develop a new electrochemical sensor platform based on large-area gold nanostructures with perfectly clean crystal surface. We expect that electrochemical signals from DNA are increased due to wide and well-arranged self-assembly monolayers of DNA complex on ultraflat and ultraclean gold nanostructures.

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Simulations on the Nitrogen-Doping of Graphene Oxide using the ReaxFF reactive force field

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

Graphene has been considered as a remarkable and promising material due to its various electrochemical applications since it is abundant and cheap. Furthermore, Nitrogen-doped graphene improves its catalytic activity after doping by regulating Fermi energy level. Thermal doping of graphene oxide with reductive agents such as NH_3 is a common and easy method to synthesize N-doped graphene.Therefore, synthesis and analysis of N-doped graphene is important. However, little is known about the synthesis mechanism of N-doped graphene in detail. Molecular dynamics (MD) study is an effective way to study chemical events at long time scale and large spatial scale. MD simulation using Reactive Force Field (ReaxFF) provides sufficient details of N-doping reaction of graphene oxide by revealing its chemical reaction pathways. Although classical MD methods could not describe the changes of chemical bonds, ReaxFF successfully describes bond breaking as well as bond formation. Statistical and chemical analysis of MD simulation results can provide us chemical intuitions about doping mechanisms of nitrogen into graphene oxide. Also, quantum mechanical analysis of possible chemical pathways supports the MD results.This study is expected to further the fundamental chemistry of graphene as well as its improved applications in experimental conditions.

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Flexibility of single-stranded DNA measured by single-molecule FRET

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서울대학교 화학부

The mechanical flexibility of single-stranded DNA (ssDNA) is crucial for understanding the biological machinery in a cell nucleus but its characterization has been difficult due to the lack of an experimental tool that measures the dynamically changing structure of ssDNA in the nanometer scale. Here, we demonstrate that single-molecule FRET can be used to probe the skeletal structures of a flexible ssDNA. We designed a double-stranded DNA system with various lengths of single-strand overhang and determined the flexibility of the single-stranded segment by measuring the FRET value between two fluorophores at specific positions of the DNA. We found that three of our ssDNAs with lengths shorter than the persistence length are indeed long enough to undergo folding. Since metal ions present in solution can affect the flexibility of DNA by reducing the repulsive interaction between the negatively charged phosphate groups, we employed Na^+ and Mg^{2+} at different concentrations. We found that there is no significant effect of charge screening by metal ion when the ssDNA is less than 9 bases in length but it becomes appreciable for longer ssDNAs. Charge screening by divalent cation was considerably more effective than by monovalent cation.

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Photodissociation Dynamics of 2-Fluorothioanisole: The effect of symmetry breaking

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한국과학기술원(KAIST) 화학과

Photodissociation dynamics of 2-fluorothioanisole has been investigated by electronic spectroscopy and velocity map ion imaging. In resonant two photon ionization (R2PI) spectrum, the low frequency mode was observed with the highest intensity, 32 cm^{-1} above the S_1 origin which situated at 34975 cm^{-1}. This implies non-planar geometry of 2-fluorothioanisole in the S_1 state. The symmetry breaking in photoexcitation process strongly affects the photodissociation dynamics since the coupling between the $^1\pi\pi^*$ (S_1) and $^1\pi\sigma^*$ (S_2) state is enhanced due to the mixing of the characters of the orbitals in the excited states. The early rising in the photofragment excitation (PHOFEX) spectrum and the early disappearance of the R2PI spectrum compared to thioanisole can be explained by this enhanced coupling. The total kinetic energy release (TKER) distributions deduced from the CH_3 ion images show the change in relative intensities; the peak at the S_1 origin decreases with increasing excitation energy, at the same time, it broadens toward the high translational energy side and eventually the high translational energy side is only survived in the S_1 state region. The peak in origin could be assigned as the cofragment A state of 2-fluorothiophenoxyl radical originated from S_1 state and the peak at the high translational energy side corresponds to the A state radical dissociated from repulsive S_2 state which is supported by the anisotropy parameters and the translational energy partitioning ratios. The $^1\pi\pi^*/^1\pi\sigma^*$ coupling facilitated by non-planar excited state minimum structure in 2-fluorothioanisole results in the coexcitation of the S_1 and S_2 states at the very early beginning of the S_1 state. Theoretical calculations with various methods have been conducted to support the experimental results.

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Monitoring of significant aging-related changes in protein expression in mitochondria by using STED nanoscopy

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서울대학교 화학부 [1]서울대학교 병원/의과대학 [2]서울대학교 의과대학

Mitochondria play an essential part in maintaining various cellular functions such as oxidative phosphorylation, respiration, and apoptosis. Since mitochondrial dysfunction is closely related with aging, we investigated the morphological dispersion of mitochondria in young vs. old skin primary fibroblast using stimulated emission depletion (STED) nanoscopy. Among the various target proteins, mitochondrial transcription factor A, which is the main component in the nucleoid of mitochondria, shows significant aging-related changes. We propose that simple morphological imaging can shed light on aging-related mitochondrial dysfunction.

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Theoretical Studies on the Bimolecular Nucleophilic Substitution Reactions for Y-substituted Benzene Sulphonyl Isothiocyanate

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The kinetics and mechanism of the pyridinolysis (XC_5H_4N) of Y-substituted benzene sulphonyl isothiocyanate ($Y\text{-}C_6H_4O(S(=O)_2)NCS$) in acetonitrile are investigated at room temperature at 25.0℃. Physical and thermodynamic parameters as well as molecular orbital overlapping indicate both the front and rear-side nucleophilic attack of pyridines and leaving group (-NCS) departure strategies. According to the literature and several experimental evidences, concerted or a stepwise mechanistic route during the expulsion of isothiocyanate (NCS) leaving group from the intermediate or TS is possible, where positive and negative ρX, and βX values including thermodynamic parameters imply the characteristics of the nucleophilic attack. In addition, the steric effects of the ligands and two S=O orbital inflation can play an important role in determining the rates of the reactions.

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Molecular sensors against evasion of innate and adaptive immunity by RNA viruses

채한화

농촌진흥청 국립축산과학원/동물유전체과

When various innate immune and non-immune cells of host recognize invading pathogens, they trigger inflammatory responses and activate entire immune system to prevent viral spread. The sentries of innate immune cells are Toll-like receptors (TLR), which have been shown to detect molecular signatures of invaders known as pathogen-associated molecular patterns (PAMPs), viral replication intermediates and serve to promote efficient signal transduction for adaptive immune response. In particular, detection of RNA viral PAMPs by the TLR3, TLR7, and TLR8 localized within endolysosomal compartments of host is essential for initiation of antiviral responses: TLR3 responds to double-stranded RNA, TLRs 7 and 8 respond to single-stranded RNA in both RNA viruses. Because of their role in a host’s defense against RNA viruses, TLR3, TLR7, TLR8 are very important targets as pattern-recognition receptors for design of antiviral drug with improved resistance or susceptibility to RNA viral infection or evasion in livestock as well as human. The main objective of this work was virtual screening of antiviral candidates based on their binding constraints within intermolecular interaction sites by considering distinct signal transduction cascades through TLRs (such as RNA viral-recognition TLRs) signaling components for regulation of RNA viral evasions.

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Theoretical Investigation of Reaction Mechanism on Photoisomerization of 1,2-Dihydro-1,2-Azaborine

문지원 임정식[1] 김중한[*]

가톨릭대학교 화학과 [1]한국표준과학연구원(KRISS) 대기환경표준센터

We investigate the photoisomerization reaction of 1,2-dihydro-1,2-azaborine using high-level ab initio and density functional methods. The intermediates (IMs) and transition states (TSs) were optimized by state-averaged complete active space self-consistent field (CASSCF) method. To obtain accurate energetics, we used multireference configuration interaction with Davidson correction. In addition, the conical intersection (CI) which plays a crucial role for the photoisomerization reaction was also optimized. On the basis of the calculated results, we propose the most favorable reaction pathways; Reactant → Franck-Condon → TS$_1$ → CI → IM$_0$ → TS$_{0P}$ → Product. These results show that the isomerization reaction of 1,2-dihydro-1,2-azaborine involves both photo- and thermal reactions. Our calculated results clarify the recent experimental observation.

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Local control of pH by light

오레나 임영빈[1] 김성근*

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

Numerous chemical and biochemical systems are controlled by pH. In this study, we developed a novel method to reversibly regulate pH within a focal volume of ~ fL (= $10^{?15}$ L) using the photo-switchable property of Cy5. Cy5 is a fluorescent dye that can be reversibly converted between a fluorescent state and a dark state. The photo-conversion of Cy5 is facilitated by forming a covalent bond with a primary thiol in solution upon irradiation of red light. During photo-switching of Cy5, we verified a local drop in pH as the concentration of the primary thiolate decreased. It was also demonstrated that the local pH was recovered upon irradiation of green light.

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Synthesis of Copper Telluride and Measurement of its Electromagnetic Property

김민진 김지환 김봉수*

한국과학기술원(KAIST) 화학과

Metal chalcogenide is a chemical compound consisting of transition metal and chalcogen anion such as sulfur, selenium or tellurium. There are many types of metal chalcogenide compound and each compound has distinctive properties. Here we report a procedure to prepare copper telluride nanowire and its electromagnetic properties. We synthesized copper telluride nanowire via chemical vapor deposition method using two precursors. The synthesized copper telluride nanowires were characterized by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The electromagnetic properties of copper telluride nanowire were also measured.

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Synthesis of BiVO4 with Facet Control for Water Oxidation under Visible Light Irradiation

서경혁 강영수*

서강대학교 화학과

Artificial photosynthesis (AP) is the one of most interest research area. The oxygen evolution reaction (ORR) in photoanode is an important part in AP. Bismuth vanadate (BiVO4) is a promising material on ORR. Advantages of BiVO4 are inexpensive, abundant and having narrow band-gap, which are able to make semiconductor absorb visible light. Herein monoclinic bismuth vanadate was synthesized. First, BiVO4 monolayer was coated on fluorine doped tin oxide (FTO) and then, secondary growth of BiVO4 was performed on monolayer by hydrothermal method. In this point, directing agent was used for selective exposure of (040) facet which is highly photoactive site in BiVO4. Finally, the properties have been demonstrated by scanning electron microscopy (SEM), X-Ray diffractometer (XRD), UV-visible spectroscopy and photocurrent measurement.

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Performance characteristics of a portable dual GC for gas mixtures in air sample

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In the present study, we developed a portable dual GC instrument for real-time and quantitative determinations of gas mixtures in air sample. Dual GC is distinguished by a set of capillary and packed columns coiled together with a heater wire and thermocouple in a small case. In addition, the detection of VOCs and permanent gases such as CO, CO2, CH4, etc. are accomplished by using a PID (Photoionization Detector) and TCD (Thermal Conductivity Dectector), respectively. By measuring the various samples. We demonstrated the high sensitivity and selectivity of this device. The results indicate that the portable dual GC module is expected to be used for a wide range of applications, particularly for in situ environmental monitoring, chemical processes, and regulation of contaminant emission.

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Development of Portable Membrane Introduction Time of Flight mass spectrometry (MIMS) for Hydrophilic compounds

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Membrane introduction mass spectrometry (MIMS) is one of the simplest way to monitoring the atmosphere. Membrane is located between sample stream part and analyzing part. Only selective acceptable analytes can through the membrane. Because of this feature, it is very important to choose the suitable membrane. In case of our study, we applied the Nafion membrane commercially available hydrophilic membrane. We analyzed the low molecular weight alcohol and other volatile polar compounds. Also, we measured the dynamic range and response time and calculated diffusion coefficient about each compounds. Finally, we compared with established hydrophobic silicon membrane in MIMS

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The correlation between the number of molecules and the line-width of SERS

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We investigate the correlation between the number of molecules and line-width of the product peak in surface-enhanced Raman scattering (SERS) spectra. We illuminated silver nanoparticle (AgNP) ? 4-nitrobenzenethiol (NBT) monolayer ? gold thin film (AuTF) junction with light at λ_{ex}=632.8 nm to drive the photo-reduction of NBT and the reaction was monitored using SERS in real-time (time resolution : 30 ms). Through the analysis of instantaneous linewidths of SERS spectra of a few molecules, and correlating them with their intensities, we were able to examine how the heterogeneous broadening in SERS spectra evolves with the number of molecules.

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Plasmon-assisted chemical reaction: how does plasmonic local field influence rate of photo-reaction?

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We investigate a photo-reaction of 4-nitrobenzenethiol (NBT) to correlate photo-reaction rate and plasmonic local field effect. To identify the correlation, we monitor surface-enhanced Raman scattering (SERS) spectra with 632.8 nm laser excitation to investigate the photo-reaction of reactant (NBT) in Ag nanoparticle (AgNP)-molecules-Au thin film (AuTF) junction. Upon excitation, the $\nu_{s,\,NO}$ peak of reactant (NBT) decays exponentially and its decay rate may be influenced by the strength of plasmonic local field. To explore such effect in detail, we investigate the correlation of initial intensity of the $\nu_{s,\,NO}$ peak and its decay rate.

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A Quantitative Decoding Logic of Spectrum Mixture from Known Raman Spectrum Library

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Raman spectroscopy has drawn interests in bio-molecular detections such as immunoassay and imaging since it can afford multiplex analysis capability owing to its highly narrow bandwidth. Current technology allows qualitative analysis and quantitative analysis is still in the development stage. In order to get quantitative information in multiplex analysis based on Raman spectroscopy, decoding of intensity ratio from mixed Raman spectra is one of essential hurdles to overcome. This work illustrates a logic of spectrum analysis to extract intensity ratios of Raman spectrum mixture proposed that the constituent Raman spectra are within known libraries and the spectral features are not altered by mixing the sample. We applied this logic to two mixtures; one consists of 2-Naphthalenethiol(2-NT), benzenethiol (BT) and 3,4-dichlorobenzenthiol (3,4-DCT) and the other consists of 4-chlorobenzenethiol(4-CBT), 4-bromobenzenethiol(4-BBT) and 2-chlorobenzenethiol(2-CBT). We used the sum of the constituent Raman spectra as the mixture spectrum. When the logic was applied to the mixtures of 4 different ratios, the estimated intensity ratios were close to the preset ratios. It indicates that if we obtain Raman spectrum of a mixture in experiment, ratios of the chemicals in the mixture can be reliably extracted.

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Monte Carlo Study of Surface Effects on the Structure of Confined Water

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The behavior of water confined between two hydrophobic surfaces is important in many natural phenomena, such as protein folding, the opening and closing of ligand-gated ion channels, and adhesion and colloid stability. However, simulations of confined water have been limited to smooth, flat surfaces, although most surfaces are rough. Here, we perform lattice gas Monte Carlo simulations of confined water between two nanoscale surfaces. We investigate the effect of surface structure and surface separation on the drying transition of water. Considering three different types of surface geometry (plate-plate, hemisphere-plate and hemisphere-hemisphere), we studied an attractive force behavior and a critical distance for cavitation. We also introduced an atomic scale (smaller than 1nm) roughness on the surfaces. We found that in every case, geometry with small roughness shows a stronger attractive force behavior and a longer critical distance than another. This result suggests that the rough surface enhanced hydrophobicity.

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Hexoctahedral Au Nanocrystals with High-index Facets and $Au_{hexoctahedron}$-Cu_2O Hetero-Nanocrystals and Their Surface-Enhanced Raman Scattering and Photocatalytic Properties

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Precise-tuning of exposed facets on the surface of metal nanocrystals (NCs) by manipulating NC shape has provoked increasing research interest, because the inherent characteristics of NCs ranging from catalytic function to plasmonic properties highly depend on their surface atomic arrangement. In recent years, the synthesis of high-index-faceted NCs has attracted a great deal of attention. High-index facets consist of surface atoms with relatively lower coordination numbers than those of low-index facets due to the presence of high-density atomic steps and kinks on them. As such, their surface atoms have higher energy than those on low-index facets. Owing to this high surface energy, high-index-faceted NCs have shown greatly enhanced performance for specific catalytic reactions over NCs bound by low-index facets. Among various high-index-faceted NCs, hexoctahedral (HOH) NCs, which are bound by 48 triangular high-index {hkl} ($h > k > l > 0$) facets, are thought to be very promising nanomaterials for a range of applications, given that they are rich in energetic sites, including tips, edges, and intraparticle gaps. In this work, we present the synthesis of HOH Au NCs enclosed exclusively by high-index {321} facets. The HOH Au NCs exhibited efficient surface-enhanced Raman scattering activities. In addition, Au_{HOH}-Cu_2O heteronanocrystals (HNCs) were prepared through the selective overgrowth of Cu_2O on the high-curvature vertices of HOH Au NCs, the generation of HNCs with unprecedented morphological characteristics was realized. The prepared HNCs exhibited excellent photocatalytic performance due to the generation of strong electric field at the interconnecting junction between Au and Cu_2O.

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Monte Carlo Simulation Study on the Hydrophobic Surface Textured with Dome Pillars

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A lattice gas Monte Carlo simulation was performed to examine the wetting properties of a surface texturized with nanometer-sized, dome-shaped pillars. The vapor and liquid phases of the gap between the pillars were related to the Wenzel and Cassie-Baxter states of a macroscopic water droplet resting on top of the pillars. With increasing inter-pillar spacing or pressure, the liquid on top of the domed pillars penetrated smoothly down into the gap between the pillars. This wetting transition contrasts with that observed for the gap between rectangular or cylindrical pillars, where a liquid abruptly fills in the inter-pillar gap at a critical inter-pillar spacing or pressure. Simple analytic expressions of the critical spacing and pressure at which the wetting transition occurs for the domed pillars were derived using continuum theory. These continuum results agreed reasonably well with the present molecular simulations, even for pillars as small as few nanometers in width.

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Efficient Photocatalytic degradation of Methyl blue by heterostructured ZnO-RGO/RuO2 under the simulated sunlight irradiation

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부산대학교 화학과

Solar photocatalytic oxidation for the degradation of water pollutants is receiving increasing attention [1]. In the present work, the ability of photocatalysis to decontaminate water using ZnO, ZnO-RGO and ZnO-RGO/RuO2 heterostructured nanocomposites is comprehensively investigated. Among these nanocomposites, the superior photocatalytic ability is obtained for ZnO-RGO/RuO2 nanocomposites which can be ascribed to an efficient charge transfer from ZnO to RGO and RuO2. We have observed 98 % degradation of methyl blue in 210 minutes for ZnO. Whereas, 99 % degradation is observed for both ZnO-RGO and ZnO-RGO/RuO2 composites within 180, 150 minutes under simulated sunlight irradiation, respectively. Fig.1 shows the schematic diagram of Eg matching and flow of photo-induced electrons from ZnO to RGO and RuO2 under simulated sunlight irradiation. The recyclability results demonstrated the excellent stability and reliability of the ZnO-RGO/RuO2. Moreover, the structural and morphological studies indicated that the obtained nano structures have good crystallinity.In addition to the excellent photocatalytic degradation properties, the synthesized samples also exhibited a strong green-yellow emission, which implies that careful design and control of the composition can lead these samples to find application as green-yellow components in near Uv-white LEDs. Overall, the present work provides a new avenue for fabricating a ternary nano composite in terms of its simplicity, as well as its good performance for photocatalysis, and photoluminescence applications.References [1] K. Anna, F.G. Marcos, C. Gerardo, Advanced Nanoarchitectures for Solar Photocatalytic Applications, Chem. Rev. 2012, 112, 1555?1614.

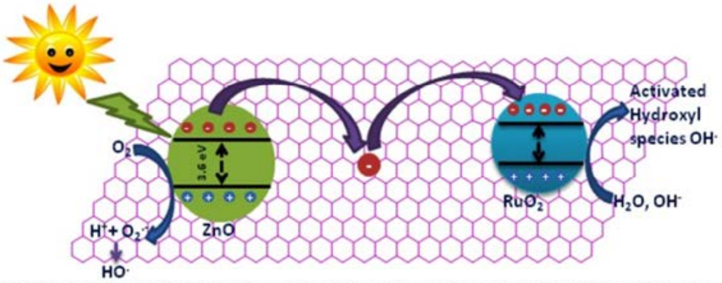

Fig.1: *Schematic diagram for E_g matching and flow of photo-induced electrons from ZnO to RGO and RuO_2 under simulated sunlight irradiation.*

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CARS Microscopy With a Femtosecond Fiber Laser

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광주과학기술원(GIST) 화학과

Coherent anti-Stokes Raman Scattering Microscopy is a powerful optical imaging technique, which allows a rapid three-dimensional chemical mapping of sample molecules without any exogenous labels. Despite the great potential of CARS microscopy, however, its applications to biomedical research and medical diagnosis have been limited due to the complicated and expensive laser instruments. Recently, an alternative CARS technique based on the so-called “Spectral Focusing Mechanism” has emerged. This technique does not only requires a much simpler laser system, but also allows a fast switching of the vibrational excitation frequency via temporal delay between two chirped laser pulses, thus eliminating the need for the expensive and complicated laser systems.Here, we present a Spectral Focusing CARS microscopy technique with a femtosecond fiber laser as a laser source. The fiber laser is of significantly lower cost than the previous picosecond laser systems and offers a possibility of a mobile CARS microscope, which can greatly help its clinical applications. Three-dimensional CARS imaging of lipid and protein inside several mouse tissues will be demonstrated.

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Effects of internal bond rotation on electronic states of Cy3 and Cy5 studied by time-dependent density functional theory

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Cyanine dyes are one of the most widely used molecules in fluorescence labeled imaging and microscopy. Despite their numerous applications, their fundamental photophysical properties related to internal rotation are still unclear. Different intermediate bonds may produce different conformations (*trans-* or *cis-*isomers) and influence the electronic states and energies. We carried out time-dependent density functional theory calculations for Cy3 and Cy5 to investigate the effect of each intermediate bond. Through the calculations, we found that the rotation of each bond distinctively changes the energies of singlet and triplet states.

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Anisotropic Diffusion Effects on the Diffusion-Influenced Reaction: Monte Carlo Simulation Studies

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Even if the latticed-based Monte Carlo simulation method is one of the simplest numerical experiments for diffusion-reaction systems, the anisotropic systems are not easy to be simulated. We find that anisotropy can be controlled by changing the probability ratio of the stay to the movement in two or three dimensional simulations. We confirm the accuracy of Monte Carlo methods by reproducing the theoretical predictions in isotropic diffusion-reaction systems. Simulation results are easily obtained and compared in anisotropic systems where theoretical predictions are absent.

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Monte Carlo Simulation Studies in Diffusion-Influenced Reaction: External Field Effects

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The external field effects including gravitational, magnetic, and electric effects on diffusion-reaction systems are ubiquitous in a broad range of chemical and biological systems. However, the theoretical approaches to study those effects have been relatively rare because of their complexities. The exact analytical results have been known only for simple systems, especially in one dimension and three dimensions. On the other hand, the computer simulations can be applied to complicated systems more easily because of its flexibility. If we want to mimic the conditions in theories with simulations for external field effects, we first have to verify the consistency between theories and simulations rigorously. In this presentation, we suggest the simulations methods dealing with the external field effects to predict the exact analytical results in one dimension.

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Surface structures of Cu-Ni binary alloy: Monte Carlo simulations with EAM potentials

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(주)인실리코 [1]고려대학교 화학과

Metal particles are the key components of conductive pastes for the transparent electrode. Now Ag paste is most widely used in industry but for cost reductions requests for the cheaper metal paste are increasing. The core-shell structure with the Ag shell is a plausible approach for that goal. Cu microsized-particles have been tested as the core, but the oxidation and Ag dewetting are the critical problems. Cu-Ni alloy could be one of the alternatives to overcome these problems. As the surface structure of Cu-Ni alloy could affect the oxidation and the compatibility with Ag shell, it is important to understand how the surface structure varies according to the compositions. In this work, we modeled the surface structures of Cu_3Ni, CuNi, and $CuNi_3$ alloys using Monte Carlo simulations with embedded-atom model (EAM) potentials. In Monte Carlo simulations, we accomplished the energy fluctuation using displacement and exchange moves. The results show that Cu is richer in the outermost plane of (111) surfaces for all alloy surfaces. For Cu_3Ni, Ni atoms gather in a couple of planes beneath the outermost plane, and for CuNi and $CuNi_3$, they disperse into the deeper inside. We conclude that to attain the quite different surface structure the bulk Ni content should be higher than 0.5.

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Real-time observation of endocytosis using total internal reflection fluorescence(TIRF) microscopy and upconversion nanoparticles (UCNPs)

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Recently, there has been great interest in studying lanthanide-doped Upconverting Nanoparticles(UCNPs) in the field of biological imaging owing to their unique optical properties. UCNPs have ability to upconvert low energy, usually near-infrared (NIR) or infrared (IR), into higher energy, ultraviolet (UV) or visible via multiphoton upconversion process. It is issued in biological application because of photostability and lower toxicity. UCNPs can be used for understanding the interaction between these nanoparticles and biological systems at the cellular level. In this study, we use a total internal reflection fluorescence(TIRF) microscope with 980-nm excitation. TIRF, it is possible to obtain images with low background steming from the cell bodies. TIRF imaging permits the monitoring of various steps and movement of vesicles composing the endocytosis pathways at the cell membrane. The combination of TIRF and UCNPs turned out to be powerful tool for the study of membrane dynamics.

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Vibrational Predissociation of AnPyW2+ and AnPyW3+: Structure and Dissociation Dynamics Analysis

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경희대학교 화학과

Vibrational predissociation spectrum of AnPyW2+ and AnPyW3+ cluster has been taken at 2700-4000 cm-1. Both case one N-H of aniline is bonded to the pi electron of pyrrole and other N-H is bonded to hydrogen bonded water. Pyrrole molecule arranged such a way that N-H of pyrrole can form another hydrogen bond with a water molecule. One water ejected channel is more preferable fragmentation pathway for both AnPyW2+ and AnPyW3+ though calculation result show pyrrole ejection channel should be more preferable for AnPyW2+. This might be due to bulky pyrrole is not good leaving solvent in these clusters. One water, two water or pyrrole molecule ejections are possible reaction pathway for predissociation of AnPyW2+ and AnPyW3+.

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Time-resolved X-ray Scattering Study of Cytochrome c Folding: Hidden Kinetic Pathway Unveiled by Thermodynamics of Solvent Heating

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Understanding the protein folding pathway with the characterization of intermediate structure is of importance in the fields of biochemistry and biophysics. Among many proteins, cytochrome c (Cytc), which is an essential component of electron transport chain in mitochondria, is an ideal model to unravel the global scheme of protein folding due to the structural simplicity relative to other complex proteins. Although the extensive experimental and theoretical studies for the Cytc folding have been performed, it is hard to establish the global folding framework of cytochrome c with respect to the global conformational change owing to the lack of experimental probe that is sensitive to the global conformational change. To overcome this, we employ time-resolved X-ray scattering to probe the folding dynamics of Cytc induced by the electron transport occurring in a wide time range from 31.6 μs to 316 ms. From the systematic analysis, the folding pathway of cytochrome c shows the two-state kinetic model (unfolded state → folded state) accompanying 117 ms as the time constant. Interestingly, the hidden pathway, which isn’t detected on the transient signal of protein structural change, can be captured by the thermodynamic analysis of the solvent heat response. From this study, we can establish the protein folding framework of Cytc with the global conformation of intermediate. Also, the calorimetry of impulsive solvent heat enables us to reveal the hidden folding pathway on the dynamics of Cytc folding.

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Photoluminescence of Band Gap States in AgInS2 Nanoparticles

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Most of binary semiconductors include toxic elementals such as Cd, Se, Te and Pb, although they have unique electronic and optical properties for application in light-emitting devices and solar cells. In this regard, non-toxic I-III-VI2 ternary semiconductors such as CuInS2, AgInS2 are investigated. In this paper, the various sizes of AgInS2 nanoparticles are synthesized upon the change of the reaction temperature. The band gap energies, which are directly obtained from photoluminescence spectra for the first time, suggest the quantum confinement effects as a function of nanoparticle sizes. The coexistence of chalcopyrite (tetragonal) and orthorhombic phase is observed in the AgInS2 nanoparticles, although the relative population of each phase depends on the reaction temperature and time. The band gap shift of the chalcopyrite phase is comparable to that of the orthorhombic phase, which indicates that the change of the band gap energy is mainly determined by the sizes. The photodynamics of the band gap states exhibits the emission wavelength dependence, which supports the coexistence of two phases. The contributions of each phase in the time profiles match with the relative population of each phase observed in the steady-state photoluminescence spectra.

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The optical properties of ZnO-Au nanocomposites for photocatalyst

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경희대학교 화학과

A great challenge facing our global future is the development of renewable energy. In this regard the various materials have been studied for the solar energy conversion. Among them the semiconductor-metal nanoparticle composites have many advantages compared to organic based structures for solar energy harvest. Because of the size-dependent optical properties and electron transfer processes the semiconductor-metal nanoparticle composites have been studied extensively. We investigated the optical properties of ZnO-Au nanocomposites for photocatalyst. We tried to find the differences of electron transfer processes with various ZnO-Au nanocomposites. And we distinguished the contribution of ZnO and Au species in ZnO-Au nanocomposites from the measurement of transient absorption spectra. We found that the rate of electron transfer between ZnO and Au is affected by the size of Au. Therefore the optimization of Au size deposited on ZnO surface is essential for the efficient photocatalytic activity of ZnO-Au nanocomposite

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Luminescence Properties of Tb(III) Complexes with TETA and phen(TETA = 1,4,8,11-tetraazacyclotetradecane-1,4,8,11-tetraaceto, phen = 1,10-phenanthroline)

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충남대학교 화학과

We synthesized complexes of [Tb(TETA)]- and [Tb(TETA)(phen)]- and investigated their luminescence properties, such as photoluminescence (PL), excitation and absolute quantum yield. The two complexes, excited by a He-Cd 325-nm, produced very typical band features, originating from the transitions from the 5D4 state to the 7FJ (J = 6, 5, 4, 3) states, peaking at 489, 545, 582 and 621 nm, respectively. Compared with [Tb(TETA)]-, [Tb(TETA)(phen)]- produced markedly enhanced the PL intensity. The excitation spectrum showed that the highly enhanced luminescence of [Tb(TETA)(phen)]- was due to the energy transfer from phen to Tb(III). The absolute quantum yield of PL of the complexes were precisely determined at room temperature on a 325-nm excitation. The quantum yield of [Tb(TETA)?(phen)]- (Q = 13.15 %) was much greater than that of [Tb(TETA)?(2H2O)]- (Q = 0.61 %).

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Formation of covalently linked artificial solid electrolyte interface using reactive force field

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(주)인실리코

The lithium ion batteries (LIB) are the most widely used power source for portable electronic devices, and many studies are carrying out to improve the performance of LIB. The fact that the solid-electrolyte interface (SEI) that forms at the anode surface as a result of electrolyte decomposition is closely related to the performance of LIB such as rate capability, cyclability and Columbic efficiency is widely known. There are reports that polymer encapsulated graphite like poly(acrylonitrile) and pyrolytic polyuria can improve the performance of LIB. (J. Power Sources 2002, 111, 350 / Electrochim. Acta 2005, 50, 4728) In this work, we carried out molecular dynamics (MD) simulations to form polymerized artificial SEI between graphite and electrolyte through thermal effect using reactive force field. We analyzed the mechanism for the formation of artificial SEI, and investigated what kind of electrolytes can create the polymerized SEI.

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Excited-State Dynamics of Carotenoids and Retinal studied by Femtosecond Stimulated-Raman Spectroscopy

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Carotenoids, which play important roles in photosynthesis like light-harvesting or photo-protection, have been known to have very complex excited-state dynamics upon photoexcitation. In order to study the photoinduced relaxation dynamics of carotenoids, transient absorption spectroscopic techniques have often been applied. However, the exact dynamics between the excited states and the ground state of carotenoids are hard to reveal mainly due to generally broad and overlapping electronic transitions and very fast kinetics.In this work, we have set up a femtosecond stimulated Raman spectroscopy (FSRS) based on a Ti:sapphire regenerative amplifier system (50 fs pulsewidth). Broadband Raman probe pulses and picosecond Raman pump pulses are combined with another femtosecond actinyl pump pulses in order to obtain a high temporal (< 10 cm-1) resolution in the different stimulated Raman spectra. Time-resolved Raman spectra of carotenoids (β-carotene and 8’-apo-β-caroten-8’-al) and all-trans-retianl will be recorded and analyzed to elucidate their excited state dynamics and structural changes upon photoexcitation.

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DFT approach for the chemisorbed hydrogen on NaY-FAU zeolite

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(주)인실리코 [1]고려대학교 화학과

Porosity and robustness of faujasite zeolites are used in the wide range of industry and NaY faujasite is one of the candidates for the hydrogen storage material. In order to store hydrogen at moderate temperature and pressure, chemisorption of hydrogen on the surface of the porous framework is required and the source of hydrogen is derived generally from the bond cleavage of H_2 molecules on the metal cluster such as Pt and Pd. Hydrogen spillover can be expected when the hydrogen atoms generated at surface of the metal cluster migrate and make a strong covalent bond to the reservoir or NaY zeolite. In this work, hydrogen atoms are assumed to be prepared by catalysts and we investigated where and how the hydrogen is located on the surface of NaY zeolite. Acidic and basic sites on NaY can influence the electronic state of hydrogen bound to the framework as chemisorption. Density functional theory (DFT) calculation showed the most hydrogen atoms bind together and make hydrogen molecules which are physically adsorbed on the surface of the NaY. Rest of hydrogen atoms donate or receive an election to or from the NaY framework and becomes proton or hydride ion. The binding sites and charge states of the protons and hydride ions by this work will be the key to understanding the characteristics of hydrogen spillover at NaY zeolite.

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Single-molecule study of the interaction between HindIII endonuclease and substituted DNA

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We studied the interaction of HindIII endonuclease with double-stranded DNA containing an AAGCTT segment, which substitutes various functional groups and is expected to be the interface between HindIII and its recognition sequence. We found that the introduction of a single substituent on the recognition site has only a small effect on binding of endonuclease. The dependence of the binding rate on the size of substituents shows a compensation relationship between the activation energy and pre-exponential factor. Different kinetics between normal vs. substituted DNA is caused by the unstable HindIII?DNA complex, which is consistent with the change in the standard free energy of the transition state. We propose that the effect of molecular changes on DNA recognition site is important in understanding how DNA modification modulates the cellular metabolism and functions of DNA binding proteins.

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Excited-state dynamics of Dyes near plasmonic nanoparticles in solution and poly vinyl alcohol

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When chromophores exist close to plasmonic nanoparticles, both absorbance and fluorescence of the chromophores increase by the locally enhanced electric field and energy transfer between nanoparticles and chomophores. These phenomena are called as metal-enhanced fluorescence (MEF) and have been used in many applications.In this work, excited-state dynamics of 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) and rhodamine6G near silver island film have been studied using an ultrafast transient absorption spectroscopy and time-correlated single photon counting (TCSPC) in visible wavelengths. DCM and Rhodamine6G in solution showed up to 30 times enhancement in fluorescence intensity and significant difference in the kinetics of transient absorption with the silver island film

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MnO2 electrode electrodeposited on 3D nanostructured Ni current collector for supercapacitors

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국민대학교 생명나노화학과

In order to improve the performance of supercapacitors, various attempts to fabricate nanostructured current collectors instead of conventional planar ones have been made since they can provide significantly enhanced contact between active electrode materials deposited on them and electrolyte. In this work, we successfully fabricated well-ordered 3-dimensional nickel (Ni) nanostructures using arrayed polystyrene nanospheres. We also fabricated half-cell supercapacitors by electrodepositing manganese oxide (MnO2) onto these nanostructured Ni current collectors and investigated their physical, morphological and electrochemical properties.

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Water-soluble D-glucuronic acid coated ultrasmall mixed (Gd/Mn) oxide nanoparticles and their application to magnetic resonance imaging

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경북대학교 화학과

Magnetic resonance imaging (MRI) is a powerful and noninvasive diagnostic technique of the human anatomy on the basis of superior spatial resolution and contrast. A large number of MRI techniques are performed employing gadolinium complexes and gadolinium nanoparticles. However, doped or alloy nanoparticles can show better contrast with enhancing relaxivity. For this purpose, we have developed ultrasmall gadolinium manganese oxide nanoparticles. The average size of prepared nanoparticles is of 2 to 3 nm, which can be dispersed homogeneously. They were coated with biocompatible and water soluble D-glucuronic acid. It shows higher relaxivity than normal ultrasmall gadolinium oxide nanoparticles. Moreover, in vivo and in-vitro tests of the sample solution, indicated clear dose-dependent contrast enhancements in both T_1 and T_2 map images, showing that the nanoparticles can be used as both T_1 and T_2 contrast agents.

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Size effect of TiO2 nanoparticles on transparency and hydrophobicity of PDMS thin films deposited on them

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국민대학교 화학과 [1]국민대학교 생명나노화학과

In this work, the surface hydrophobicity and transparency of polymer films coated on the substrates covered with titanium dioxide (TiO2) nanoparticle layers were studied. Firstly, we synthesized various sizes of TiO2 nanoparticles using sol-gel hybrid method and spray-coated them onto ITO/glass substrates. The crystallinity and size of the TiO2 nanoparticles were examined using x-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively. The polydimethylsiloxane (PDMS) thin films were then spin-coated on the TiO2 nanoparticle layers and their transparency and surface hydrophobicity were studied using UV-visible spectroscopy and water contact angle measurements, respectively.

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Photodissociation Dynamics of Oxalyl Bromide at near 265 and 234 nm: an Application of Velocity Map Ion Imaging Technique

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부산대학교 화학과

Velocity map ion imaging (VMI) is an advanced technique which allows simultaneous measurements of both speed and angular distribution. VMI technique makes easier to keep the laser and the molecular beam stable and increase the signal-to-noise ratio. In the field of photodissociation dynamics, velocity map ion imaging is the state-of-the-art technique.In this study, we have revealed the photodissociation dynamics of oxaly bromide (C2O2Br2) at near 265 and 234 nm using VMI technique. The [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme was used for state selective detections of Br (2P3/2) and Br* (2P1/2) generated after photolysis of C2O2Br2 at two wavelengths. The nascent Br (2P3/2) atoms stem from the primary C-Br bond fission as well as secondary dissociation of their corresponding C2O2Br radicals which are energized from the ultrafast primary photodissociation steps at both pump energy. The measured total translational energy distributions, recoil anisotropic parameters, and the relative quantum yields were used to explore photo-induced stepwise multi-body dissociation processes. In excited state translational energy distribution can be fitted by single Guassian distribution, where as three Guassian functions at ground state. The translational anisotropy parameter, β, values are 0.90 (0.79) for Br and 1.38 (0.97) for Br*, respectively, at 265 (234) nm. The resultant quantum yields for Br* are 0.42 and 0.33 at 265 and 234 nm, respectively.

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Synthesis and Characterization of cRGD Conjugated Gd_2O_3 Nanoparticles for the Detection of Cancer Cell

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경북대학교 화학과

Cyclic RGD shows high affinity and specificity for several cancer cells and bind selectively to their target cell. The selective labeling of cancer cells is performed in suspension, allowing a fast interaction between the Gd_2O_3 nanoparticles (GNPs) labels and the target proteins expressed at the cell membrane. We synthesized two types of GNPs system; cRGD conjugated GNPs and then amine group of cRGD was coupled with fluorescent compound. The additional coupling of the cRGD to fluorescent compound offers an excellent and highly sensitive method for detecting cancer cells. In order to prove the potential of this rapid and low-cost method for diagnostic purposes, confocal microscopy was used to confirm the specific collection and detection of target cells. The final fluorescence of the cells labeled with the nanoparticles was quantified using a fluorescence microplate reader.

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Synthesis and Characterization of Glycine-Folic Acid Surface-modified Gadolinium Oxide Nanoparticles as A MRI Contrast Agent

Xu Wenlong 이강호*

경북대학교 화학과

A MRI contrast agent, glycine-folic acid coated Gadolinium oxide nanoparticles were reported which were synthesised in triethylene glycol. They were characterized with XRD, FT-IR, TGA, MPMS, TEM and MRI instrument. We hope that they can only target the cancer cells but not normal cell. These nanoparticles have enhanced relaxivity. Hence, it can be used as a MR imaging contrast agent.

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D-Glucuronic acid coated Tungsten oxide, Dysprosium oxide and Barium oxide nanoparticles as CT Contrast Agent

김성준 이강호*

경북대학교 화학과

We have searched for improved CT contrast agents and we discovered some materials. The materials are Tungsten, Dysprosium and Barium. They have considerably high x-ray attenuation coefficients. So, we synthesized Tungsten oxide, Dysprosium oxide and Barium oxide nanoparticles for using improved CT contrast agent. To be used as clinical CT contrast agent, they were coated with D-glucuronic acid which is hydrophilic and biocompatible ligand. They characterized by using MP-XRD, TGA, FT-IR, HRTEM, Phantom images and In vitro cytotoxicity test.

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Apoferritin coated Gd_2O_3 nanoparticles as MRI contrast agent

MiaoXu 이강호*

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Gadolinium oxide nanoparticles which were prepared by coating the apoferritin cavity were reported. They were characterized with XRD, FT-IR, TEM, TGA, MPMS and MRI instrument. Because the apoferritin can be dissociated into subunits by extremes of pH. By using this property, can be better coated Gadolinium oxide nanoparticles as MRI contrast agent.

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Small Angle X-ray Scattering study of the lamella phase separation for alcohol binary mixture

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인천대학교 화학과

Splitting of the scissoring as well as rocking band has been considered a useful probe for micro-phase separation of a binary mixture of long chain hydrocarbons. The extent of splitting reflects the size of the micro-domain, which grows with time, and the earlier reports show that the difference in chain length should be at least 4 to observe a band split. In contrast, The IR spectra of alcohol-n-alkane mixtures indicate immediate phase separation regardless of the difference in length and mixing ratio. While chain disorders increase with approaching to the melting point, the spectra suggest that phase separation still remains. The SAXS (small angle X-ray scattering) method is also newly employed to investigate the lamellar structures from the Q-vector spectra. It is interesting that two Q-vector points (lamellar thicknesses) are observed from an alcohol binary mixture, instead of three (three possible combinations via hydrogen bonding of two long chain alcohols). Noticeable changes in the Q-vector spectra also occur after annealing (50℃, below the melting point). The results along with our interpretation will be presented.

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Effects of bovine serum albumin on the antioxidant activity of phenolic compounds

천태민 조한국 정병서*

인천대학교 화학과

Phenolic compounds show a variety of biological activities including antioxidant, anti-inflammatory, anti-fibrosis, and so on. While there have been many studies to determine the antioxidant activity for a variety of dietary phenolic compounds, the protein binding may affect the activity of antioxidants in foods. In the present study, the effect of bovine serum albumin (BSA) on the antioxidant activity of selected phenolic compounds, ellagic acid and propyl gallate, was investigated using the Trolox equivalent antioxidant capacity (TEAC) assay. Antioxidant activities of ellagic acid and propyl gallate with binding to BSA were measured and the results were compared to those of free phenolic compounds. In addition, the binding interactions of these phenolic compounds with BSA were studied using fluorescence spectroscopy. The observed behavior in the antioxidant activity of the protein-phenolic compound systems was discussed on the basis of interactions between the protein and phenolic compound.

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Spectroscopic properties of fluorescent dyes and proteins in polymer and sugar matrices

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인천대학교 화학과

In order to correlate how the solvent affects emission properties of fluorescent dyes, the fluorescence emission spectra of carboxytetramethylrhodamine (TAMRA) and rhodamine B (RhB) as well as myoglobin conjugated with TAMRA were measured in methanol, polyvinyl alcohol (PVA) polymer matrix, trehalose and trehalose/sucrose sugar glass matrices. The fluorescence properties and spectral shifts observed in the TAMRA and RhB spectra were compared and analyzed to provide information on the environment and dynamics of the matrices. The fluorescence spectra of myoglobin conjugated with TAMRA in sugar glasses were examined to gain insight into the behavior of protein in sugar films. Efforts were also made to discern the changes in fluorescence characteristics, e.g. the fluorescence intensities and emission maxima, depending on the drying condition of films, thereby revealing the effect of residual water in the films.

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Synthesis and characterization of silver nanoparticles with complex shapes for SERS applications

이승장 조한국 정병서*

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Synthesis of silver nanostructures in various morphologies has received much attention because of the shaped- and size-dependence of physicochemical, optical, and electronic properties. In this study, we prepared the silver nanoparticles of different shapes and sizes for applications to surface-enhanced Raman scattering (SERS) by controlling the concentrations and mixing ratios of the reducing agents and stabilizers, and the silver nanoparticles with highly roughened surfaces were characterized by scanning electron microscopy (SEM) and dark-field microscopy as well as UV/Vis absorption spectroscopy. The SERS spectra of rhodamine 6G and p-aminothiophenol were obtained using the nanoparticles synthesized as active SERS substrates, and the enhancement of SERS effects was evaluated. They were also compared with the SERS spectra in silver colloid solutions.

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Water Soluble Ultrasmall Mixed Gadolinium Dysprosium Oxide Nanoparticles for MRI Contrasting Agent

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Surface coated magnetic nanoparticles have been very intensively investigated so far due to their potential applications to a variety of biological and biomedical areas.In this work we synthesized ultra small water soluble GdDy mixed oxide nanoparticles with biofunctinalized surface coating. D-glucuronic acid was used for the surface coating of the nanoparticles. The water soluble and biocompatible D-Glucuronic acid coated GdDy mixed oxide nanoparticles have drawn tremendous attraction in the application of magnetic resonance imaging.The structural, morphological and magnetic properties of these synthesized products were characterized by using X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy (FTIR), TGA, and SQUID magnetometer. To confirm the validity of mixed gadolinium dysprosium oxide nanoparticles for T_1, T_2 dual MRI imaging ,we performed in vitro and in vivo imaging and relaxivity measurements.

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Distance-dependent enhancement of fluorescence on silver island-coated surfaces

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The metal-enhanced fluorescence (MEF) occurs by surface plasmon resonance and this plasmonic phenomenon is strongly correlated with the distance between the fluorophore and metal nanoparticles. In this study, we have investigated the distance-dependence of MEF of fluorophores, fluorescein and rhodamine B, on silver island films (SIF). Fluorophore molecules are dispersed in the polyvinyl alcohol (PVA) polymer matrix, and spin coated on the SIF substrate, controlling the distance by varying the concentration of PVA from 0.5% to 5.0%. We have observed that the fluorescence emission of both fluorescein and rhodamine B is considerably enhanced on SIFs, and the fluorescence enhancement depends on the thickness of PVA films or the average distance between the fluorophore and metallic silver particles.

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Photodissociation Dynamics of Thioanisole-d_1,-d_2 and 2-Fluorothioanisole using Velocity Map Ion Imaging (VMI) and Slow-Electron Velocity-map Imaging (SEVI)

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Photodissociation dynamics of the two rotational isomers of both thiosnisole-d_1 and thioanisole-d_2 have been investigated using Velocity Map Ion imaging (VMI) and slow-electron velocity-map Imaging (SEVI) spectroscopies. Increasing of nonadiabatic transition probability in symmetric and asymmetric stretching modes of S-CH_3 bonds results in sharp resonances of X/A ratio of SC_6H_5. The mode dependence and intramolecular vibrational redistribution (IVR) induce qualitative and quantitative change of product branching ratio. Also, VMI and SEVI of 2-Fourothioanisole are in progress to identify the excited state photodissociation dynamics.

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Resistive Switching Behavior in chalcogenide nanostructures

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Resistive switching (RS) behaviors of chalcogenide nanostructures have studied by conductive atomic force microscopy (C-AFM). The chalcogenide nanostructures were prepared by chemical vapor deposition and their crystal structure were determined from X-ray diffraction, scanning electron microscopy and transmission electron microscopy. Dielectrophoresis was used for the alignment of the nanostructures between patterned Au electrodes. The electrical contacts between the nanostructures and Au electrodes were made by focused ion beam assisted Pt deposition. After all fabrication steps are complete, the prepared samples present a structure of Pt/Pt-coated nanostructure/Au. The electrical properties of the devices were obtained in the contact mode by C-AFM with Pt/Ir-coated tips at room temperature and in air. As a result of C-AFM measurements, the devices exhibit both reversible resistive switching behaviors with bipolar switching characteristics and electrical bistability. The ratio between the currents during high resistance state and low resistance state (at a positive voltage) was compared respectively. These results indicate that the electrical bistability and memory phenomena can be seen from the simple device structure of Pt/Pt-coated nanostructure/Au. Finally, it can suggest the possibility of developing simple nanostructure-based resistance memory devices.

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Real-time observation of the conformational change of T7 RNA polymerase for understanding the mechanism of transcription initiation

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Transcription plays a key role in gene expression by transferring the genetic information of DNA into mRNA. Especially, understanding the transcription initiation, which determines the rate of the transcription, is important. Although it has been extensively studied by using X-ray crystallography and numerous biochemical techniques, it is still difficult to fully understand the mechanism of transcription because those techniques provide only the information about the static states but not about the dynamics. In order to elucidate the complete mechanism of the transcription process of T7 RNA polymerase, we investigated its real-time dynamical changes in structure using TIRF microscopy.

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Surface-Enhanced Raman Study of Adsorbates on Gold and Silver Nanosurfaces

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Surface Enhanced Raman spectroscopy (SERS) is an effective tool to study vibrational aspects of molecules adsorbed on noble metal surfaces. The SERS enhancement mechanism involves the local surface plasmon and/or the formation of a charge-transfer between the metal and the adsorbates.In this work, silver and gold nanoparticles have been synthesized by various reducing agents including borohydride and citrate and silver and gold island films by immersing aminopropyltriethoxysilane (APS)-coated glass slides in colloidal solutions. Concentration and pH dependent SERS spectra of orange dye coumarin 343 have been observed and the absorption geometry related to the carboxylic and carbonyl groups of coumarin 343 will be analyzed and compared with simulated Raman spectra from DFT methods at the B3LYP/6-311+G(d, p) level. SERS of amino acids including glycine and alanine have been observed on silver and gold nanosurfaces and the surface adsorption geometry will be also discussed.

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Concentration-Dependent H-Bond Structure and Dynamics of Water in Aqueous $NaPF_6$ Solutions

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There has been a difficulty in studying the individual dynamics of water in bulk and ionic hydration shells in most of aqueous ionic solutions because the hydroxyl stretch (-OH or -OD) bands of water molecules in bulk and ionic hydration shells are very broad and substantially overlapped with each other in FTIR spectra. Water molecules in bulk, cationic and anionic hydration shells (OD_W, OD_C, and OD_A, respectively) were able to be spectrally separated in aqueous $NaPF_6$ solutions. These spectral features allow us to study the structure and dynamics of water in bulk, cationic and anionic hydration shells separately. The vibrational lifetimes of water in three different configurations were successfully determined and found to be well characterized in bulk and ionic hydration shells. The orientational relaxation dynamics of water were found to be dependent on the solution viscosity and were reasonably well described by the Debye-Stokes-Einstein equation. Frequency-dependent transition dipole moment of the OD stretching vibration was obtained from the IR and Raman spectra.

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Carbon-13 isotope separation using photo-dissociation of formaldehyde

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한국원자력연구원 양자광학연구부

자연계에 존재하는 많은 동위원소들이 의학, 산업, 기초과학 분야 등에서 널리 사용되고 있다. 특히 NV-diamond 제조를 위한 고순도의 탄소-12, 생물학과 의학 분야에서 탄소의 표지자로 사용되는 탄소-13 의 수요가 늘어나고 있기 때문에 효율적인 탄소 동위원소 분리 방법 개발의 필요성이 대두되고 있다. 동위원소를 분리하는 여러 방법 중 하나인 분자 레이저 동위원소 분리법(MLIS)은 특정 동위원소를 포함하는 분자가 주로 흡수하는 파장의 빛 조사하여, 광분해를 촉진시켜 동위원소를 분리하는 방법이다. 이 방법은 생산물을 빠르게 얻을 수 있고 경제적이기 때문에 기존에 널리 사용되던 원심분리법이나 증류법 등을 대체할 수 있을 것이라 생각된다.탄소 동위원소 분리를 위해 폼알데하이드(HCHO)의 자외선 광분해를 이용하였다. 폼알데하이드는 근자외선 영역(~350nm)에서 매우 높은 양자효율(~90%)로 일산화탄소(CO)와 수소(H_2)로 분리되기 때문에 탄소(^{12}C, ^{13}C ^{14}C)와 산소(^{16}O, ^{17}O, ^{18}O), 수소(H, D, T) 동위원소 분리에 적합하다.이번 실험에서는 다이오드 기반의 파장가변 광섬유 레이저를 이용하여 352 nm 영역에 있는 ^{13}C-폼알데하이드의 전이선에 파장을 고정하여 ^{13}C-폼알데하이드를 선택적으로 광분해하는 방법으로 ^{13}C 분리 실험을 수행하였다. 약 30W 정도의 자외선을 15 분간 조사한 결과 ^{13}C 는 약 74%정도 광분해되었고, ^{12}C 는 0.5%정도 광분해 되었음을 확인되었다. 그 결과 ^{13}C 의 농축계수는 약 155, 감손계수는 약 3.8, 분리계수는 약 592 정도로 계산되었다.이번 실험을 통해 근자외선 영역의 광섬유 레이저를 이용하여 폼알데하이드를 선택적으로 광분해함으로써, 탄소-13 동위원소를 효과적으로 분리할 수 있음을 실증하였다.

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CO oxidation over mesoporous NiO/Al_2O_3

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We deposited NiO layers on mesoporous Al_2O_3 using atomic layer deposition (ALD) which can form homogeneous film on complex surfaces such as porous materials. Chemical and physical properties of the fabricated NiO/Al_2O_3 were analyzed by inductively coupled plasma optical emission spectrometry (ICP-OES), X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM). The Al_2O_3 supported-NiO was used as a catalyst for CO oxidation at various temperatures, and the catalyst showed high catalytic activity and stability at 250 ℃ for 24 h. Even at 30 ℃, NiO/Al_2O_3 catalyst showed about 90% CO conversion in the first 10 min of CO oxidation reaction. Reactivity of the deactivated NiO/Al_2O_3 catalyst during CO oxidation was regenerated after post-annealing at 300 ℃ for 2 h in air condition. It implies that ALD-prepared Ni/Al_2O_3 could be one of the promising catalysts for low temperature CO oxidation.

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Smart shield: Gas permeable superhydrophobic film

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We report a simple method for fabricating superhydrophobic film with gas permeability. PDMS (Polydimethylsiloxane) coated silica nanoparticles were deposited on various substrates using dip coating method. The water contact angle of coated substrates was over 150°, which implies that the surface of these substrate is superhydrophobic and highly repellent to water. In order to improve adhesion of PDMS coated silica nanoparticles on substrate, PDMS with curing agent was added to the solution as adhesive. Enhanced mechanical stability of the films was revealed by sand abrasion test and the films were highly resistant toward degradation under acidic and basic environments and UV-exposures. We also showed that the superhydrophobic film can permeate gas. The surface structure of the particles formed on substrate was analyzed using SEM (Scanning electron microscopy) and AFM (Atomic force microscopy).

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Excited-state dynamics of carotenoid and alizarin sensitized with TiO2 nanoparticles by transient absorption spectroscopy

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Photoinduced electron transfers between chromophore molecules and semiconductor nanoparticles have been studied by a femtosecond transient absorption spectroscopy. Carotenoids, often found in the photosynthetic complexes of plants and photosynthetic bacteria, are known to lose an electron upon photoexcitation and become a cation, especially when TiO2 nanoparticles have been attached to the chromophore as an electron acceptor.In this research, all-trans-8'-apo-β-caroten-8'-oic acid (ACOA) has been synthesized from its aldehyde and from TiO2 nanoparticles of 2-3 nm diameter prepared from a hydrolysis reaction have been attached to ACOA and alizarin. Femtosecond transient absorption measurements at different excitation wavelengths of 400 and 480 nm have revealed the ultrafast photoinduced electron injection to TiO2 and much slower recombination kinetics.

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Electrospun RuO2-Co3O4 hybrid nanotubes for enhanced electrocatalytic acitivities

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We report a facile synthesis of electrospun RuO2-Co3O4 hybrid nanotubes as well as their enhanced electrochemical responses. Among the various compositions of the relative atomic ratio(Ru/Co), polycrystalline RuO2-Co3O4 hybrid nanotubes of the relative atomic ratio(Ru/Co=2.30:1) prepared by electrospinning shows the highest efficient catalytic activity in terms of the onset potential and the slope for oxygen reduction reaction (ORR). In addition, the electrochemical sensing of ascorbic acid was carefully performed, resulting in the high sensitivity, low detection limit, broad dynamic range without the interference from other biological relevant species.

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Optimal control of catalytic reaction via in silico molecular modeling: Succinyl CoA Synthetase in the rTCA cycle

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Solar energy has been known to be one of the most invaluable resources on the earth. Unfortunately, the overall efficiency of natural photosynthesis is rather low. Increasing the efficiency of any one of the processes involved in photosynthesis would be invaluable to human being. Succinyl CoA synthetase (SCoA Syn) catalyzes the reversible reaction of succinly CoA to succinate in the tricarboxylic acid (TCA) cycle. Through the rTCA cycle, SCoA Syn participates in the photosynthesis. SCoA Syn has $\alpha 2\beta 2$ heterotetrameric structure and His246 of the enzyme has been known to play an important role in the catalytic reaction at the active site. The complementarity of an enzyme and a substrate could be very important in the enzymatic reaction. The enzyme-substrate complex, stabilized due to favorable complementarity, may result in the retardation of the catalytic reaction, while structural instability induced in the enzyme-substrate complex may contribute to the acceleration. Based on the theoretical model, we use in silico molecular modeling to control the catalytic efficiency of SCoA Syn in the photosynthesis. We proposed the criteria of selecting effective mutants for maximal activity of SCoA Syn by adjusting the stability of a substrate, coenzyme A (CoASH), at the binding site of SCoA Syn.

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Electronic circular dichroism spectroscopy of 2-amino-1-phenylethanol in a supersonic jet

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We obtained the electronic circular dichroism (CD) spectrum of (*R*)-(-)-2-amino-1-phenylethanol (*R*-AP) and its hydrated clusters produced in a supersonic jet using resonant two photon ionization spectroscopy. The *R*-AP and its clusters were irradiated by left and right-handed circularly polarized (LCP and RCP) laser pulses generated using a photoelastic modulator and the difference between the ion signals produced by LCP and RCP pulses was recorded as a function of the wavelength to obtain the CD spectra. We identified the origin bands of the S_0-S_1 transition for two different conformers of *R*-AP present in the jet. Theoretical calculations were carried out to predict the structures of the conformers as well as their CD signs of the origin bands.

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Electron Transport Characteristics of Nano-flake embedded Graphene Nanoribbons

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We have designed nanoelectronic devices having characteristic electron transport behaviors based on the graphene nanoribbons (GNRs) and their derivatives. We have performed a systematic analysis of electron transport characteristics for GNR and nano-flake embedded graphene nanoribbons (NF-GNR) considering the chirality of GNR and the symmetry of the edge structure of zigzag GNRs. In these works, we found that the electron transport characteristics strongly depend on the edge structure of zigzag GNR with semiconducting, metallic and varistor behaviors, and the embedded nano-flake induces a negative differential resistance (NDR), which is a characteristic feature of the Esaki-like diode. We believe that our results will give an insight in to the design and implementation of various electronic logic functions based on GNRs for applications in the field of nanodevices.

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Tautomerism of Adenine Complexes with Alkali Metal Cations

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We obtained ultraviolet (UV) photodissociation (PD) and UV-UV hole burning (HB) spectra of adenine complexed with a potassium cation produced by electrospray ionization (ESI) using quadrupole ion trap reflectron time-of-flight (QIT-reTOF) mass spectrometry. The UV PD spectrum exhibits well-resolved vibronic peaks, which coincide well with those in the UV-UV HB spectrum, indicating the presence of a single isomer in the QIT at ~10K. Although the most stable tautomer of adenine is 9H-adenine (9HA), we found that the most stable adenine complexes with alkali metal cations (M^+A, M=Na and K) in water was M^+7H-adenine (M^+7HA) by theoretical calculation and experimental results on 9-methyladenine and 7-methyladenine complexes with K^+. On the basis of density functional theory calculation on K^+9HA clusters with three water molecules, we suggest that the binding of K^+ ion to 9HA accelerates its tautomerization to 7HA in water by lowering the reaction barrier.

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Enzyme Catalyzed CO_2 Conversion: QM/MM Simulation Studies

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The conversion of carbon dioxide into more valuable materials is an important issue in both global warming and green chemistry. Conventionally, organometallic catalysts or electrochemical methods have been used for this conversion. Despite their high catalytic efficiency, these methods are expensive, require harsh reaction conditions, and have less control over the final products. On the other hand, the enzyme catalyzed carbon dioxide conversion can be processed under the mild condition and has specific final products. Especially, the NAD-dependent formate dehydrogenase from *Thiobacillus* sp. (TsFDH), which originally catalyzes the conversion of formate into CO_2, has been reported to have the best performance on the reverse reaction (or the conversion of into formate) among the same family. Hence, we investigated several FDH enzymes including wild type and mutated TsFDH with semi-empirical (SCC-DFTB) and ab initio QM/MM simulations to understand the catalytic mechanism of the conversion reaction and to improve its catalytic efficiency in CO_2 conversion.

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Rebinding dynamics of CO with Cytoglobin in aqueous solution using ultrafast vibrational spectroscopy

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Recently, Cytoglobin, a heme-containing protein, was found in vertebrates. It is found in a wide range of mammalian tissues and is also available to bind with external ligands. Unlike myoglobin Fe in heme plane of Cgb is six coordinated with distal and proximal histidine. In this study, We measured the rebinding dynamics of the CO complex of Cytoglobin in aqueous solution using femtosecond and nanosecond vibrational spectroscopy.The stretching mode of CO bound to the protein shows three stretching bands at 1924 $cm^{-1}(A_0)$, 1899 $cm^{-1}(A_1)$ and 1884 $cm^{-1}(A_3)$. Ligand binding to Cgb is a multiphasic process with fast geminate rebinding taking place on the nanosecond timescales and slower bimolecular rebinding occurring on microsecond timescales. The geminate rebinding of CO to Cgb is about 40%, more efficient than that of myoglobin(4%), ligand binding protein has primary heme pocket. The fast geminate rebinding of CO to Cgb was from the distal histidine imidazole oriented out of the heme pocket in a similar way as observed for the distal histidine in Mb at low pH, open conformations(A_0). It suggests that according to conformations of protein affects rebinding kinetics of photolized CO.

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Simulated NMR order parameters in proteins with knowledge-based potentials

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It is rather paradoxical that a protein interacts with high selectivity in spite of its floppy side-chains. As a result, protein side-chain dynamics is worth studying to understand protein-protein and protein-chemical interactions along with protein functions. In this study, we proposed a computational method to predict accurate order parameters in a protein: a simulated annealing (SA) protocol using target energy function based on knowledge-based Statistical Torsion Angle Potential (STAP). The side-chain motions of methyl carbons were mainly investigated, and their order parameters (S^2) and correlation coefficients were evaluated and compared with experimental values. We predicted χ_1 and χ_2 order parameters for two target proteins, α_3D and protein L. While α_3D has many buried side-chains, protein L has many exposed side-chains. Although these proteins have contrary characters, the proposed method produces good correlation coefficients with experimental data: 0.39 (α_3D) and 0.7 (protein L). The computational method based on knowledge-based potentials can be used to characterize the χ_1 and χ_2 conformation of side-chain residues and to understand side-chain motions.

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Protein structure refinement of CASP target through structure selection

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The protein structure is closely related its functions. For detailed structural studies, the high resolution structure is required. In general, molecular dynamics (MD) simulation is useful for the refinement of low-quality protein structure in many studies. In this study, we performed CASP10 targets refinement using the MD simulation on time scales of 10ns with implicit solvent model (EEF1). The knowledge-based potential (STAP) and distance restraints were also used refinement simulation. All of the simulation were executed using CHARMM. After simulation, best structure which has best performance is selected by using several criteria. The selection of best refined structures without knowledge of the native structure is still remained challenge. We selects the best structure with “protein-like scores”. There are two kind of important factors, the one is factor associated with protein packing quality (nDOPE, dDFIRE and WHAT CHECK packing score) and the other is clash score. The TM-score of best value was increased by 1.5%, from 0.785 to 0.800. Using the clash score, the TM-score of best performance structure was increased by 0.5%.

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Quantitative dissection of RNA polymerase-controlled gene expression variability

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Transcriptional initiation, at the end of which RNA polymerase (RNAP) is ready to synthesize a mRNA molecule, is an important regulatory step for downstream gene expression. The question of how noise in intracellular RNAP level is propagated into the downstream gene network has attracted experimental and theoretical interests. Here, we present how to quantitatively understand the effect of RNAP-promoter interaction fluctuation on the gene expression statistics. By making use of the fact that various moments characterizing the downstream gene expression statistics are essentially a function of the mean and noise of RNAP level, as was recently found for synthetic *E. coli* with T7 RNAP transcritpion machinery, we introduce the non-perturbative method to efficiently take into account the effect of the higher-order moments of RNAP-promoter interaction fluctuation. The resulting analytic expressions provide a quantitative explanation of the mean and noise of protein level. Furthermore, we could explain that the susceptibility of the protein noise to the RNAP noise decreases with RNAP level while the normalized correlation between RNAP and protein levels increases.

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A Theoretical Study for the Binding Energies of Ni, Pd and Pt-decorated Fullerenes

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The chemical reactivity of 2-D carbon materials depends on their curved surface properties. For example, the inherently curved surface of a CNT has different chemical reactivity from the planar sheets of graphene layers. It has been shown that the hydrogenation energies of various CNTs depend on the curved surface structure, which were described by pyramidalization angle. In this study, we focused on the binding energy of metals depending on the surface structure of fullerenes. The binding energies of Ni, Pd and Pt on fullerenes with various surface structures, C_n (n=20, 26, 30, 36, 60, 70, 84), were calculated using the DFT methods. This study showed that the binding energies increased with the pyramidalization angle of fullerene surface. The overlap of metal d-orbitals and fullerene p-orbitals also depends very much on the surface structure.

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Ruthenium 을 도입한 Titanium Oxide의 합성과 산화제 사용 여부에 따른 유기 산화반응 연구

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Titanium 과 Ruthenium 의 합성 시 몰 비율(Ru/Ti=0.01, 0.03, 0.05, 0.07)을 조절하여 Ruthenium 이 도입된 Titanium Oxide(Rux/TiO_2)를 수열합성법을 이용하여 합성하였다. TEM 이미지를 통하여 합성된 샘플이 나노 크기임을 확인하였으며 ICP 원소 분석을 통하여 Titanium 과 Ruthenium 의 조성비을 확인하였다. XRD 실험을 통하여, Ruthenium 이 도입된 Titanium Oxide 은 모두 Anatase 구조만이 관찰되었지만, 700 °C 이상의 열을 가하였을 경우, Titanium Oxide 와 Ruthenium Oxide(RuO_2)의 상분리가 일어나는 것을 확인하였다. 본 연구에서는 Ruthenium 이 도입된 Titanium Oxide 을 이종상촉매로 사용하여 산화제로서 산소분자의 사용 여부에 따른 Benzyl alcohol 및 Benzyl amine 의 산화반응에 적용하였다. Benzyl alcohol 의 산화반응을 수행하였을 경우, 산화제를 사용하여 여부와 관계없이 Benzaldehyde 가 주로 생성되었지만 Benzyl amine 에 대한 산화반응의 경우 Benzaldehyde, Benzonitrile, N-benzylidenebenzylamine 의 3 가지 물질이 생성되었다. 뿐만 아니라 Benzyl amine 의 산화반응에서 산화제를 사용하였을 경우, 주생성물로서 benzonitrile 이 생성되었지만, 산화제를 사용하지 않았을 경우, Oxidative Self Coupling 반응을 통하여 N-benzylidenebenzylamine 이 주로 생성되었다.

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Hydrophobicity of Amino Acids in Protein Context

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숙명여자대학교 화학과

Hydrophobicity is a major driving force in protein folding, protein self-assembly and protein-ligand interaction. Moreover, hydrophobicity is the key point to understand the role of water in protein interaction. Commonly, protein hydrophobicity is evaluated as a sum of hydrophobicity scales for component amino acids, and it is based upon the premise that the hydrophobicity scales determined for individual free amino acids have not changed when amino acids are embedded in a protein. Here, we investigate how the hydrophobicity of amino acids depends on the protein context by computing the solvation free energy (SFE) of a protein and by decomposing it into contributions from constituent amino acids. We find that the negatively charged residues show decreased SFE and the positive ones show increased SFE when the protein total charge is negative, whereas this trend is reversed when the protein total charge is positive.

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니켈과 질소를 도핑 함으로써 염료흡착성을 가지는 TiO_2 합성 및 특성연구

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TiO_2 에 니켈과 질소가 도입된 촉매를 합성하여 특성과 광촉매 활성을 연구하였다. XRD 관찰 결과 니켈과 질소가 도입된 TiO_2 는 anatase 와 rutile 그리고 brookite 가 동시에 나타났으며 HRTEM 으로 원소분석 결과 모든 원소가 골고루 분포 되어있었다. 상용 TiO_2 인 Degussa 는 methylene blue 분자에 대하여 흡착능력을 거의 나타내지 않았으나, 니켈과 질소의 양이 최적화된 촉매에서는 최대 흡착량이 13.01mg/g 에 달하였다. Zeta potential 측정 결과 최대 ?25.46mV 의 음전하를 나타내었으며, 각각의 촉매흡착성은 이와 비례하는 것으로 나타났다. 특히 니켈이 도입된 TiO_2 는 흡착능력뿐만 아니라 가시광선을 이용한 MB 분해 실험에서 우수한 광촉매 특성을 나타내었다. 뿐만 아니라 환경오염물질인 Bisphenol A 와 Tetrachloroehthylene 의 광분해 실험에서도 촉매활성을 나타내었다.

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수산화인회석에 Ru를 도입한 이종상 촉매의 합성및 특성 평가

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산화인회석(Hydroxyapatite)는 뼈와 이빨의 무기물의 주성분으로서 칼슘과 인산염으로 구성된다. 본 실험에서는 다양한 농도의 염기조건 (NaOH 0,2,4,5,10,15,20M)하에서 서로 다른 형태의 수산화인회석을 수열합성법(hydrothermal method)을 이용해 합성하였다. 합성된 각각의 수산화인회석을 XRD 로 확인하였고 일정농도 이하에서는 dicalcium phosphate 이 함께 존재한다는 것을 확인 할수 있었다. 수산화인회석 표면에 Ru 를 Ion-exchange 반응을 통하여 도입하였으며, 도입된 표면을 TEM 을 확인하였다. Ru 를 도입한 수산화인회석을 일차알콜과 이차알콜, benzyl amine 을 산화반응에 응용하였다. 이 실험을 통해 NaOH 2,4,5M 이 도입되어진 수산화인회석이 다른 농도의 NaOH 수산화인회석보다 반응성이 뛰어나다는 것을 확인할 수 있었다.

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The effect of *ortho* groups in the solvolyses of benzyl dervatives using the extended Grunwald-Winstein equation

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A kinetic study was carried out on the solvolysis of *ortho* and *para* benzyl dervatives in a wide range of solvents. The *l/m* values of the extended Grunwald-Winstein equation for solvolysis of *ortho* and *para* benzyl dervatives in solvents without fluoroalcohol content are all significantly larger than unity while those in all the fluoroalcohol solvents are less than unity. The role of the *ortho*-groups as an internal nucleophile (intramolecular nucleophilic assistance) in promoting solvolytic reaction of benzyl halides has also been evaluated. These observations were compared with those previously reported for the corresponding carboxybenzyl bromides.

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Contrasted fluctuations in product number:Non-renewal versus renewal birth process

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The conventional reaction kinetics with rate constants no longer can provide an exact description of product number statistics when reaction times are distributed in a non-Poissonian manner. Depending on if individual reaction times are correlated with each other, non-Poisson statistics of reaction times can be classified as non-renewal and renewal processes. The former can be generated by considering a general situation where reaction rates are coupled to environmental fluctuation. In this case, we study how the product number fluctuation is influenced by stochastic properties of the environmental process and product decay rate. Based on a generalized master equation where creation rate is not a constant but a stochastic variable, a series of moments characterizing the counting statistics of product molecules can be exactly calculated. Our analyses show that the non-Poisson indicator,Δ(t) defined by the difference between variance and mean of product number at time t undergoes a kinetic phase transition from fully heterogeneous phase to pure renewal-like phase. It is shown that depending on product decay rate, variation in the relaxation rate of associated environmental variable can greatly amplify or depress the product number fluctuation quantified by the maximum Mandel’s Q parameter over time, Q(t*) in comparison with the randomness, R of reaction time interval distribution. The renewal counterpart defined by the distributions of first reaction time and time interval between two consecutive reaction events, which are obtained from the non-renewal case, shows a similar qualitative behavior in terms of Δ(t) but the magnitude of Q(t*) cannot be greater than that of R, which is distinctly contrasted to the non-renewal case.

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Adsorption of DPCl and CPCl on negatively charged solid surfaces under geometric confinement: A comparison of SBA-15 and Ti-substitued SBA-15 studied by SANS

신태규

한국원자력 연구원 중성자과학연구부

The adsorption behaviour and organisation of the cationic surfactants dodecyl and hexadecyl pyridinium chlorides adsorbed in the cylindrical pores of a periodic mesoporous silica SBA-15 and Ti-substituted SBA-15 were studied by SANS. The combination of attractive solid-wall interaction and repulsive electrostatic interaction between the charged head groups leads to a characteristic adsorption behaviour for Si surface. For Ti-substituted SBA-15 a different adsorption behaviour is expected due to the influence of Ti-substitution on the electrostatic attraction and structural distortion of SBA-15.

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Facile Synthesis and Optical Properties of Carbon Nanodots

이경진 주태하*

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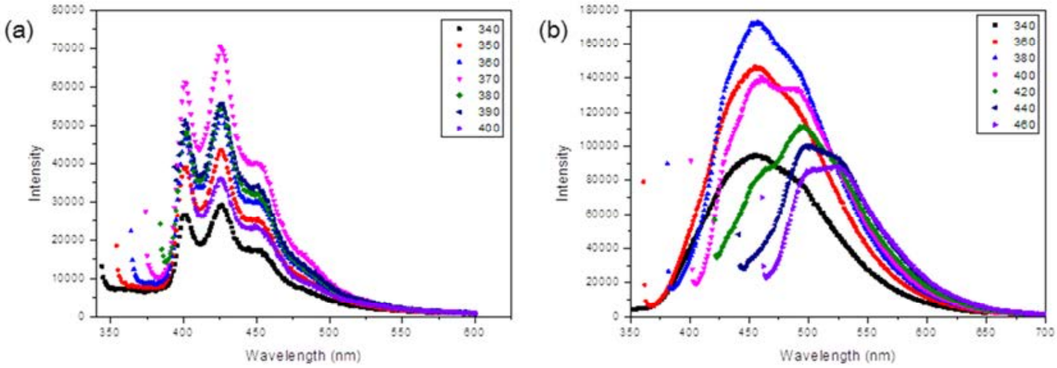
Photoluminescent carbon nanodots (CNDs) have received great interest because of their photostability, low toxicity, and excellent biocompatibility, compared with organic dyes and other semiconductor nanodots. CNDs can be used in a broad range of optoelectronic application fields, such as bioimaging, photocatalysis, sensing, light-emitting diodes, and energy conversion/storage devices. However the understanding of fluorescence origins of CNDs is still remaining unclear. Nevertheless, the involvement of surface states in the radiative transition of CNDs has been widely proposed to origin of fluorescence. Surface groups can introduce trapping states with different energy levels, making CND’s photoluminescence(PL) varies with excitation wavelength. The excitation-dependent emission was frequently observed, whereas excitation-independent emission was seldom observed in CNDs.If all surface states are completely passivated, the emission will take place only through the radiative transition of sp2 carbon, so that CND’s PL will show excitation independence. The surface states of the CNDs could be engineered so that their photoluminescence was either excitation-dependent or distinctly independent. This was achieved by changing the density of amino-groups on the CND surface. We synthesized fluorescent CNDs via a “water-in-oil” emulsion as a self-assembled-soft template. The PL spectrum of CNDs synthesized with citric acid and oleylamine shows strong peaks between 400-600 nm. The emission peaks of CNDs-oleylamine are dependent of excitation wavelength. The PL spectrum of CNDs synthesized with citric acid and urea also shows PL peaks between 400-500 nm, but emission peaks are independent of excitation wavelength. There is a series of single peaks spaced by ~1450 cm-1 corresponding to the average of D band and G band. Further study is in progress including picosecond time-resolved fluorescence, femtosecond transient absoption spectroscopy which may allow more detailed structures and origin of fluorescence of CNDs.Fig. 1 PL emission peak positions are either independent (a) or dependent(b) of excitation wavelength for the urea and oleylamine for capping molecule, respectively.



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Discovering the Mechanisms of Carbon Dioxide Binding to Hydrazine

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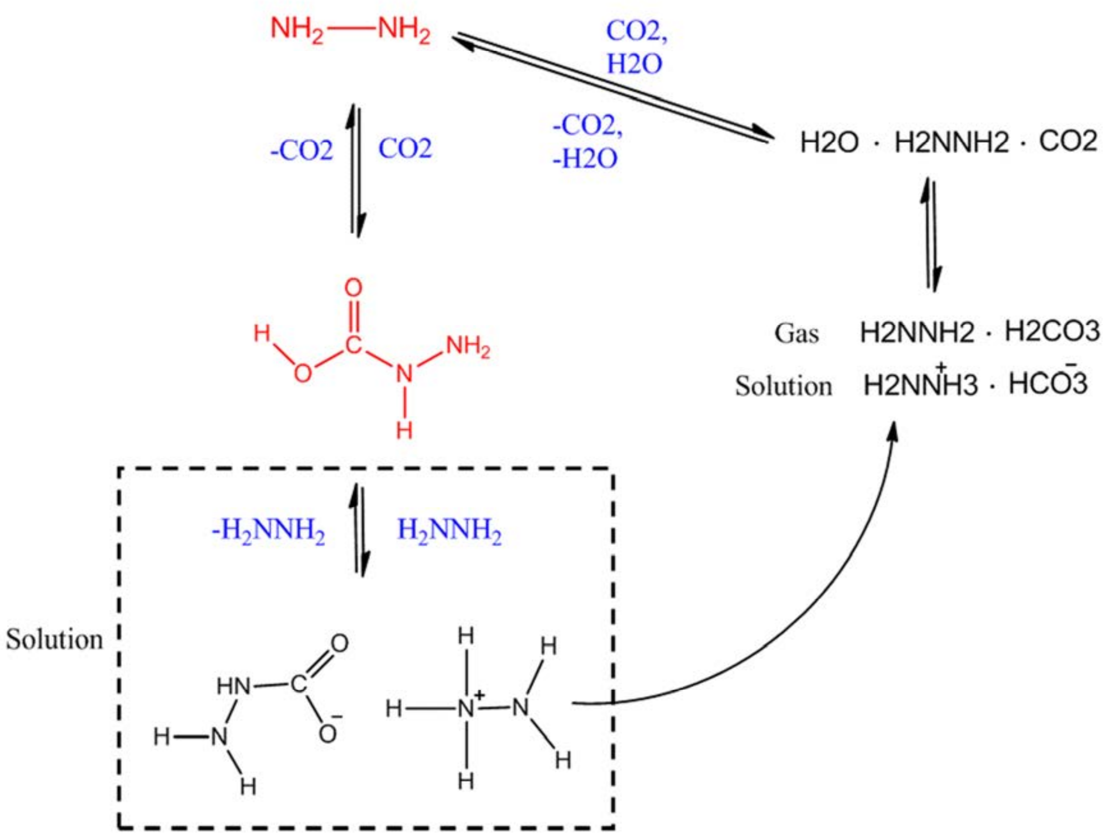
To reduce the concentration of CO_2 in the air, which is considered as a main cause of greenhouse effect and global warming, industrial science has applied various methods of cutting the CO_2 emission to their systems and also has searched for other new ways recently. There has been an experimental study where the reaction between CO_2 and Hydrazine results in solids, but the mechanisms were still unknown. In this study, we discovered several mechanisms which take place differently in gas phase or in solution and found that water molecules have a very important role to the mechanisms. Related calculations were performed to know how the energies in water catalysis and specific solvent effect change along the reaction coordinates.We are going to present you what we achieved as conclusions from all of those data including the mechanism which is the most possible way in the binding reaction between Hydrazine and CO_2.


NH_2—NH_2
CO2,
H2O
-CO2,
-H2O
H2O · H2NNH2 · CO2
-CO2
CO2
Gas H2NNH2 · H2CO3
Solution H2NNH3 · HCO3
-H_2NNH_2
H_2NNH_2
Solution

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High-Yield Preparation of Heterodimers with Tunable Interparticle Distances and Probing Quantum Plasmon Coupling

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금나노입자와 은나노입자로 이루어진 이종 이합체(heterodimer)에서 발생하는 플라즈몬 커플링 현상을 입자간 거리에 따라 측정하고 최근 본 연구실에서 발표한 금-금 이합체(Cha, H.; Yoon, J. H.; Yoon, S. *ACS Nano* 2014, *8*, 8554)와 비교 분석하였다. 이합체는 조립체 중 가장 단순한 구조로 입자간 거리에 따라 달라지는 플라즈몬 커플링을 연구하기 좋은 모델이다. 그러나 이합체를 높은 수율로 만드는 것이 어려울 뿐만 아니라 입자간 간격이 1 nm 이하가 될 경우 고전 전자기학 모델에 맞지 않아 많은 연구를 필요로 한다. 우리는 입자간 거리를 유기 분자의 사슬 길이로 조절하여 다양한 입자간 거리를 갖는 이합체를 높은 수율로 만들었으며 구성하는 나노입자의 종류를 금과 은으로 달리하여 이종 이합체를 조립하였다. 또한 입자간 거리에 따라 변화하는 플라즈몬 커플링을 확인 하였으며 입자간 거리가 1 nm 이하일 때 발생하는 양자 터널링 효과를 실험적으로 관찰하여 분석 하였다.

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Assembly of Gold Nanocube-Nanosphere Dimers and Their Plasmonic Properties

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비구형(nonspherical) 금 나노입자나 이를 이용해 만든 조립체는 구형 금 나노입자와 비교해 다중 표면 플라즈몬 공명 모드를 나타내며 가시 영역에서 근적외선 영역까지 그 범위를 폭넓게 조절할 수 있는 장점을 가진다. 또한 비구형 금 나노입자의 한 종류인 금 나노큐브는 빛이 입사될 때 12 곳의 모서리와 8 곳의 꼭짓점에서 발생하는 피뢰침 효과에 의해 비슷한 크기의 구형 금 나노입자보다 더 강한 표면 플라즈몬 공명 성질 및 전기장 증폭을 나타낸다. 우리는 이러한 금 나노큐브의 모서리나 꼭짓점에 선택적으로 구형 금 나노입자를 조립하여 평균 70% 수율의 이합체를 만들었으며 근적외선 영역인 785-790 nm 에서 조립 축 방향 플라즈몬 커플링 모드(longitudinal Plasmon coupling mode)를 관찰하였다. Finite difference time domain(FDTD) 계산을 통해 큐브-구형 나노입자 사이에 발생하는 강한 전기장을 시뮬레이션 하고 이를 바탕으로 라만 단면적이 작은 알킬사슬 분자의 표면증강 라만 산란(SERS)을 측정하였다. 끝으로 비슷한 크기의 구형 금 나노입자 이합체와의 비교를 통해 큐브-구형 나노입자 이합체의 우수한 플라즈몬 특성을 논하고 라만과 형광증폭체로서의 다양한 응용 가능성을 제시하고자 한다.

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Moving Nanoparticles with Photons: Light-Induced Changes in the Interparticle Distance of Au Nanoparticle Dimers

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Alkanedithiol 로 연결된 금나노입자 이합체(dimer)에 빛(UV-vis-IR)을 쬐어주면 입자간 거리가 맞닿을 때까지 점점 가까워지고 이에 따라 두 입자 사이에 발생하는 플라즈몬 커플링도 고전적인 전자기 영역에서 양자 영역으로 전환된다는 것을 발견하였다. 금속 나노입자 조립체를 이용한 플라즈몬 커플링 조절은 매우 중요한 일로 널리 연구되고 있다. 특히 높은 수득율로 조립체를 만드는 것과 입자 간격을 1 nm 이하로 정밀하게 조절하는 것은 매우 의미 있는 일이다. 최근 본 연구실에서는 서로 다른 사슬 길이의 유기분자를 이용해 입자간 거리를 조절한 나노입자 이합체 합성법을 개발하여 보고한 바 있다 (Cha, H.; Yoon, J. H.; Yoon, S. *ACS Nano* 2014, *8*, 8554). 이러한 나노입자 이합체의 경우 연결 분자를 바꿔줌으로써 입자간 거리를 일정한 간격으로만 조절할 수 있다. 본 연구에서 우리는 나노입자 이합체의 입자간 거리를 빛을 조사함으로써 연속적으로 변화시킬 수 있음을 제시하고자 한다. 입자간 거리 변화는 플라즈몬 커플링 밴드의 이동(shift)을 통해 관찰하였으며, 관찰 결과 입자간 거리가 점점 가까워져 전자 터널링에 의한 charge transfer plasmon(CTP) mode 가 형성되는 영역까지 그 간격이 좁아짐을 알 수 있었다. 빛에 의한 나노입자의 움직임은 연결분자들의 탈착(desorption)에 따른 분자층(self-assembled monolayer)의 구조변화에 기인한 것으로 보인다.

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Highly branched RuO2 Nanorods on Electrospun TiO2 Nanofibers toward Electrochemical Catalysts

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We report a facile growth route to synthesize hierarchically grown single crystalline metallic RuO2 nanorods on electrospun TiO2 nanofibers via a combination of a simple vapour phase transport process with an electrospinning process. This synthetic strategy could be very useful to design a variety of highly branched network architectures of the functional hetero-nanostructures for electrochemical applications. Particularly, Ruthenium oxide (RuO2) 1-dimensional nanostructures can be used as the effective catalysts or electrochemical electrode materials. Thus, we first synthesize TiO2 nanofibers from mixture of titanium isopropoxide precursor and polymer and then ruthenium hydroxide precursor on TiO2 nanofibers are transformed into RuO2 nanorods by thermal treatment at 250oC in air. The crystalline structures of products are confirmed using scanning electron microscopy (FE-SEM), X-ray diffraction (XRD) spectrum, Raman spectroscopy, and high resolution electron microscopy (HRTEM). The fundamental electrochemical performances are examined using cyclic voltammetry (CV).

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Different effects along the similar para-methoxy substituents in benzoyl chloride derivatives

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A lot of benzoyl chloride derivatives are studied using kinetic solvolysis methods by our research group. Specifically para-methoxy group and similar ones on benzoyl chloride were chosen to study the different effects of substituents. The case of 4-methoxybenzoyl chloride (1) is the basic substrate, another case of (4-methylthio)benzoyl chloride (2) is that the oxygen atom in methoxy group of 1 is switched with sulfur atom, and the last case of (4-trifluoromethylthio)benzoyl chloride (3) is that the three hydrogen atoms of 2 are switched with three fluorine atoms. Depends on these substituents, each substrate had shown different computing calculation and kinetic results, like solvolysis rates, the Grunwald-Winstein equation analysis, the kinetic solvent isotope effect (KSIE), and the activation parameters (enthalpies and entropies). We summarized and compared all these results about all three substrates.

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Pulsed laser ablation synthesis of hcp and fcc Ni nanoparticles in liquids

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We report a simple and controllable preparation of face centered cubic (fcc) and hexagonal close-packed (hcp) Ni nanoparticles by a pulsed Nd-YAG laser ablation method in various solvents, such as deionized water, methanol, hexane, and acetonitrile. We generate Ni/NiO and fcc/hcp Ni nanoparticles by a laser ablation to a Ni plate submerged in various solvents, followed by a post-ablation to the colloidal solutions. Interestingly, the phases of Ni nanoparticles prepared via PLAL show a strong dependence on the solvents used in the ablation process. Ni/NiO, pure fcc, and mixture of fcc and hcp Ni nanoparticles were generated in DI water, methanol, and hexane or acetonitrile, respectively. After the post-ablation, however, pure fcc Ni nanoparticles were generated in methanol and hexane; while pure hcp Ni was formed in acetonitrile. We think that the solvent dependence on the phase of Ni nanocrystals is related to the specific heat of solvents that plays an important role kinetically and thermodynamically in the process of cooling the plasma plume where the nanoparticles nucleate and coalesce to a specific phase. Formation of graphite layers on Ni nanoparticles fabricated in hexane and acetonitrile is also discussed. The Ni nanoparticles prepared from PLAL were analyzed by X-ray diffraction (XRD) measurements, X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HRTEM), and fast Fourier transform (FFT) analysis.

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Structure and Dynamics of DOPC and DSPC Mixture Membranes: Atomistic Molecular Dynamics Simulation Studies

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The non-thermal plasma technology is the emerging field of biomedical application such as cancer therapy. It has been shown recently by experiments that the treatment of DBD plasma on membrane disturbs the fine structure, alteration integrity, fluidity, and permeability of cell membranes. [1, 2] Especially, it is reported that 1,2-dioleoyl-sn- glycero-3-phosphocholine (DOPC) lipids are converted into 1,2-distearoyl-sn-glycero-3-phosphocholine (DSPC) lipids by the DBD plasma treatment. Hence, we investigated various physical properties such as order parameter, area per lipid, and lateral diffusion coefficients using the atomistic MD simulations of model DOPC:DSPC mixture membrane systems. We used 6 membrane models with different % of DSPCs: 0%, 20%, 40%, 60%, 80%, and 100% of DSPC lipid bilayer membranes. The potential of mean force (PMF) was also calculated between DOPC lipids or between DSPC lipids using umbrella sampling techniques to understand the clustering mechanism of lipid mixtures. [3]References[1] Panngom, M.; Baik, K. Y.; Nam, M. K.; Han, J. H.; Rhim, H.; Choi, E. H. Preferential killing of human lung cancer cell lines with mitochondrial dysfunction by nonthermal dielectric barrier discharge plasma. Cell Death and Disease 2013, 4, e642.[2] Greenberg, M. E.; Gugiu, B. G.; Gu, X.; Qin, J.; Salomon, R. G.; Hazen, S. L. The lipid Whisker model of the structure of oxidized cell membranes. J. Biol. Chem. 2008, 283, 2385-2396.[3] Torrie, G. M.; Valleau, J. P. Nonphysical sampling distributions in monte carlo free-energy estimation: umbrella sampling. J. Comput. Phys. 1977, 23, 187-199.

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Resistance of covalently linked organic dyes against photobleaching

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Relatively fast photobleaching of organic dyes compared with nanoparticles is a great disadvantage for their applications in bio-imaging. Earlier, we have reported unusual resistance of covalently linked Alexa647 and Cy3 heterodimers against photobleaching. Although the mechanism behind their photostability is not clear, we attempted to verify the generality of the phenomena by conducting the stability test to check photophysical characteristics using various combinations of a photoswitching dye and a conjugated dye.

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Origin of oscillatory feature in bacterial transcription rate fluctuation

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Recently, we revealed that transcription rate autocorrelation function can show an oscillatory behavior over time by quantitatively analyzing the steady-state statistics of mRNA copy number per cell in Escherichia coli. In terms of time-dependent standard deviation of mRNA copy number, which is closely related to the transcription rate autocorrelation, we found from stochastic simulation that such an oscillatory behavior can be produced when the respective distributions of times required to complete successful initiation and elongation have a highly sub-Poissonian character and the mean time of RNA polymerase (RNAP) binding to promoter is sufficiently small compared with the mean initiation time, leading to a well-separated sequential alignment of RNAPs on a single gene. In addition to the experimental evidences showing that the successful initiation time distribution can be narrow enough to generate such an oscillatory behavior in the standard deviation, we investigate if the transcriptional elongation time distribution is also really the case by using the stochastic simulation algorithm constructed with the results of single-RNAP tracking experiments. Transcriptional pausing, which is contrasted to active elongation phase, is a key ingredient to realize heterogeneity in transcriptional elongation time in silico. It is shown that the resulting transcriptional elongation time distribution is highly sub-Poissonian.

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CRASY:Correlated Rotational Alignment Spectroscopy of Acetylaceton Tautomers

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CRASY is a new type of spectroscopy which correlates high-resolution rotational spectra with femtosecond time-resolved mass or electron spectra. CRASY provides the information of molecular composition, photochemical dynamics, electronic structure, and nuclear structure in a single optical experiment. Therefore, we can identify each component in an impure sample. First, we will look at the mechanism of photochemical reactions in acetylaceton tautomers. CRASY is sufficiently sensitive to identify minority compounds, for instance the minor tautomer of acetylaceton. Photochemical reactions of different tautomers will give a deeper understanding of the atmospheric chemistry of acetylaceton.

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Photochemical reactions of Cytosine tautomers, investigated with CRASY

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There is a hypothesis that photostability of DNA and RNA bases was crucial for the evolution of life on the sunlit surface of earth. To investigate this hypothesis in our lab, we experiment with Cytosine. Cytosine has three different tautomeric structures, only one of which occurs in DNA or RNA. With correlated rotational alignment spectroscopy (CRASY), we will obtain high resolution rotational spectra for each tautomer and observe photochemical reactions proceed in real time. Thereby, we can obtain information about photochemical reactions for each Cytosine tautomer. We aim to assign the fragmentation products of photochemical reactions and the electronic structure of the electronic excited states involved in the reactions. This poster presents our experimental concept and the expected results of the first tautomer-resolved spectroscopic experiment.

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Ultrafast Internal Conversion Dynamics of Reduced Cytochrome *c*

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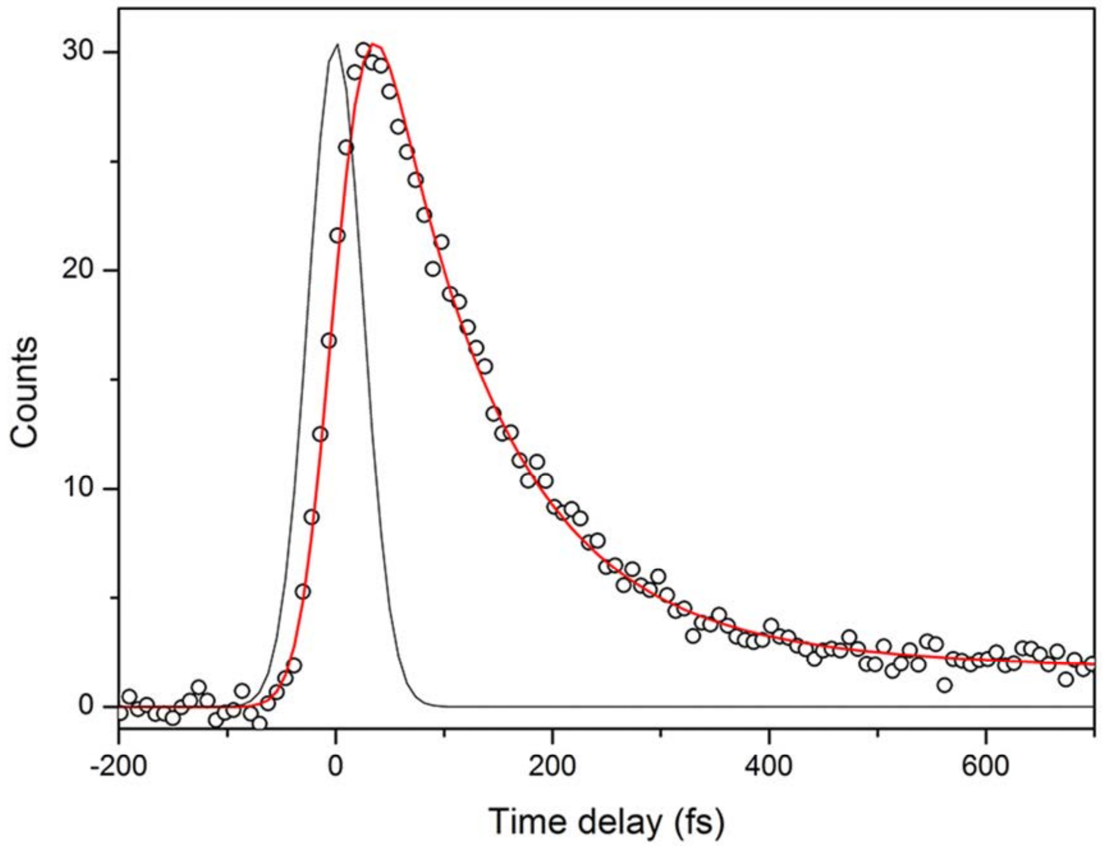
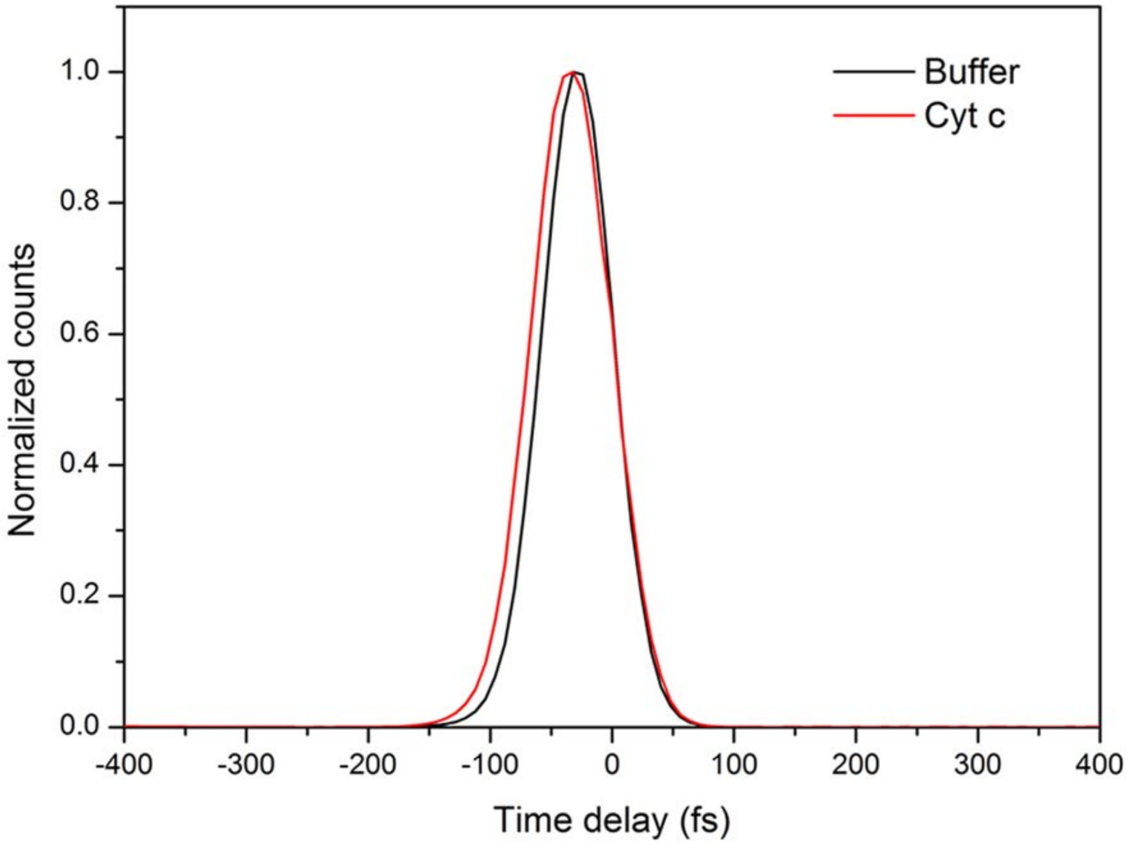
Cytochrome *c* (cyt *c*) is one of the most important heme proteins which function as reversible redox carriers in electron-transport chains. In the absorption spectrum of reduced cyt *c*, the strongest band is B (or Soret) band of porphyrin at 414 nm and two peaks in the visible region are Q(1,0) and Q(0,0) bands at 520 nm and 549 nm. We investigate ultrafast internal conversion dynamics (B→Q→ground) of reduced cyt *c* by highly time-resolved fluorescence after Soret excitation. Lifetime of Q state is determined to be 100 fs (figure 1(a)). Also, Soret band lifetime of reduced cyt *c* has been expected by comparing the experimental result (figure 1(b)) with numerical simulation of the third-order response functions.

(a) Time-resolved fluorescence at 600 nm (Q band)



(b) Time-resolved fluorescence at 445 nm (B band)

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Effects of urea on the fluorescence properties of organic dyes

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Organic fluorescent dyes constitute a class of useful compounds for many purposes. They are particularly useful in the studies of biological systems through fluorescence labeling. Since organic dyes often exhibit subtle differences in their properties as a result of their interaction with surrounding chemicals, elucidating the dye-medium interaction is important for better understanding of the target system as it may imply corresponding changes in the dynamics and kinetics of the molecule. We found that a significant degree of enhancement in fluorescence takes place when a DNA-protein sample was treated with urea. To unravel the underlying cause of this novel phenomenon, we investigated the fluorescence decay of several dyes in different solvents with urea and measured their lifetime distributions.

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Noble Organic-Inorganic Hybrid Thin Film Fabrication as Encapsulation using TMA and Adipoyl Chloride

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We fabricate organic-inorganic hybrid thin film for the purpose of encapsulation by molecular layer deposition(MLD) using Trimethylaluminium(TMA) and Adipoyl Chloride(AC). Molecular layer deposition (MLD) is a gas-phase process analogous to ALD and also relies on sequential saturated surface reactions In the MLD method, the high quality organic thin films can be quickly formed with monolayer precision under ALD conditions (temperature, pressure, etc). We found that desirable organic thin film fabrication is possible by MLD surface reaction in monolayer scale. Purging was carried out after dosing of each precursor to form monolayer in each sequence. Ellipsometry was employed to verify self-limiting reaction of MLD. Linear relationship between number of cycle and thickness was obtained. We deposit TMA and AC at 70 °C and that 1.78Å root mean square was obtained which indicates that uniform organic thin film was formed. We calculated WVTR of organic-inorganic hybrid super-lattice epitaxial layer using Ca test. WVTR indicates superlattice film can be possibly use as encapsulation in flexible devices.

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Prediction of crystal density and explosive performance of high energy density molecules using the modified MSEP scheme

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Fast screening to identify a promising high energy density molecule (HEDM) is of significant importance in developing high performance explosives and propellants. Our molecular surface electrostatic potential (MSEP) method applies well to various physicochemical properties of organic and energetic molecules. In order to apply our method in an efficient way, we utilize molecular structures optimized by semi-empirical methods to develop a fast screening approach that is applicable to a large number of HEDM candidates. As a benchmarking test, solid densities, heats of formation, and explosive performances of HEDMs are calculated using the ‘modified MSEP scheme’. In validating this new scheme, the absolute average errors in crystal densities based on our new scheme are a range of 0.041-0.055 g/cc, which serves fairly good input data in estimating accurate explosive performance. The fast screening procedure based on our modified MSEP scheme with the semi-empirical methods provides quite similar results to the original MSEP scheme in various aspects of explosive performance.

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Coherent Phonon Oscillations in Single-Chirality (6,5) SWNT

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Single-walled carbon nanotubes (SWNTs) are standards for ideal one-dimensional system in both scientific research and industrial applications. Optical properties of SWNTs, in particular, have been of a great interest as a non-invasive non-contacting approach since the discovery of suspended SWNTs [1]. With pump/probe transient absorption techinique (TA), the assignment of chirality of SWNTs was available by the frequencies of the radial breathing modes (RBM) excited by the E22 excitation [2]. Coherent phonon wavepackets are created by impulsive excitation and their motions can be recorded in a probe pulse in a pump/probe transient absorption (TA) experiment.

Here, we report the features of coherent phonon oscillations of (6,5) single chiral SWNTs at room temperature with TA experiments in the E11 and E22 optical regions. The E11 resonant excitation allows the direct observation of many vibrational modes. For the E11 excitation, RBM is excited by coherent superposition between the ground state and the first excited state. And it is remarkably different from for E22 excitation, which probes exclusively the ground state since the lifetime of the E22 state is rather short (~100 fs). It supports that the excitonic picture should be account for the E11 excitation.

1. Reigh, S; Thomsen, C.; Maulzsch, J. *Carbon Nanotubes :Basic Concepts and Physical Properties;* Wiley-VCH: Berlin, 2004
2. Lim, Y.S.; Yee, K. J.; Kim, J. H.; Haroz, E. H.; Shaver, J.; Kono, J.; Doorn, S. K.; Hauge, R. H.; Smalley, R. E. *Nano Lett.*2006, *6*, 2696

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Multifarious effort for optimization of expression, purification, and structural characterization of disease related human transmembrane proteins

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한국외국어대학교 화학과

Human transmembrane proteins (hTMPs) are closely related to transport, channel formation, signaling, cell to cell interaction, so they are the crucial target of modern medicinal drugs. In order to study the structure and function of these hTMPs, it is important to prepare reasonable amounts of proteins. However their preparation is seriously difficult and time-consuming due to insufficient yields and low solubility of hTMPs. We tried to produce large amounts of human amyloid-β (hA?? that is related to the dementia and human melanocortin-4 receptor (hMC4R) that is related to the severe early onset obesity. The hA? transmembrane protein shows membrane-bound oligomeric state, and the Ca2+-permeable ion channel formation of non-fibril in the cell membrane. It plays a central role in pathogenesis of dementia and Alzheimer disease. The hMC4R has a critical role in part of energy homeostasis like the food intake and energy consumption. Heterozygous mutation D90N located in second transmembrane domain of hMC4R relate in genetic cause of human obesity. In this research, we succeed to produce the trans-membrane domain of the hAβ and second trans-membrane domain both of the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). To assess the structural characterizations of these proteins in the membrane-like environments, we were obtained enough quantities of proteins by using a recombinant DNA technology and highly purified proteins were applied to a few biophysical analysis techniques like PAGE, CD, MS, solution and solid-state NMR spectroscopy. In addition, we could get 1H-15N 1D, 2D SAMMY and SMAPI spectra using home-built solid-state NMR probe.

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Quantum Computational Screening for Organic Dye Materials

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서울대학교 화학부

Organic dyes with the core of various metals (rhodium, paladium, platinum, copper and others) are used in applications such as organic light-emitting devices and dye-sensitized solar cells. In order to design and screen materials for such dyes, computational approaches can helpful by predicting electron/energy transfer rate or excited state energy levels. Practically, accurate prediction of the properties of metal-cored organic dyes takes lots of computational resources. In the present study, we investigated the performance of various computational methods in calculating physical quantities such as HOMO-LUMO energy gap used for predicting the functionalities of metal-cored organic dyes.

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[발표취소] Excited State Proton Transfer Dynamics of Coumarin 183

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고려대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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Expression, Purification and NMR Structural Studies of syndecan-4 as a cell surface receptor

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한국외국어대학교 화학과

Syndecans as cell surface receptors participate in biologically important cell-cell and cell-matrix interactions. They have a common basic structure including modified extracellular domains, conserved transmembrane and cytoplasmic domains. One of them, syndecan-4 may affect tissue development and repair as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4(Syd4) consists of 25 hydrophobic amino acids. It performs the formation of dimer or oligomer and is crucial for transduction of signals. Even though, a lot of efforts to elucidate the structure and function of them, it has been hindered by insufficient yields and low solubility. Thus, we demonstrated an optimized method for recombinant expression and purification of three kinds of Syd4 like wild type Syd4-TM(wt-Syd4), mutant Syd4-TM(mSyd4), and Syd4-eTC. The mSyd4 has a partially modified sequence of wt-Syd4 and the Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of syndecan-4. All peptides were released from the fusion protein, and then purified by semi-preparative reversed-phase HPLC. Enough amounts of purified Syd4 series for the analysis of peptides was obtained from 1L of M9 minimal media under optimal conditions. Their biophysical properties of peptides were studied by CD, MS and NMR spectroscopy. Analysis of CD spectra presents that all types of Syd4 series adopt a stable α-helical structure in micelle environments. The solution NMR studies show wSyd4 and Syd4-eTC form an asymmetric dimer in micelles and mSyd4 present monomer. Optimized 3D structure and absolute tilt angle on membrane bilayers of Syd4 based on 2D SAMPI4 solid-state NMR and Molecular Dynamics Simulation are underway.

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Synthesis and thermal properties of Silicon Nitride Precursors

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충남대학교 화학과

Reaction of the secondary amine NHR_2 (R = Me, Et), and symmetric and asymmetric β-diketiminate (nacnacR, R = *n*-Pr, i-Pr, *n*-Bu, i-Bu), with one equivalent of tetrachlorosilane yielded the silicon precursor $(nacnacR)_x Si\text{-}(NR2)_y$ ($x = 1 - 2$, $y = 2 - 3$).All complexes were characterized by NMR, TGA and DSC studies The phase of the synthesized Si Precursor was dependent on the number of equivalent of nacnacR ligand in the complex: on equivalent formed as powder state and two equivalent ligand formed as liquid state. The thermal properties of the precursors will be discussed in terms of the decomposition temperature.

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Theoretical Study for Geometric Structures and Characteristics of Hlothiophene derivatives

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Bithiophene, terthiophene, and their derivatives were optimized at the HF and MP2/6-311+G** levels using Gaussian 09 program.Optimized structure, geometric parameters, atomic charges, relative energies, tendency of HOMO and LUMO energies with increasing halosubstituent, and relative stability of isomers were investigated. Equilibrium structures of the halosubstituted bithiophene derivatives were optimized to anti- and syn-isomers. Anti-form was more stable. The stable structures of the halosubstituted terthiophene derivatives were optimized to (anti-,anti-), (syn-,anti-), and (syn-,syn-)isomer. (anti-,anti-)form was more stable than the others.With increasing halosubstituted group, dihedral angles of between two rings in the stable thiophene derivatives were approximately optimized to perpendicular. With increasing substituents, the HOMO energies of thiophene derivatives become to lower. HOMO-LUMO gaps of thiophene derivatives substituted with one to three halogen atoms were decreased, while the energies of thiophene derivatives substituted with four to six halogens were increased. The tendency of HOMO-LUMO gaps is similar to those of the UV-vis and PL spectra.

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IR Correlation Spectroscopy using Microgratings to detect target gases

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For the past couple of years, we have devoted to develop microgratings, each of which can provide a reference IR spectrum of a target gas in the correlation spectroscopy. Each micrograting pattern was designed using a gradient searching error minimization method and a Fraunhofer diffraction equation. It consists of 1441 reflecting lines of 13.323 μm width, whose depths were discretized into 16 levels between 0 and 6.9 μm. The microgratings for SF6, NH3 , and CH3OH were fabricated by a series of etching process using four masks on a silicon wafer in 19.2×19.2 mm2 size. When monitored at 15o angle, each micrograting generated the IR spectrum in good agreement with the reference one. To apply it for the correlation spectroscopy, a 10 cm long gas cell containing a target gas is placed in the middle of the optical path in our micrograing test setup and a broad band IR is introduced. The detected signal changes as the detection angle off the micrograting varies. Particularly at 15o, the signal shows a dip, whose intensity is proportional to the target gas concentration. This is the correlation signal. We have compared the performances, such as signal to noise ratio, of the correlation IR spectroscopy to conventional dispersive transmission IR spectroscopy.

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pH 조절을 통한 다양한 형태를 지닌 수산화인회석의 합성과 물성 연구

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본 실험에서는 다양한 농도의 염기 조건 (NaOH 10^{-3}, 10^{-2}, 10^{-1}, 1, 10, 30 M)에서 서로 다른 형태의 수산화인회석을 수열합성법을 통하여 합성하였다. X-Ray powder Diffraction(XRD), Transmission Electron Microscopy(TEM)을 통하여 합성된 물질의 물성을 평가하였다. XRD 관찰 결과 NaOH 농도 10^{-1} M 이상에서부터 수산화인회석이 합성됨을 확인하였다. TEM 을 이용하여 HAP 의 모양과 표면을 관찰해본 결과 NaOH 의 농도가 진해질수록 육각기둥 형태에서 사각형으로 변화하였다.

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First-principles calculation of charge transfer rate of push-pull copolymer

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Low-band-gap copolymers having both electron-rich and electron-deficient units, so-called push-pull-type copolymers, are promising donor materials for bulk heterojunction organic photovoltaic cells. Two push-pull copolymers 1-2, in which a common pushing group, cyclopentadithiophene (CPDT), is connected to a different pulling group, either benzothiadiazole (BT) or thienopyrroledione (TPD), are compared. Their structure, electronic structure and optical properties are calculated with density functional theory (DFT) and time-dependent DFT (TDDFT) methods. Both 1 (CPDTBT) and 2 (CPDTTPD) show a highly planar backbone structure. The absorption spectra predicted from the calculated HOMO and LUMO energy levels match very well the experimental UV/visible spectra of both polymers. From those HOMO and LUMO energy levels, almost the same power conversion efficiencies (PCE) are predicted for both polymers, but in fact a higher PCE has been observed for 2 than for 1 especially after a morphology control. It appears that a better-controlled morphology of 2, which is not considered in electronic structure calculations, improves the charge transfer and in turn the PCE. Therefore, in this work, we compare the charge transfer properties of the copolymers 1-2 by (1) building a set of π-π stacked pairs of their monomer and dimer units, (2) performing DFT calculations on those pairs to obtain their intermolecular interactions, reorganization energies and the transfer integrals, and finally (3) estimating their charge transfer rates and mobilities. Indeed, the copolymer 2 exhibit a higher hole mobility than the copolymer 1.

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Development of a miniature fourier transform IR spectrometer based on Lamella grating

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The interferometers which conventional fourier transform IR spectrometers adopt occupy a large space and may be prone to misalignment under external shocks, which are undesirable as a miniature spectrometer to be used for on-site spectrum acquisition and analysis. There have been interests and efforts in replacing the bulky interferometer by an optical component fabricated by MEMS techniques. In this respect, Lamella grating may be a good candidate. The Lamellar grating consists of a pair of transmission gratings, in which one pair is translated while the other is fixed. The relative distance of the two gratings produce the phase difference of the reflected lights off the two; the interferogram is recorded as the distance is varied. One limitation of the fourier transform spectrometer in this new optical arrangement, as a tradeoff for miniaturization, is in the spectral resolution. The maximum distance between the two gratings is limited, as an AC voltage must be used to drive one grating translation. The other resolution limit arises since the light field transmitted from the front grating forms an undesirable field image (e.g. Talbot image) before the rear grating. Such undesirable field image may distort the spectrum and limit the spectral resolution. In a preliminary work, we calculated the light field using 1-dimensional scalar diffraction theories such as Rayleigh-Sommerfeld approximation or Fresnel diffraction. We will discuss the spectral resolution of the Lamellar grating fourier transform IR spectrometer based on the field calculation. We will also show the current stage of the developing the miniature fourier transform spectrometer based on the Lamella grating.

References[1] Ferhanoglu, O.; Seren, H. R..; Lutterjohann, S.; Urey, H. Lamellar grating optimization for miniaturized fourier transform spectrometers Opt. Express. 2009, 17, 21289-21301.

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

Dynamics of Water in Aqueous $NaPF_6$ SolutionAt Different Temperatures

남다영 이치호 박성남*

고려대학교 화학과

Direct measurements of the dynamics of water in ionic hydration shells apart from those of bulk water have been experimentally quite challenging because of the poor spectral distinction among water molecules in bulk and ionic hydration shells. Here, the dynamics of water in aqueous $NaPF_6$ solution were studied at different temperatures by FTIR and IR pump-probe spectroscopy. The OD stretch band in the FTIR spectra of aqueous $NaPF_6$ solution was able to be separated into the contributions from three distinct subsets of water: (1) water molecules in bulk (OD_W), (2) water molecules in the hydration shells of Na^+ ions(OD_C), and water molecules hydrogen-bonded to PF_6^- ions (OD_A). Temperature-dependent FTIR experimental results indicate that the water structure around ions is more rigid and less changed than in bulk water with increasing temperature. Polarization-controlled IR pump-probe experiments were used to study vibrational population relaxation, P(t), and orientational anisotropy decay, r(t), of water in different subsets. The vibrational lifetimes of OD_W, OD_C, and OD_A in aqueous 5.0 M $NaPF_6$ solution were directly determined and found to be independent of temperature up to 50 ℃. In contrast, orientational relaxation dynamics of water became faster when the temperature was increased in aqueous $NaPF_6$ solution and the activation energies for water orientation were determined from the temperature-dependent orientational relaxation time. In our present experiments, the individual dynamics of water in bulk and ionic hydration shells in aqueous $NaPF_6$ solutions were able to be studied in more detail.

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Dynamics of photoexcited $Co(CO)_3(NO)$ by 266 nm probed by femtosecond IR spectroscopy

이태곤 권다예 임만호*

부산대학교 화학과

Nitrosyl metal complex is important in surface chemistry, biochemical systems and environmental chemistry. Its structures and excited states have been studied with laser-ablation and photolysis. Nitrosyl metal forms N-bound nitrosyl, isonitrosyl (ON), and side-on nitrosyl (η^2-NO). Recently, it is known that M-N-O structure is bent when metal complex is photo-excited with 400 nm. Photochemical processes were also known in gas phase. In gas phase, nanosecond time-resolved spectroscopy was studied to understand NO-release process. We used femtosecond UV pump - mid-IR probe spectroscopy to observe the early processes of photoexcited $Co(CO)_3(NO)$ in n-hexane. We mainly observed C?O vibration regions, from 1720 cm^{-1} to 2150 cm^{-1}. Based on the vibrational frequency of carbonyl or nitrosyl complex in gas phase and observed kinetics, we assigned new peaks and drew photochemical and photophysical processes up to 1 ns. Detailed dynamics of photoexcited $Co(CO)_3(NO)$ in solution by 266 nm was unveiled.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Optimized Parameters for Functionalization of Silver Nanorod Array Substrates in Surface Enhanced Raman Spectroscopy (SERS)

De Ranjit 이창렬 신용석[1] 오명규[*]

광주과학기술원(GIST) 고등광기술연구소 [1]광주과학기술원(GIST) 고등광기술연구소 바이오광학

Oblique-angle-deposited Ag nanorod (AgNR) array which is uniform, reproducible, containing large SERS-active area, and capable of high Raman signal enhancement has been successfully fabricated as SERS substrate. Bare surfaces of metal and metal oxides have the tendency to adsorb adventitious organic materials readily altering the interfacial properties; it can also play significant influence on the stability of metal nanostructures. Taking these advantages into consideration, the AgNR nanosubstrate was functionalized by organic thiols as the sulfur can form strong bond with silver. To form defect minimized self-assembled monolayers (SAMs) on the AgNR array surface, the condition parameters such as choice of solvent, concentration of thiol, incubation time, temperature, reaction in presence of inert gas, surface stability and uniformity, etc. were optimized. The characterization of nanorods before and after functionalization was done by field emission-scanning electron microscopy (FE-SEM) and found that the functionalization does not alter the morphology of the AgNR array. SERS spectra were also acquired. The functionalized AgNR nanosubstrate has shown to be an excellent SERS substrate with an enhancement factor of ~ 108. Electromagnetic as well as chemical effect contributes to the total enhancement factor. The contribution of chemical effect to the total enhancement factor has been studied using spacer layer in between AgNR surface and SAM. Advantages of SAM are discussed in the light of wettability, corrosion resistance, and molecule detection.

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

Chemically enhanced Raman scattering of rhodamine 6 G molecule adhere to graphene, MoS2 and WSe2: efficiency dependence on pressure and carrier density

김현민

대구경북과학기술원(DGIST) 나노바이오연구부

Recently, graphene enhanced Raman scattering (GERS) is very popular as a method to extract chemical information from dye molecules due to its excellent quenching effect on otherwise superfluous fluorescent backgrounds. Here, we aintroduce a new method to enhance Raman signals of a graphene-rhodamine 6G (R6G)-graphene sandwich structure by creating a magnet-induced static pressure to maximize the chemical contact of the R6G molecules with graphene. The increase in pressure in the graphene-R6G-graphene sandwich geometry plays a crucial role in enhancing the Raman signal by approximately up to 30 times in comparison to that acquired from a R6G/graphene layered film.The enhancement effect diminished with an increase in the number of graphene layers (on the bottom side), clearly discernible upon imaging the graphene/glass sandwiched structures placed on top of exfoliated multilayered graphene coated with R6G. We also studied the surface enhanced Raman scattering of R6G using 2-dimensional hexagonal honeycomb layers such as MoS2, WSe2 systems to compare with graphene. The fluorescence quenching factor of R6G molecules coated on MoS2 and WSe2 systems was measured by approximately 100 times higher than that of solution-state R6G molecules. We also investigated the thickness dependence of MoS2 and WSe2 layers on the enhanced Raman signals of adsorbed R6G, showing that the enhancement effect of MoS2 systems was maximized in the single layered nanosheets, demonstrating almost a linear-scale tailoring of Raman signals with the increase of the numbers of layers, while that of WSe2 still remained substantial until the double layered nanosheets followed by a drastic decrease above them.

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

Triple Layer Detection Using Spetially Offeset Raman Spectroscopy

이희수 송시원[1] 김형민[1,*] 박찬량[2,*]

국민대학교 자연과학대학 생명나노화학과 [1]국민대학교 생명나노화학과 [2]국민대학교 화학과

We develop a simple methodology for the effective investigation of Raman spectra of triple layers. Collecting scattered light from surface that are diffused from the laser spot on the sample is the basic technique of this experiment. In this technique, the Raman signals of each component of triple layers are obtained, and all spectrums provide specific characteristics of the components. Using 1mm glucose is the surface of the layer, and polyethylene and trans-stilbene are composed the experimental triple layer in serial order. The applications are suggested that biomedical detection underneath skin tissue, also industrial investigation of mixing process in large scale.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **PHYS.P-483**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Spectroscopic Studies on Upconversion Process of Upconversion Phosphors

조영호 배보람 황진건 박찬량[1,*] 김형민[*]

국민대학교 생명나노화학과 [1]국민대학교 화학과

We demonstrate upconversion mechanism of upconversion phosphors (UCPs), which $NAYF_4$: Er, Yb, through spectrally-resolved and temporally-resolved spectroscopy. To suggest the upconversion process, we conduct power dependence and wavelength dependence experiment. Furthermore one-photon spectroscopy is given more information about upconversion mechanism. As a result, we indicated that blue, green and red upconversion process of UCPs. Especially red upconversion process, which has many debates, is focused.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of multicolor upconversion thin film that prepared controlling humidity and temperature

김범진 조영호 임수영 김형민[*] 박찬량[1,*]

국민대학교 생명나노화학과 [1]국민대학교 화학과

Upconversion of $NaYF_4$:Er,Yb converts infrared region light to visible region. Because the upconversion process needs the IR, it has not any harmful effect on human body. We made a upconversion thin film with pulsed laser deposition that are used as an identification chip and it applied underneath the human tissue. Also, a simple patterning and making various color tuning through annealing give each chip a specific identification. Non-contact temperature measurement is possible by using the temperature depended change of green to red signal ratio.

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H-atom release dynamics from the gas-phase radical-radical reaction of $O(^3P)$ + C_2H_3

김장운 최종호*

고려대학교 화학과

The gas-phase radical-radical reaction dynamics of ground state atomic oxygen [$O(^3P)$ from the photolysis of NO_2] with vinyl radicals [C_2H_3 from supersonic flash pyrolysis of C_2H_3I] was studied by applying a combination of vacuum-ultraviolet laser-induced fluorescence (VUV-LIF) spectroscopy in a crossed beam configuration, together with *ab initio* calculations and statistical calculations.The average translational energy of the products and the average fraction of the total available energy were respectively revealed to be 7.03 ± 0.30 kcal mol^{-1} and 7.2 % using the nascent hydrogen atom Doppler-profile analysis under the kinetic energy release of the nascent hydrogen atom products from the title reaction $O(^3P) + C_2H_3 \rightarrow H(^2S) + CH_2CO$ (ketene). The experimental data combined with CBS-QB3 level *ab initio* theory and statistical calculations demonstrated that the title oxygen-hydrogen exchange reaction is a major reaction channel, through an addition-elimination mechanism involving the formation of a short-lived, dynamical complex on the doublet potential energy surface.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Diabatic electronic population and its application in describing nonbonded interactions in complex systems

박재우 이영민*

포항공과대학교(POSTECH) 화학과

Modeling the nonbonded interactions between electronically excited molecules and their environments is of great importance in theoretically studying systems with fluorescence and luminescence. Although the computational demand required for using molecular mechanics is much smaller than that needed for employing costly ab initio calculations, the associated accuracy is often not satisfactory for describing the excited molecules. The main problem is that the electronically excited systems normally have complex potential energy surfaces. Moreover, the electronic properties ofteh change drastically as the molecules travel on the surfaces. Here, we present a formalism for improving the description of nonbonded interactions between an electronically excited chromophore and its environment within the fixed point charge model. We introduce a diabatic electronic population matrix, which is analogous to the atomic partial charges in the adiabatic states. To obtain the electrostatic interaction energies of the adiabatic states, we first compute Coulombic responses of the diabatic states to the presence of external charges in the environment using the diabatic electronic population matrix, and then diagonalize the diabatic Hamiltonian. We demonstrate the performance of this formalism in comparison with QM/MM reference values toward calculating the electrostatic interaction energies in the solvated green fluorescent protein chromophore.

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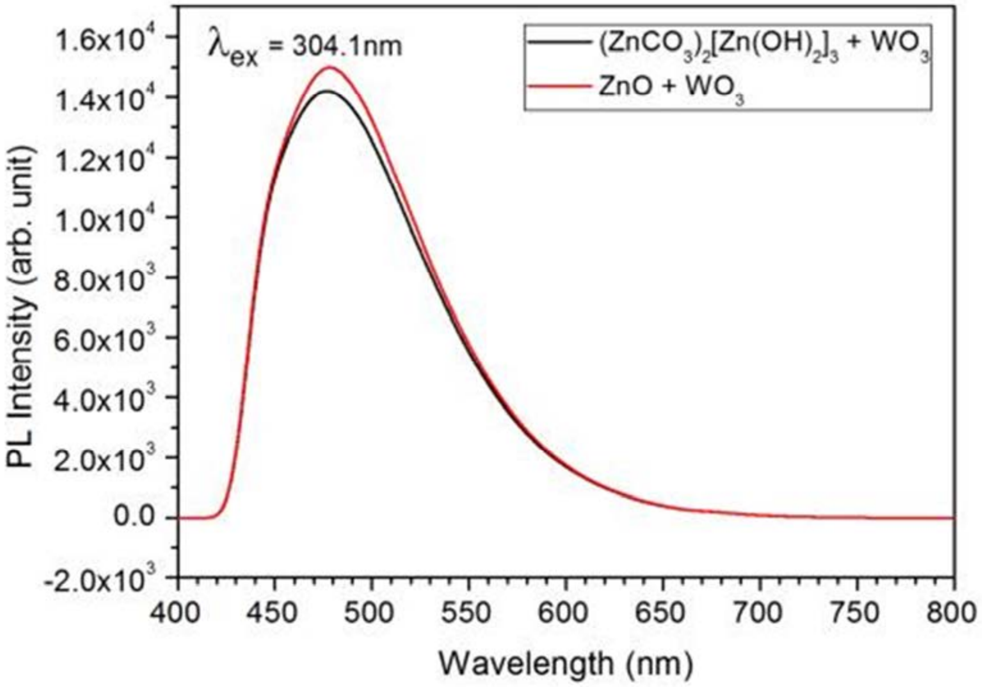
ZnWO4 합성과 박막제작Synthesis and Fabrication of ZnWO4 Thin Films

이국진 조선욱*

신라대학교 신소재공학과

광학적 디스플레이나 에너지 소재로서의 응용을 염두에 두고, ZnWO4 박막제작을 위해 고상법으로 ZnWO4 를 합성하였다. 반응 ZnO + WO3 --> ZnWO4 과 반응 (ZnCO3)2-[Zn(OH)]2-3 + 5WO3 --> 5ZnWO4 + 2CO2 + 3H2O 중에서 훨씬 더 좋은 PL 특성을 보이는 ZnWO4 가 형성되는 소결온도가 달랐다. 최고 950 도에서 3 시간 소결을 거쳐 만들어진 ZnO + WO3 --> ZnWO4 분말시료를 타겟으로 만들어 RF magnetron sputtering 방법을 이용하여 기판에 증착을 시도하였다. 박막은 증착온도 25, 100, 200, 300, 400 도에서 네 가지 종류의 기판 글라스, 쿼츠, 사파이어, 실리콘에 만들어졌다. 300 도에서 증착한 것이 박막이 잘 형성되었고, 500 도에서 30 분간 RTA 를 거쳐 박막이 성공적으로 제작 되었다. PL 과 흡광도를 측정하여 ZnWO4 박막의 물성을 확인하였다.



λ_{ex} = 304.1nm
$(ZnCO_3)_2[Zn(OH)_2]_3$ + WO_3
ZnO + WO_3
PL Intensity (arb. unit)
1.6x10^4
1.4x10^4
1.2x10^4
1.0x10^4
8.0x10^3
6.0x10^3
4.0x10^3
2.0x10^3
0.0
-2.0x10^3
400
450
500
550
600
650
700
750
800
Wavelength (nm)

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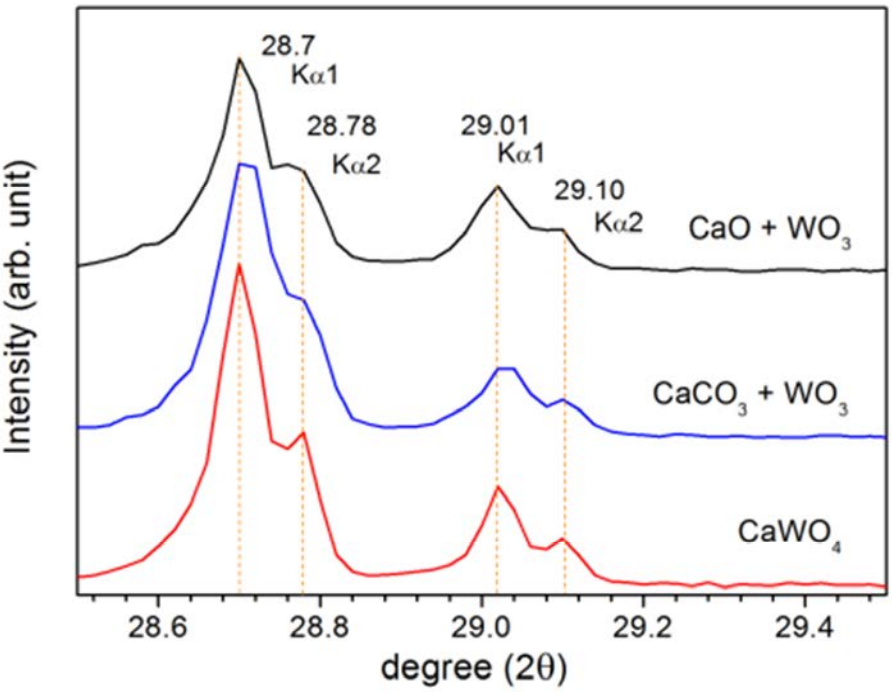
CaWO4 합성과 박막제작Synthesis and Fabrication of CaWO4 Thin Films

김민기 조선욱*

신라대학교 신소재공학과

CaWO4 박막제작을 위해 고상법으로 CaWO4 를 합성하였다. 반응 CaO + WO3 --> CaWO4 보다는 반응 CaCO3 + WO3 --> CaWO4 + CO2 를 택하는 것이 훨씬 더 좋은 PL 특성을 보이는 CaWO4 가 만들어졌다. 확대한 XRD 주 피크인 (112)면의 2theta 와 intensity 그림에서 Cu K alpha 1 과 K alpha 2 피크들을 비교하니 결정구조가 잘 만들어졌음을 확인하였다. 박막은 증착온도 25, 100, 200, 300, 400 도에서 네 가지 종류의 기판에 스퍼터링 장치를 이용하여 만들어졌다. 500 도에서 30 분간 RTA 를 거쳐 박막이 성공적으로 제작 되었고, PL 과 흡광도를 측정하여 CaWO4 박막의 물성을 확인하였다.


28.7
Kα1
28.78
Kα2
29.01
Kα1
29.10
Kα2
CaO + WO_3
$CaCO_3$ + WO_3
$CaWO_4$
Intensity (arb. unit)
28.6
28.8
29.0
29.2
29.4
degree (2θ)

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A@C20H20(CH3)2-trans2 isomers in the physical and chemical properties (A: He, Ne, Ar)

김성후 이기학[1,*]

원광대학교 자연과학대학/바이오나노화학부 [1]원광대학교 화학과

C20H20(CH3)2-trans2 cage 구조에 gaussian 프로그램을 이용하여 b3lyp method 로 계산 해보았다.cage 구조에 비활성 기체를 넣음으로써 에너지 변화 및 구조 변화를 설명 하고 대칭성에 대해서 조사를 해보았다. cage 구조와 비활성기체의 상호작용을 조사해보고 상호작용에 따른 물리화학적 성질의 경향성에 대해서 설명 할 것이다.이러한 시뮬레이션 결과로 fullerene 에도 적용 할 수 있는 좋은 기회가 될 것이다.

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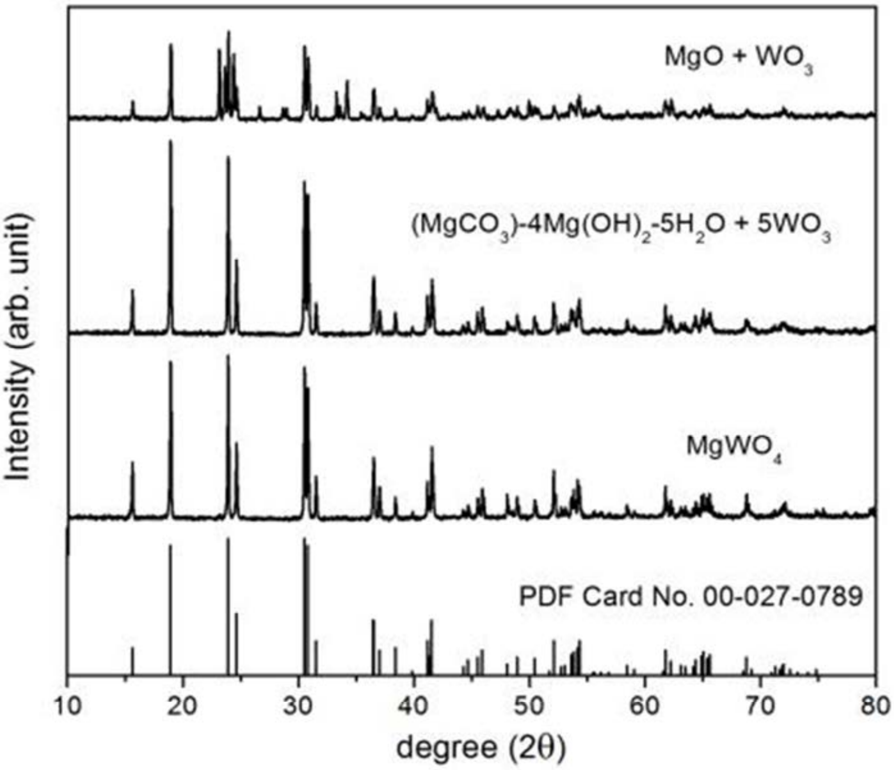
MgWO4 합성과 박막제작Synthesis and Fabrication of MgWO4 Thin Films

강은주 백경래 조선욱*

신라대학교 신소재공학과

스마트 윈도우나 광학적 디스플레이 응용을 염두에 두고, MgWO4 박막제작을 위해 고상법으로 MgWO4 를 합성하였다. 반응 MgO + WO3 --> MgWO4 보다는 반응 (MgCO3)4-Mg(OH)2-5H2O + WO3 --> 5MgWO4 + 4CO2 + 6H2O 를 택하는 것이 훨씬 더 좋은 PL 특성을 보이는 MgWO4 가 만들어졌다. 최고 950 도에서 3 시간 소결을 거쳐 만들어진 분말시료를 타겟으로 만들어 RF magnetron sputtering 방법을 이용하여 기판에 증착을 시도하였다. 박막은 증착온도 25, 100, 200, 300, 400 도에서 네 가지 종류의 기판글라스, 쿼츠, 사파이어, 실리콘에 만들어졌다. 300 도에서 증착한 것이 박막이 잘 형성되었고, 500 도에서 30 분간 RTA 를 거쳐 박막이 성공적으로 제작 되었다. PL 과 흡광도를 측정하여 MgWO4 박막의 물성을 확인하였다.


MgO + WO_3
$(MgCO_3)$-4$Mg(OH)_2$-5H_2O + 5WO_3
$MgWO_4$
PDF Card No. 00-027-0789
Intensity (arb. unit)
10
20
30
40
50
60
70
80
degree (2θ)

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발표코드: **PHYS.P-491**
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Analysis low concentration of Bio molecule based on compact designed SPR

진성일 박찬량[*] 김형민[1,*] 황진건[1]

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Since the first application of SPR phenomenon for sensing, various application and design has been developed. Designed focused on low-cost, compact, and relatively higher sensitive liquid bio sensor allows the general use of SPR bio-sensing. We designed SPR not only the size small enough to be moved by hand, relatively sensitive. SPR system is a highly significant instrument for applicable for immunoassay-type analysis, enzyme mimics, characterizing and quantifying biomolecular interactions and so on.

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Structural characteristics of thermoactive L-Arabinose Isomerase from Geobacillus Kaustophilus

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조선대학교 약학과

GKAI (Geobacillus Kaustophilus Arabinose Isomerase; L-AI) is an enzyme to convert L-arabinose into L-ribulose in vivo and has high activity and stability at 60 ℃. Though L-AI structure was solved by X-ray, the experimental temperature as 20℃ is not reliable to understand a mechanism of the thermoactive enzyme. Therefore, molecular dynamics simulation is performed at the active temperature using GROMCAS software. The monomer consists of 493 amino acid residues and a total system is a trimer with TIP3p water box. The protein system is modelled by amber99sb-nmr-ildn force field. Since the ligand sbbinding site with a metal (Mn^{2+}) is located at monomer boundary surface, monomer-monomer interaction would be important to open the enzyme gate. According to the simulation results, it is shown that the hydrophobic core between helixs as the tertiary structure is broken in the boundary of a monomer and the monomer secondary structure is still conserved. In the opposite side of the other monomer with a metal binding site , a hydrophobic core formed by loops is rearranged as a new hydrophobic core. To conform the opening mechanism of L-AI, we run the single mutation simulation with modification of Tyr20 into Ala20. However, there was no remarkable difference between the two results and then we try to run other simulations with other residues.

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Interferometric Scattering Microscopy for Investigating Self-Assembly Dynamics

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Self-assembly is a type of spontaneous association of components via non-covalent interactions (e.g. van der Waals interaction, hydrogen bonds, π-π interaction) where a disordered state becomes an organized one. For example, in an organism, self-assembly occurs at tissue formation where helical and chiral macromolecules such as collagen are secreted. The exact dynamics of self-assembly processes are still unclear, although they are very common and fundamental in nature. The goal of this experiment is to directly visualize the processes of self-assembly and to comprehend their dynamics better.

For this goal we choose the M13 phage as a model system mainly because of its dimension (800nm-length and 10-nm diameter) that allows optical observation. Since the M13 phage is transparent, we use a scattering microscope to observe it, and the scattered light is detected in the form of interference with the reflected light on a substrate. Thus, the name of the apparatus is interferometric scattering (iSCAT) microscope. Furthermore, we focus the narrow interfacial region between M13 phage solution and a solid substrate where the M13 phage self-assembles as its concentration increases by solvent evaporation. One of the possible setups is that M13 phage forms a film by pulling substrates vertically from phage solution at exactly constant controlled speeds.

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LC-MS-based in-vitro quantitative eicosanoid signatures on inflammatory responses of simvastatin

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Statins reduce low-density lipoprotein cholesterol in the mevalonate pathway and one of their pleiotropic effects, anti-inflammation, have been concerned with additional benefits of the clinical outcomes preventing cardiovascular events. Eicosanoids are oxygenated metabolites of membrane-released arachidonic acid through the cyclooxygenase (COX), lipoxygenase (LOX), cytochrome P450 ω-hydroxylase (CYP ω-hydroxylase) and non-enzymatic free radicals. In contrast to the conventional circulating inflammation markers, evaluating the broad spectrum of lipid signaling mediators may give better understanding the biological functions of inflammation. A liquid chromatography-mass spectrometry (LC-MS)-based metabolic profiling in the liver microsomal S9 fractions have been developed to measure 33 eicosanoids in the liver S9 fraction. The limit of quantification is 0.5~20 ng/mg proteins, while the precision (% CV) and accuracy (% bias) ranges from 4.7 to 10.8% and from 88.4 to 110.9%, respectively. Eicosanoid signatures resulted in the COX metabolites were increased in inflammation-induced model rabbits against the control rabbits, whereas 20-HETE catalyzed by CYP ω-hydroxylase was significantly decreased. In contrast, all detected eicosanoids catalyzed by COXs and LOXs showed no significant alterations, whereas the levels of 20-HETE were significantly increased (9.33- and 11.85-folds in response to 50 and 100 μM treatments, respectively; P

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Enzyme linked aptamer assay for the determination of Tetracycline residue in foods

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서울여자대학교 화학과

Enzyme-linked immunosorbent assay (ELISA) is the most commonly used tool for protein detection and quantification in complex solutions. Here we applied oligonucleotide, aptamer as a capture binder based on avidin/biotin interaction on multi-well polystyrene plates, and three different oligonucleotide [prove 1, 2 and 3] as a detecting binder, in its standard "sandwich" set up. Tetracyclines (TCs) are a group of broad-spectrum antibiotics which prevent and control many bacterial infectious diseases. So, they are widely used to treat many infections and growth promotion in animal husbandry. However, an abuse of antibiotics can increase the risk of TCs remaining in foods and cause serious problems on drug tolerance. To ensure the safety of food, it is necessary to establish a reliable analytical technique with specificity and sensitivity. This work represents enzyme linked aptamer assay (ELAA) by sandwich design for the determination of TC residue in foods. Aptamers are functional single-stranded oligonucleotides (ssDNA or RNA), which are selected in vitro by SELEX process. And they binds to a specific target molecule with high affinity and selectivity, from small molecules to proteins. A 76mer DNA TC aptamer was utilized as capture and three complementary oligonucleotides (36mer-ssDNA, 37mer-ssDNA and 76mer-ssDNA) were used as detector. Various assay conditions were optimized and a proposed assay design is expected to become a promising method for the determination of TCs in contaminated food product. From those results, a binding site of 76mer-DNA TC aptamer also could be identified indirectly.

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Combination of Comprehensive 2D Gas Chromatography and High Resolution Mass Spectrometry Applied to Analysis of Oils Sourced from Different Shale Facies in the Molecular Level

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Unconventional petroleum reservoirs often contain multiple productive intervals with differing lithofacies that reflect changes in the depositional environment through time. These changes lead to variations in source rock character and other factors in the reservoir relevant to the properties of the petroleum generated and its production. Lithofacies variations can be determined from well log data and through visual assessment or geochemical analysis of core and outcrop rocks. Petroleum chemical characteristics are also known to vary with source rock properties; therefore, interpretation of oil geochemistry can be used to obtain information on the nature of the source rocks in a particular reservoir. In this study, molecular level characterization was performed by combination of comprehensive 2D gas chromatography and positive-mode atmospheric photoionization Fourier transform ion cyclotron resonance mass spectrometry on oils produced from different lithofacies within the lacustrine Green River Formation in the Uinta Basin of Utah, USA. These source rocks include the Mahogany zone oil shale, the Black Shale facies and the informal Uteland Butte member. The Mahogany zone and Black Shale were deposited during periods when the lake was more saline while the Uteland Butte was deposited during an earlier time when the lake was fresher. Significant differences in chemical composition were observed between oils obtained from different wells and these differences are consistent with other analyses indicating which of the three source rock lithofacies each originated oil. Our results show that the combination of multidimensional gas chromatography and ultrahigh resolution mass spectrometry provides a more complete assessment of oil constituent compounds over a wide mass range ($50 < m/z < 1100$).

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Fabrication and Characterization of PZT Thin Film with RF Magnetron Co-sputtering at Various O_2 Gas Ratio

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부경대학교 화학과

Lead zirconate titanate (PZT) is significant material in electrical and optical devices for their ferroelectric, piezoelectric and dielectric properties. In this research, PZT films were fabricated by reactive RF magnetron co-sputtering method by using metallic lead, zirconium and titanium targets at various O_2 gas ratio and post-annealing treatment. And the O_2 gas was used for reactive gas and Ar gas was used for sputter gas and the deposited PZT films were annealed at 723, 823, 923 and 1023 K for 2 h in ambient atmosphere. The deposited PZT films were investigated the change of chemical environment, morphology and electrical properties with respect to O_2 gas ratio and annealing temperature. By proceeding depth profile, the composition of PZT was investigated from surface to bulk. At XPS spectra, oxidation states of lead, zirconium and titanium were depending on O_2 gas ratio. And the thickness of PZT films was measured with surface profiler and the thickness decreased when O_2 gas included with reactive gas. After oxygen gas was introduced, the thickness of the PZT films did not depend on O_2 gas ratio. And the resistivity of PZT thin films was increased and the conductivity was decreased.

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Investigation of molybdenum nitride thin films deposited by reactive r.f. magnetron sputtering at various nitrogen ratio

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Molybdenum nitride (MoN_x) thin films were deposited on p-type Si(100) wafer by reactive r.f. magnetron sputtering at various nitrogen gas ratio in ultra high vacuum (UHV) chamber. Surface properties of MoN_x thin films were investigated by alpha step measurement, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and 4-point probe measurement. Thickness of MoN_x thin films was decreased from 180 to 20 nm with increasing nitrogen gas ratio measured by alpha step measurement. The structure of MoN_x thin films was γ-Mo_2N phase assigned by XRD. Mo and nitrogen species were confirmed by deconvolution of high resolution XPS spectra of Mo 3d, Mo 3p and N 1s. And conductivity of MoN_x thin films was increased after nitrogen gas involved in the sputter gas.

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Separation of gold polyhedral nanoparticles using gel electrophoresis

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본 포스터에서는 기존의 젤 영동 분석법에 계면활성제의 종류와 농도 및 젤 매트리스의 농도를 체계적으로 조절하여 금 나노입자들 중에서 특히 불균일한 다각형 모양의 금 나노입자를 균일한 크기로 분리하고자 하였다. 분리된 금 나노입자의 형태와 크기 및 농도를 투과전자현미경(TEM)과 UV-vis 분광법으로 확인하였으며 그 예비결과를 나타내었다.

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Free radical initiated peptide sequencing (FRIPS) studies for phosphorylated peptides

오한빈

서강대학교 화학과

Post-translational modifications (PTMs), particularly, phosphorylations, are the important step that plays an important role in biological system in vivo. Phosphorylation PTMs are involved in cell death, cell-cell signaling, and various biological processes. Due to its importance, extensive investigations have been made towards the development of phosphorylation PTM analysis. On the other way, our group has development a new radical-based peptide backbone dissociation method, the so-called, ‘free radical initiated peptide sequencing (FRIPS)’. In this method, a TEMPO-containing radical initiator is conjugated to the N-terminus or lysine side chain. Upon collisional activation, a benzylic radical can be generated and this radical species can initiate peptide backbone dissociations upon the secondary application of collisional activation. In this study, we have explored the opportunity of using FRIPS for the analysis of phosphorylated peptides. We have examined the peptides phosphorylated at serine or tyrosine site. For the phosphopeptides modified at tyrosine, it was found that the phosphor-ether bond could survive even at the collisional activation with which the benzylic radical was generated. As a result, the phosphorylation site could be determined in FRIPS MS experiments. In the case of peptides with a phosphoserine residue, dephosphorylation was found to occur extensively. The detailed results will be presented in the symposium.

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Development of a simple ANS-based displacement assay for the characterization of druggability

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Development of a simple, inexpensive, robust, and high throughput method to characterize promiscuous drug candidates is described. The method utilizes a fluorescent probes, 1,8-anilinonaphthalene-8-sulfonate (ANS), in which its inherent fluorescence intensity increases upon binding to protein targets. The fluorescence signal diminution when they are displaced by small competing chemicals provides a quantitative tool to compare, or rank, non-specific binding affinity and is therefore directly applicable to assess druggability of chemical compounds. As a proof of principle, 446 chemical compounds from NIH clinical collection were screened and the displacement activity was evaluated. Most compounds did not show significant activities against ANS displacement. This result demonstrated that comparative biological analysis on non-specific binging affinities allows us to quickly examine druggability of small molecules and prioritization of compounds from commercial or house-produced libraries at very early drug development stage. Key words: Fluorescence, displacement, high throughput screening, drug, promiscuous inhibitors

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Enantiomer separation of acidic chiral compounds on a quinine-zirconia hybrid monolith by capillary electrochromatography

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영남대학교 화학과

An organic-inorganic hybrid zirconia monolithic capillary column was prepared by sol-gel process in a fused-silica capillary with 3-triethoxysilylpropylisocyanato quinine as chiral selector. The column was employed for electrochromatographic enantioseparation of a set of acidic chiral drugs. Effects of the composition of the eluent, concentration of electrolyte, applied voltage and capillary temperature on enantioseparation were investigated to find optimal separation conditions.

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Comparative study of oxidized phospholipids in lipoprotein classes between controls and patients with coronary artery disease by flow field-flow fractionation and nanoflow liquid chromatography-tandem mass spectrometry

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Since several decades ago, lipoprotein particles in blood that transports lipids, has been treated as one of the most critical topics in terms of coronary artery disease (CAD). Lipoproteins can be classified into three classes by their densities and specific roles they play. High density lipoprotein (HDL) transports lipids from body to liver for decomposition of the fats. Very low density lipoprotein (VLDL) is synthesized in liver for storing the remaining fat, and low density lipoprotein (LDL) is formed by loss of TGs from the VLDL. When excess amount of lipoproteins build up on blood vessels, they are oxidized by either non-enzymatic or enzymatic processes and start to malfunction. According to recent clinical studies, the oxidized lipoproteins are critical biomarkers of CAD because they promote the formation of the plaque on blood vessels. Studying oxidized phospholipids (PLs) within the oxidized lipoprotein is the main objective of this study.Due to the capability of increased amount of injection and disposability, a multiplexed hollow-fiber flow field-flow fractionation (MxHF5) system was applied for the separation and collection of lipoprotein particles from blood plasma. HDL, LDL and VLDL from two groups of pooled blood plasma samples, 10 controls and 10 patients with CAD, separately, were successfully separated by MxHF5 system without any pre-treatment.Nanoflow liquid chromatography-tandem mass spectrometry was used to identify the oxidized phospholipids from the collected lipoprotein classes of blood plasma. Oxidation, peroxidation and cleavage of fatty acid from PLs were successfully profiled from the fragmentation patterns of collision-induced dissociation and comparative analysis of oxidized PLs between controls and patients were carried out.

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Discrimination analysis of fire retardant and fake expandable polystyrene materials by chemometrics and FT-NIR and XRD spectrometer as Non-invasive analyzer

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Sandwich panel as Building material is widely used to factory and warehouse building. Above all, the sandwich that could be made from side plates of steel and the core of EPS(expandable polystyrene) is applied the most. Because of complex material, the weight is light and the method of building is simple, and it has the advantage of good adiabatic performance. However, owing to combustible properties of the core properties, the risk of fire was too high. Also, as the fire was happened into steel plate, it was difficult to have the fire fighting. Recently, after fire retardant properties were supplied for improving it. Fire retardant sandwich panel has been built on-site. But because it is impossible to determine whether it is safe on fire by the naked eye or not, through it was built by fake panel, fire accidents were happened. Therefore it is necessary to become a social issue. It was studied to analyze the discrimination of fire retardant EPS on-site by XRF and FT-NIR spectrometer as hardware. Also, PLS-DA and PCA of chemometrics as software was used. As the analytical result, in the case of XRD, it was sure to discriminate the fake in fire retardant sandwich by PCA method. And in FT-NIR spectrometer, the fake could be discriminated in sandwich by only PLS-DA.

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Effects of fluorine substituted LiFeBO3 as a cathode material for lithium rechargeable battery

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In Lithium rechargeable battery, LiMBO3 (M=Fe, Mn and Co) is increasing to interest due to its strong boron-oxygen covalent bond, high theoretical specific capacity, environmental friendly benefit, and less expensive. The fluorine substituted LiFe(BO3)1-xF3x composites have been synthesized by solid-state reaction using planetary mill method without carbon coating. It was characterized by XRD, SEM and cycling test. The XRD results of composite indicate fluorine anions have been successfully substituted to BO33- sites without structural modification. Electrochemical analysis has been also performed with various C-rates and cycleability.

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Characterization of Oxidized Water Accommodated Fractions by High Resolution Mass Spectrometry

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경북대학교 화학과

Crude Oil and petroleum products chiefly enter the environment through oil seeps and oil spills and their chemical compositions are changed by biodegradation and photodegradation. Besides, the water soluble oil compounds(WAF) (e.g. BTEX, naphthalenes, PAHs, phenols and polar components) have high bioavailability towards marine organisms. It is well known that oxidation of compounds plays an important role for biodegradation, photodegradation and change of toxicity. However, little is known about photodegradation process of crude oil compounds and their oxidized products. It is mainly because of crude oils' extreme complexity and lack of suitable analytical technique. In this study, high resolution mass spectrometry is utilized for characterization of oxidized WAF. Oxygen containing functional groups such as alcohols, aldehydes, ketones are major parts in the oxidation of crude oil. So we will focus on oxygen containing compounds.

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Prediction of vapor pressure and phase transition enthalpy of plasticizer

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In the system of melt castable explosives, thermal properties are very important. Because of this reason, analysis of explosives and plasticizers is needed. Recently, studies of energetic plasticizers are very active. And calculation or determination of thermal properties of these energetic plasticizers is also needed. TGA(thermal gravimetric analysis) method is easy to measure and handle. From TGA data, in this presentation we will show calculation of vapor pressure and phase transition enthalpy of plasticizers. Vapor pressure and phase transition enthalpy can be calculated using derivation of ideal gas equation and Clausius-Clapeyron equation. Benzoic acid was used as standard material for taking important two constants. And using those constants, we could calculate vapor pressure and phase transition enthalpy of plasticizers.

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Growth and electrochemical properties of CNFs on electroplated Co-Ni and Co-Cu/C-fiber textiles

장건호 남기목 박희구[1] 홍석주[2] 이창섭[*]

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In this study, we have grown carbon nanofibers(CNFs) on Co-Ni and Co-Cu catalysts electroplated on C-fiber textiles by chemical vapor deposition(CVD) and applied the CNFs to an anode material of Li secondary batteries. Prior to the growth of CNFs, Co-Ni and Co-Cu catalysts were electroplated on C-fiber textiles. The CNFs were then grown by thermal CVD on Co-Ni/C-fiber textiles and Co-Cu/C-fiber textiles, respectively. Temperature of the furnace was increased up to 700℃ under N_2 atmosphere and H_2/N_2 mixed gas for reduction process of oxidized surface was flowed for 1h at 700℃. CNFs were then grown on electroplated Co-Ni/C-fiber textiles and Co-Cu/C-fiber textiles by flowing ethylene/N_2 mixed gas as carbon source for 1h at 700℃. SEM and EDS were measured to investigate the growth and compositions of CNFs. Physicochemical properties were characterized by XRD and BET. The As-grown CNFs onto C-fiber textile without any binder were used as an anode material of a conventional three-electrode cell. Cyclic voltammetry and galvanostatic charge-discharge experiments were performed to investigate electrochemical properties of the cell.Acknowledgment : 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(NO.2012026209).

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Fabrication and Characterization of an Anode Material for Li Secondary Batteries Based on CNF and CNT - Si composites

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We have performed a study on the characteristics of CNF and CNT-Si composites that used as an active anode material for lithium secondary batteries. Samples employed for the battery test were commercial products of GNF(Herring bone), GNF(Antler), CNT, CNF and lab-prepared CNF. Lab-prepared CNF was synthesized by Chemical Vapor Deposition(CVD) using Co and Cu catalysts. The test results of the samples were compared with the Si composites of each sample. The Si particles were ball-milled to a micron size and coated with pyrolytic carbon using by acetylene gas. Then it was finely mixed with respective five samples using ball mill. PTFE(Polytetrafluoroethylene) was used as the binder and glass fiber separator was used as the separator membrane for the composition of three electrode cell. As the electrolytes, 1M $LiPFH_6$ was dissolved in a mixture of ethylene carbonate (EC) : propylene carbonate (PC) : ethyl methyl carbonate (EMC) in a 1:1:3 volume ratio. The five different CNF and CNT-Si composite materials were evaluated as the anodic material in three electrode cells. The morphology and composition of samples were analyzed by SEM and EDS measurements. Physicochemical properties were investigated using XRD, Raman spectroscopy and XPS. The electrochemical characteristics as an anodic material of Li secondary battery were investigated using the galvanostatic charge-discharge and cyclic voltammetry measurements.Acknowledgment: 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(NO.2012026209).

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A trial for disposable microcolumns in liquid chromatography

홍성훈 정원조*

인하대학교 화학과

The purpose of this study is to investigate the possibility of disposable micro-columns. A permanent frit (2 ㎛ pore) was welded to the column outlet of glass-lined stainless steel tubing, and then 5 ㎛ commercial silica particles were packed in the column. After packing, a second frit was welded to the inlet of the packed column. In order to reduce the production cost of disposable microcolumns, partially sub-2 ㎛ silica monolith particles were prepared in a large scale and modified to C18-bound silica monolith particles as low cost packing material. The strategy of permanent attachment of frit to the column is the critical step for the preparation of disposable microcolumns. The possibility of realization of disposable microcolumns has been examined by comparing the efficiency of this column with that of the column with non-welded frits.

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C18 modified silica monolith particles of high chromatographic separation efficiency

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Partially sub-2um porous monolithic silica particles have been prepared by sol gel process with controlled multi-step heating followed by grinding and calcination. The production scale has been increased four times than our previous work. These particles were subject to C18 modification (chlorodimethyl octadecylsilane) in anhydrous toluene under reflux followed by end capping with HMDS (hexamethyl disilazane) and TMCS (trimethyl chlorosilane). The resultant phase was washed, filtered, dried and packed in a micro-column (1.0 mm ID and 300 mm length). The optimized mobile phase was found to be 60/40 (v/v) acetonitrile/ water containing 0.1% TFA at a flow rate of 25?L/min. The column efficiencies as high as 123,000 N/m were achieved for separation of benzene and its derivatives in HPLC. The separation efficiency of this stationary phase (C-18 bonded partially sub-2um porous monolithic silica particles) was better than that of commercial C-18 bonded silica particles.

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Progresses in ground organic monolith particles as new chromatographic separation media

김윤성 정원조*

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We have recently reported a pioneering study on ground organic monolith particles as new chromatographic separation media in our laboratory. The reaction mixture was composed of methacrylic acid (MAA) as funtional monomer, ethyleneglycol dimethacrylate (EDMA) as crosslinker, azobis-isobutyronitrile (AIBN) as initiator, polyethyleneglycol as special porogen, and toluene-isooctane mixture as solvent. In this study, we have prepared different stationary phases by changing formulation of reaction mixture in a variety of different ways. For example, trimethylpropane trimethacrylate (TPTM) was used as a new crosslinker, or polyvinylpyrrolidone was used as a new porogen. The variations of morphology and chromatographic separation performance of the resultant organic monolith particles will be comparatively discussed.

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Formation of a layer of N-phenyl acryl amide - styrene co-polymer on the inner surface of silica capillary for excellent separation of saccharride isomers by CEC

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인하대학교 화학과

The initiator moieties were successfully attached on the inner surface of silica capillary (50?m ID and 50 cm length) by binding 4-chloromethylphenylisocynate to the silanol groups via isocyanate-hydroxyl reaction with an aid of dibutyl tin dichloride as a catalyst, followed by reaction with sodium diethyl dithiocarbamate. Then a N-phenylacrylamide-styrene co-polymer layer was attached via reversed addition-fragmentation chain transfer polymerization. The resultant open tubular silica capillary column showed excellent separation performance for saccharide isomers. Five structural isomers were separated for maltotriose, and α and β anomers were separated for D-glucose with very high separation efficiency (N-values over one million) in CEC in 90/10 (v/v) ACN/30mM sodium acetate of pH 6.6.

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Monitoring of surfactants in wet tissues and detergents by liquid chromatography-electrospray ionization/mass spectrometry

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Surfactants are the active ingredients in personal hygiene products and detergents for industrial and household cleaning. Some of them are known to be toxic to animals, ecosystems, and humans, and can increase a diffusion of other environmental contaminants. For this reason, they are widespread environmental pollutants. Their separation and identification can be difficult due to both the diversity of surfactants and the complexity of sample matrices. A variety of methods have been developed, it is challenging to choose proper methods for specific applications. The aim of this study was to develop a direct measurement of amphoteric, cationic and nonionic surfactants in detergents by liquid chromatography-electrospray ionization/mass spectrometry. The compounds were well separated through a reverse-phase column within the rate of 40 mins providing good peak shape, and were well quantified using a full-scan mode in ion-trap MS. The solvent system used was composed of water and acetonitrile or methanol with 0.1% formic acid as an ionization solvent to improve ion strength. The detection limits of surfactants were 0.003-0.2 ug/mL which could be detected down to 1~20 ug/mL. The calibration curves were linear in the working range of 0.01 ug/mL- 20 ug/mL with correlation coefficient values of above 0.99. The precision (% CV) and accuracy (% bias) of the assay were 0.2-9.9% and 92.3-117.8%, respectively. The proposed method allowed a sensitive and rapid detection of surfactants and it could be applied to monitoring surfactants from various cleaning agents, wet wipes and detergents.

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Water contents in Nafion Investigated by ^{2}H Nuclear Magnetic Resonance Spectroscopy

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대표적 고분자 전해질 막인 나피온(Nafion)은 과불소화된 고분자 부분(perfluorinated polymer backbone)과 전해질 성질을 갖는 -SO_3H 그룹으로 구성되어 있다. -SO_3H 그룹을 매개로 하여 발생하는 나피온의 수소이온 전도성은 나피온에 함유된 물의 양과 그 분포도에 의존한다. 따라서 물의 양과 그 분포도에 대한 상관 관계를 알 필요가 있다. 그러나 나피온에 흡수된 물은 빠르게 증발하기 때문에, 분포도를 알기위한 분석 실험 과정에서도 함수량이 변한다. 따라서 무게 측정 후 위의 분석 실험을 하면 함수량과 분포도에 대한 상관 관계를 올바르게 구할 수 없다. 또한 저울의 동적 측정 범위(dynamic range) 한계로 인하여 상대적으로 무거운 시료의 무게에서 소량의 함수량 차이를 무게 측정으로 구별 하기 힘든 점이 있다. 본 연구에서는 위의 문제점을 극복하기 위하여, 중수소(^{2}H) 핵자기공명 (nuclear magnetic resonance: NMR) 분광법을 이용하여 물의 분포도를 측정하는 과정에서 동시에 함수량을 정량하는 방법을 연구하였다. 먼저, 나피온의 실제 부피와 함수량의 관계를 관찰하였다. 그리고, 나피온에 D_2O 를 흡수시켜, ^{2}H 고체 NMR 신호를 얻었다. ^{2}H NMR 신호의 화학적 이동 값, 신호 면적, ^{2}H NMR 신호들간의 간격과 나피온의 함수량에 대한 관계식을 구하여 나피온의 함수량에 대한 검정곡선법(calibration curve method)을 완성하였다.

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Synthesis and Electrochemical Characteristics of Carbon nanofibers based on Ni and Mo Catalysts by Chemical Vapor Deposition

장은이 현유라 박희구[1] 정재원[2] 이창섭[*]

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This study reports on the synthesis of carbon nanofibers by chemical vapor deposition using Ni and Mo as catalysts. In order to investigate the suitability of their growth temperature and catalytic activity for the synthesis of carbon nanofibers, we prepared catalysts for the synthesis of carbon nanofibers with nickel nitrate and ammonium molybdate. We found the optimum growth temperature and concentration of each catalyst. The catalysts were sparsely and thinly spread on a quartz tube boat to grow carbon nanofibers by thermal chemical vapor deposition. The surface morphology and composition of synthesized carbon nanofibers were investigated by SEM and EDS analyses. The crystal quality of synthesized carbon nanofibers was analyzed by Raman and XRD. The chemical state of the surface was investigated by XPS. Specific surface areas of prepared metal catalysts and carbon nanofibers were measured by BET. It was verified that the characteristics of the synthesized carbon nanofibers were greatly influenced by the concentration ratio of catalysts. When the concentration ratio of Ni and Mo was 6:4 at 800 ℃ of calcinations temperature, the most uniform carbon nanofibers of 50 nm in diameter with the best crystallizability was grown. The three-electrode cell for Li secondary battery was fabricated with the CNFs grown on catalysts (Ni:Mo=6:4) as an anode material. The cell was composed of Polytetrafluoroethylen (PTFE) as a binder and Li metal used as the counter and reference electrode. The electrolyte consists of a 1M $LiPF_6$ solution in ethylene carbonate (EC): propylene carbonate (PC): ethyl methyl carbonate (EMC) with 1:1:3 volume ratio. The electrochemical characteristics of CNFs were investigated by cyclic voltammetry and galvanostatic charge-discharge.Acknowledgment : 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(NO.2012026209).

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Sensitive and selective detection of NO2 ion using modified gold nanoparticle as a colorimetric sensor

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A sensitive and selective colorimetric method for determination of nitrite ion in aqueous samples was developed using 1-(2-mercaptoethyl)- 1,3,5-triazinane- 2,4,6-trione-functionalized gold nanoparticles (MTT-GNPs). The nitrite ion seems to be used as a “molecular bridge”, which can form NH?N and NH?O hydrogen bonds with the MTT-GNPs, shorten the interparticle distance, and induce the aggregation of the MTT-GNPs. This aggregation results in a dramatic change from wine-red to purple?gray color. Therefore, the concentration of nitrite ion in environmental samples can be quantitatively detected using the MTT-GNPs sensor by the naked eyes or UV?vis spectrometer. Moreover, investigations have revealed the sensitivity of the detection could be clearly improved by modulating pH of the solution, which led to a more rapid color change in the optimized GNPs system. The absorption ratios (A790/A535) of the modified GNPs solution exhibited a linear correlation with nitrite ion concentrations and the limit of detection was 1ppm. This cost effective sensing system allows for the rapid and facile determination of the concentration of NO2 ions in aqueous samples.

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SERS-Fluorescence Dual-Mode Immunoassay of Graphene Quantum Dots Labeling on 1D-aligned Magnetoplasmonic Nanoparticles

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A novel dual mode immunoassay based on surface enhanced Raman scattering (SERS) and fluorescence was designed using graphene quantum dot (GQD) labels to detect tuberculosis (TB) antigen, CFP-10, using a newly developed sensing platform of linearly ? aligned magnetoplasmonic (MagPlas) nanoparticles (NPs). The GQDs were excellent bi-labeling materials to carry out Raman scattering and photoluminescence (PL), simultaneously. The 1D alignment of MagPlas NPs simplified the immunoassay process and faster signal transducing and enhancement. With a sandwich type immunoassay using dual mode nanoprobes, both SERS signals and ?uorescence image were recognized in high sensitive and selective manner with a detection limit of 0.51 pg mL-1.

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Rapid Detection of DNA by Magnetophoretic Assay

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Recently, marine environmental pollution has become more and more serious due to oil spills or the collapse of nuclear power plant resulting in a massive release of hazardous materials to the ocean. These harmful radioactive materials are associated with the random mutation of genes leading to deformity of individuals. So far there has been no effective system for monitoring this marine pollution. Therefore, rapid detection of DNA mutations has become increasingly important in a variety of fields including medical diagnostics and food safety. Herein, we report a rapid, sensitive, qualitative and quantitative approach for DNA detection based on the magnetophoretic assay. The Au-magnetic microparticles (MMPs) nanocomplex was used to generate a color signal and uncombined Au NPs contributed an optical signal that could be directly quantified by UV-Vis absorption spectroscopy of the supernatant after the sample was placed in a magnetic field for 2 min. The linear relationship between signal intensity and the target DNA concentrations (0.1 nM ~ 1.0 ?M) was investigated and a limit of quantitation of 0.1 nM was achieved using this method.

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Discrimination of Geographical Origin and Authenticity of Sesame Oils Using ^{1}H NMR Spectroscopy with Discriminant Analysis

이윤희 진경수 김지은 신지영 전재경 이효진 정용애 장석규 안상두*

중앙대학교 화학과

The geographical origin and authenticity of sesame oil are important issues in Korea because its price is decided by the geographical origin of sesame seeds and ratio of sesame oil. Especially, the price between domestic and imported sesame seeds is significantly different. Also, flavored oil which has a low ratio of sesame oil is more cheaper than pure sesame oil. In this study, we prepared sesame oils from 72 Korean, 20 Chinese, and 18 Indian white sesame seeds and flavored oils from 44 different commercial products in the deuterated chloroform solvent and obtained their ^{1}H nuclear magnetic resonance (NMR) spectra at 600 MHz NMR spectrometer. And the discriminant analysis of the SPSS statistics 21 was used to discriminate geographical origin and authenticity.The NMR spectra showed the existence of fatty acids and lignans which are ingredients of the sesame oils. We measured the ratio of double bonds in fatty acids and the amount of some lignans (sesamol, sesamolin) by integrating the NMR peaks and found they are important factors to discriminate the origin and authenticity of sesame oils. The geographical origin of sesame oils from Korea, China, and India was well defined by using two discriminant functions at 92.7 %, and Korean sesame oils were distinguished from the other imported sesame oils by using discriminant functions. Also, pure sesame oils were distinguished from flavored oils at 100% by using discriminant functions.These results suggest that NMR-based discrimination is a useful method to categorize sesame oil according to its geographical origin.

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Application of 2D-NMR (HSQC-DEPT) Spectroscopy and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Separation of Crude Oil by Normal Phase HPLC

김다애 조윤주* 김성환*

경북대학교 화학과

Crude oil is mixture of various compounds and its complexity makes it difficult to be analyzed at a molecular level. Therefore, it is advantageous to separate crude oils into ring-type groups for understanding details about crude oil sample. For this reason, the separation of crude oil is regarded as important part in petroleum industry. Compounds in crude oils were separated into five different groups (saturates and 1-ring, 2-rings, 3rings, 4-rings and polar compounds) according to aromatic ring number. Normal phase HPLC, two six port valves and two columns (PAC column and DNAP column) were used for separation. Five different groups were collected by using fraction collector and these samples were purged and dried using nitrogen. After this step, oil samples were further characterized by 2D NMR and 15T FT-ICR MS coupled to atmospheric pressure photo ionization (APPI). Carbon number and DBE distribution plots generated from FT-ICR MS data showed that ring type separation was successfully performed. The conclusion was further confirmed by application of NMR. Generally, NMR could determining molecular structure when analyzing complicate and large sample. In this characterization step, we used Heteronuclear single-quantum correlation spectroscopy (HSQC)-DEPT which is one of 2D NMR methods. Additionally, ^{1}H-^{13}C HSQC-DEPT spectra agrees with the FT-ICR MS data very well.

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The separation and analysis of crude petroleum-oil by combining HPLC and ion mobility mass spectrometry and theoretical CCS calculations

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In this study, the potential of combining ion mobility spectrometry (IMS), high resolution mass spectrometry and theoretical calculation in combination with high performance liquid chromatography (HPLC) for Petroleum-Oil analysis is investigated. HPLC has been widely used as a method for aromatic ring types study and ion mobility and theoretical calculation can add additional dimension of information to differentiate isomers of the same mass but with different molecular geometry. The ring type separation is performed by using 6-port value and normal phase mode column. In the next step, the obtained fractions were further characterized by use of IMS and theoretical CCS calculations. This study shows that aromatic ring types of crude oil compounds can be successfully separated and characterized by using these combined approach.

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압타머 혼성화를 활용한 새로운 방법의 도파민 샌드위치 분석법

김지은 이인숙*

서울여자대학교 화학과

압타머는 SELEX 과정으로부터 얻어진 한 가닥의 올리고뉴클레오타이드이다. 이것은 면역분석법에서 사용되는 항체보다 더 많은 이점을 가지고 있다. 따라서 분석물질을 인식하는 새로운 결합체로 이용된다. 도파민은 카테콜아민에 속하는 신경전달물질 중 하나이다. 하지만 저분자량 물질인 도파민은 항원결정기(epitope)가 한 자리이기 때문에 항체를 이용한 샌드위치 분석법에는 적용할 수 없다. 그렇기 때문에 새로운 결합체인 압타머를 사용하여서 샌드위치 분석법을 진행하고자 한다. 이제까지 진행된 실험으로는 두 가지의 방법이 있다. 하나는 항체를 capture 로 압타머를 detector 로 사용한 실험이고, 또 다른 실험은 압타머를 capture 로 항체를 detector 로 사용하였다. 본 연구에서는 capture, detector 로 모두 올리고뉴클레오타이드를 사용하였다. Capture 로 사용한 압타머는 57mer DNA 압타머이고, 이것은 57mer RNA 압타머 서열에 상응한다. Capture 에 상보적인 배열을 갖는 올리고뉴클레오타이드(probe)는 detector 로 사용하였다. 여기서 probe 는 4 가지의 서로 다른 상보적인 올리고뉴클레오타이드로 구성되었다(19mer ssDNA, 21mer ssDNA, 24mer ssDNA, 57mer ssDNA). 각각의 probe 들은 압타머와 혼성화를 이루며 서로 다른 혼성화 자리를 가지게 된다. 이것을 통해 일반적인 샌드위치 분석법의 디자인을 나타내고자 한다. 따라서 압타머의 도파민 결합자리와 상보적인 배열을 갖는 probe 를 이용한 결과와 도파민이 결합하지 않는 자리와 상보적인 배열을 갖는 probe 를 이용한 결과를 비교하고자 한다. 이 분석법을 통해서, 도파민 검출을 위한 새로운 방법의 샌드위치 분석법에 접근하고자 한다.

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Evaluation of correlation structure between a column selection method and an RP-LC analysis of a real pharmaceutical system

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Due to a vast variety of reversed-phase liquid chromatographic stationary phases on the market, it is paramount to select an appropriate chromatographic column. One of the recent attempts of RP-LC column ranking/selection was a method developed at the Katholieke Universiteit Leuven (KUL method), which was in this work correlated to retention parameters obtained for a real pharmaceutical analysis of alfuzosin hydrochloride and its impurities (column performance analysis). Thirty-six stationary phases were evaluated, and for this purpose two multivariate chemometric methods: Partial Least Squares, and Canonical Correlation Analysis, were utilized. Results of the analyses, for the first time, revealed a correlation structure between the KUL method parameters and retention parameters of a column performance analysis. Thus, a strong correlation between the afore-mentioned has been confirmed. The tested stationary phases organized into groups based on their physical and chemical characteristics, which verifies the obtained correlations. Analyzed correlation structure is especially important in cases when two or more chromatographic columns have identical or nearly identical values, and serves as a valuable extension of the KUL method. Thereby, applicability of the KUL method as an invaluable asset in proper RP-LC column selection is confirmed.

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The dynamic and static analysis of the Interior Film VOCs for the performance evaluation of visible photo-catalyst by using Thermal Desorption GC/MS

양진석

LG Hausys Analysis PJT

산업화에 따라 환경오염은 단순한 지구환경 문제를 떠나 개인의 삶의 질에도 큰 영향을 끼치고 있으며 자연 정화로는 한계가 있는 실정이다. 따라서 인위적인 방법을 통해 오염물질을 무해한 성분으로 분해하여 완전 제거하는 기술에 대한 연구가 전세계적으로 주목받고 있다. 특히, 실내공기질 부분은 1970 년대 초 새집증후군이라는 새로운 증상이 보고되었으나 최근에서야 본격적으로 이슈화 되었다. 현대인이 실내에서 생활하는 시간이 하루중 90% 이상을 차지하고 있으며, 이에따라 실내공기질은 현대인의 건강에 직접적으로 영향을 미치기 때문에, 실내공기 오염 문제와 해결 방안에 대한 논의는 최근 나날이 늘어가고 있으며, 국가차원의 관리를 집중하고 각종 제제 조치를 통해 의무화 하고 있는 실정이다. 우리나라에서도 환경부를 중심으로 2004 년 실내공기질 관리법을 정하였고, 점차 그 규제가 강화되고 있다. 이에 근본적인 오염원을 제거 할 수 있는 방법 중 하나로 광촉매가 떠올랐으며, 특히 실내 거주환경에서 감응 할 수 있는 가시광촉매의 합성 및 성능 평가가 중요해 지기 시작하였으며, 광촉매의 성능 평가를 위해 small chamber 를 이용한 dynamic 분석법과 gas bag 을 이용한 static 분석법을 비교하여 유해 물질들의 정성 및 정량법을 구성하고자 한다.

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SERS based immunoassay using Single Crystalline Gold Nanoplate and Cysteine-tagged Protein G for Detection of C-reactive Protein (CRP)

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C-reactive protein (CRP) is ring shaped, which is a five repeat pentameric protein found in the blood plasma. CRP is used mainly as a nonspecific biomarker for the diagnosis of infection and acute inflammation. Recent research suggests that CRP can be used as a potential risk predictor of cardiovascular disease. In immunoassays, antibody immobilization on a solid support is a vital process. Because it strongly influence the antigen-sensing ability of immobilized antibodies. For highly sensitive detection of CRP, we employ surface enhanced Raman scattering (SERS) sensor based on Au nanoparticles-on-Au nanoplate platform. Particularly, as synthesized single-crystalline gold nanoplate arrays are provided as atomically smooth surface substrate. It can reduce zero-signal extremely due to highly suppressed non-specific bindings. Anti-CRP were immobilized on Au nanoplate using cysteine-tagged Protein G. Protein G is an antibody binding protein, which specifically targets the Fc region of an antibody. And cysteine residues at the N-terminus of protein G can form well-orientation of immobilized antibodies on atomically smooth surface of single crystal Au nanoplate.. By using this platform, being enable to detection of the target biomarkers with sub-fM level of detection limit.

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[발표취소] Copper Nanoparticles Functionalized Conducting Polymer Film Based Electrochemical Immunosensor

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발 표 취 소

본 논문은 발표취소된 논문입니다.

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Stimulated Bienzymatic Catalysis Based Highly Sensitive Quartz Crystal Microbalance Detection of Interleukin-6 in Serum

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충남대학교 분석과학기술대학원 [1]충남대학교 분석과학기술대학원 분석과학기술과

A highly sensitive quartz crystal microbalance (QCM) detection of interleukin-6 (IL-6) in serum based on enormous biocatalytic precipitations of 4-chloro-1-naphthol (CN) using magnetic bead (MB)-supported horseradish peroxidase (HRP) and glucose oxidase (GOx) conjugate was developed. The IL-6 detection was made with a QCM immunosensor, which was fabricated by immobilizing a monoclonal interleukin-6 antibody (anti-IL-6) on a protein A (PA) attached self-assembled monolayer (SAM) of 3-mercaptopropionic acid (MPA)-modified gold coated QCM crystal. The bioenzymatic conjugate was prepared by the covalent linkage of a secondary anti-IL-6 antibody, HRP, and GOx with carboxylic acid functionalized MBs. The QCM IL-6 immunosensor exhibited a linear dynamic range between 1 and 50 pg/mL and a detection limit of 0.6 ± 0.036 pg/mL in serum. The proposed QCM immunosensor could be a promising tool for the detection of IL-6 and other protein biomarkers in serum.

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Pharmacokinetic study of n-butanol extract from Panax notoginseng injection and simultaneous determination of saponins in rat serum using LC-MS

설희진 전승원*

전남대학교 화학과

Five saponins are the main active components of n-butanol extract from Panax notoginseng (PN-BE) and its pharmacokinetics were studied following the oral administration of extract in a rat with doses of 200 mg/kg using liquid chromatography mass spectrometric (LC-MS) method for simultaneous quantification. The five saponins were extracted from rat serum using methanol, and determined by mass spectrometry with negative electrospray ionization (ESI) in the linear concentration range of 6.3-1000 ng/mL with a good correlation coefficient higher than 0.995 and the lower limits of detection (LLOD) less than 2.6 ng/mL. The validated method was successfully applied to investigate the pharmacokinetics of five sponins in a rat after oral administration of ‘PN-BE’ injection. The Cmax and AUC(0-∞) for five saponins were 1.07, 0.21, 0.93, 8.42, and 5.62 ng/mL, and 1.05, 0.79, 0.84, 285, and 316 (h ng/mL), respectively.Keywords: Saponins; Panax notoginseng; LC-MS; Pharmacokinetics; Bioavailability.

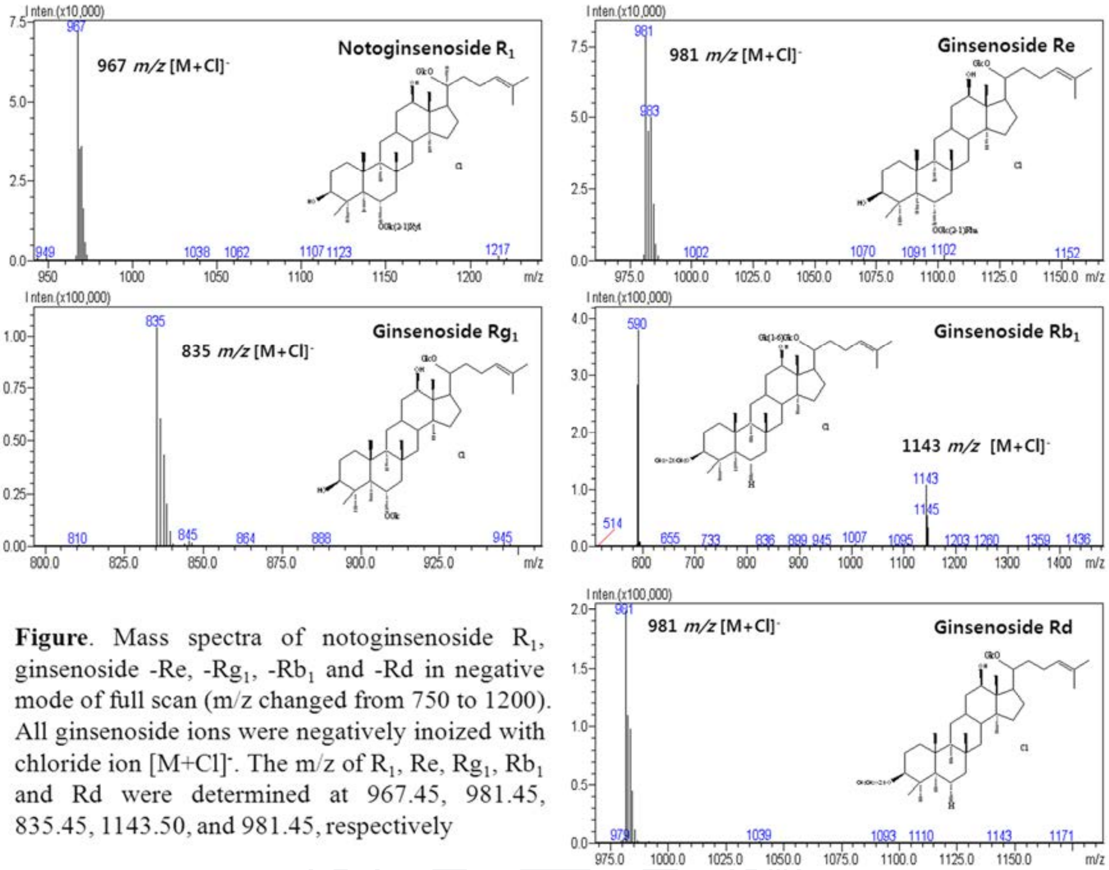

Figure. Mass spectra of notoginsenoside R_1, ginsenoside -Re, -Rg_1, -Rb_1 and -Rd in negative mode of full scan (m/z changed from 750 to 1200). All ginsenoside ions were negatively inoized with chloride ion $[M+Cl]^-$. The m/z of R_1, Re, Rg_1, Rb_1 and Rd were determined at 967.45, 981.45, 835.45, 1143.50, and 981.45, respectively

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Application of FT-IR, ^{1}H and ^{13}C NMR spectroscopy to analyze biodiesel

박은수 오세웅*

목포대학교 화학과

Biodiesel has attracted attention as an alternative to petroleum-based diesel. Two kinds of biodiesels were made from soybean oil and lard with methanol under potassium hydroxide catalyst at 70 oC. FT-IR, ^{1}H and ^{13}C NMR spectroscopy applied to confirm biodiesel, and analyze blended biodiesel with petroleum-based diesel. We present ^{1}H NMR spectra of some vegetable oils, animal oils and fish oils. We also compare the ^{1}H spectra of some fatty acids such as stearic acid, linoleic acid and linolenic acid, and a method to detect ω-3 fatty acid in oils is examined by ^{1}H nmr technique.

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Rapid and sensitive detection of CFP-10 in culture media of *Mycobacterium tuberculosis* with Magnetophoretic immunoassay

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A sandwich-type colorimetric magnetophoretic immunoassay (MPI) is introduced to monitor tuberculosis (TB) antigen, CFP-10, in cultures of *Mycobacterium tuberculosis* (*Mtb*) using nanoparticle complexes of Au nanoparticles (NPs), magnetic microparticle (MMPs), and TB immuno-moieties. The MPI can monitor the target antigen quantitatively and qualitatively within 10 min in the detection range of 10^1 ~ 10^4 pg/mL. Furthermore, the quantitative analysis of the MPI in Mtb culture showed that there was linear relationship between the concentration of the secreted CFP-10 from 10^6 CFU/ml of Mtb and culture time. From these data, it is suggested that the MPI analysis can carry out TB diagnosis within 3~7 days, based on antigen secretion from *Mtb*. These data suggest that our MPI kit is able to be applied in early TB diagnosis through detection of TB specific antigen during culture.

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DSC 샘플 crucible type 에따른 고에너지물질의 열분석결과 비교연구

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고에너지물질의 특성 중 열적특성이 가장 중요하다. 열적특성을 측정하는 가장 일반적인 방법으로는 DSC 를 사용하여 승온속도별로 승온후 이때 얻은 thermogram 의 점을 이용하여 Arrhenius plot 으로부터 활성화 에너지를 구하고, 이 활성화에너지를 다른 열적특성을 계산하는데 적용하여 열적특성을 계측한다. 그리고 일반적으로 에너지물질은 분해서 급격히 분해가스가 발생하는데 이 분해가스를 배출하기 위하여 일반적으로 알루미늄 crucible 에 hole 을 내고 실험을 한다. 최근 연구결과에 의하면 내부압력에 따라 열분해 결과에 많은 차이가 있을 수 있으며, 따라서 생성가스에 의한 내부압력을 견딜 수 있는 내압 crucible 을 적용하면 고압 상태의 열분석 결과를 얻을 수 있다고 알려져 있다. 본 연구에서는 고에너지물질로서 RDX 를 이용하여 샘플 crucible 에 따른 열분석 결과를 비교하였다.

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Comparison of two types utilizing combination antibody and aptamer as binder in sandwich assay

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서울여자대학교 화학과

Sandwich (Two-site immunometric) assay designs have the obvious advantage of increasing the specificity of the assay. To applying sandwich assay, analytes should have multiple epitopes that are sufficiently well spatially separated. However dopamine (DA), small molecule, is not the case. Aptamers as a new binder are artificial nucleic acids such as functional single-stranded oligonucleotides (ssDNA or RNA), which are selected in vitro by SELEX process. From the results of our previous DA assay studies (a competitive assay based on both RNA DA aptamer and its homolog DNA aptamer as bio-recognizers), the better stability and sensitivity was observed with DNA aptamer. Here, we present a sandwich assay for DA by utilizing antibody and aptamer (57mer homolog DNA aptamer) as a new combination binder. Antibody and aptamer are used as capture and detecting binder, or vice versa. In case of using aptamer as capture, it is possible to combination antibody and aptamer without steric hindrance. In inverse study using antibody as capture, we expect a steric hindrance because antibody is larger than aptamer. Two sandwich assay designs are thoroughly examined and compared for the determination of DA and its metabolites. The optimizations in both designs assay were conducted on various conditions. This presentation describes optimized analytical data.

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Synthesize metal/dye-doped silica nanoparticle and metal doped magnetic nanoparticles for the determination of CA15-3 in serum using ICP-MS

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단국대학교 화학과

Nanotechnology is a rapidly progressing technique for bioanalysis. Especially, nanoparticle has been shown to be an excellent tool to investigate various bio-targets such as biomarker, antibiotics, etc. Recently various analytical techniques for bio-targets are introduced. Most of all, Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is known as a highly sensitive and almost interference-free technique, for which metal particles and magnetic nanoparticles are needed. In this work, we synthesized Metal/dye -doped silica nanoparticles for tagging and metal-doped magnetic nanoparticles (MNPs) for target extraction. In particular, the doped metal MNPs was used as an internal standard for the ratiometric measurement of the tagged particle. Various metal/dye doped silica nanoparticle with silica shell, such as Eu/FITC, Gd/FITC, Ce/FITC, Cs/FITC-doped silica nanoparticles, were synthesized by microemulsion method and functionalized with amine groups APTMS. The estimated average number of doped Eu, Gd, Ce and Cs atoms in each nanoparticle were 6.3*103, 1.3*104, 7.5*102, 1.8*104. The LOD of ICP-MS was 1.3*104, particles for Eu, 2.2*105 for Gd, 3.3*104 for Ce, 3.3*103 for Cs when 10μL sample was injected. We also synthesized Cd-doped MNPs and Cs-doped MNPs using St?ber method. The estimated average number of Cd and Cs atoms in each particle was 1.7*103 and 3.8*103, and LOD was 1.6*107 and 8.7*105 respectively, when 10μL sample was injected.With these nanoparticles, we developed analytical technique to determine Carbohydrate antigen 15-3 (CA 15-3) in serum, which is known as tumor marker for breast cancer.

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Analysis of hybride organic compounds on the silica material by using TOF-SIMS

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한국기초과학지원연구원 부산센터 [1]부산대학교 화학과

We have been studied the heliced silica nanotubes via polycondensation of tetraethoxysilane (TEOS) on self-assembled structures that were composed 1,2-diphenylethylenediamine based neutral (G1) and cationic (G1N) gelators. On the other hand, a chiral stationary phase (CSP) prepared by bonding (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid to silica gel was successfully employed in resolving various chiral compounds.In this study, we analyzed helical silica nanotubes and derivatized chiral stationary phases by using TOF-SIMS. We discussed products of each steps for the derivatized organic compound on the silica surface in order to confirm the reactions.

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Electrochemically reduced graphene oxide and chitosan composite modified disposable immunosensors for the detection of sildenafil and vardenafil

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Disposable amperometric immunosensors based on screen-printed carbon electrodes by one-step deposition of electrochemically reduced graphene oxide/chitosan (ErGO-CS) composite were developed. The sensors developed were applied for the sensitive detection of viagra drugs namely sildenafil and vardenafil (SDF/VDF, phosphodiesterase type 5 enzyme inhibitors) based on a non-competitive sandwich type enzyme immunoassay format by using horseradish peroxide (HRP) as an enzyme label. The sensors developed, for the first time, were successfully demonstrated for the determination of SDF/VDF. Electrochemical impedance spectroscopy, cyclic voltammetry and amperometry were used to evaluate and confirm the electrochemical characteristics of the sensors as well as all the experimental parameters such as optimum pH and operation potentials will be presented in the poster. The sensors showed a good linear response SDF/VDF concentrations ranged from 10 pgmL-1 to 100 pgmL-1 and LOD was found to be 0.2 pgmL-1. The proposed sensing chemistry strategy and the sensor format could be used as a simple, cost-effective, and potent method for the in-field or in-situ analysis of SDF/VDF in clinical and designed food samples.

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Charaterization of N-linked and O-linked glycans in Darbepoetin alfa(NESP) by MALDI MS/MS

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Glycosylation of two major types of glycosylation, N-linked and O-linked, are both involved in the maintenance of protein conformation and activity, in protein protection from proteolytic dgradation, and in protein intracellular trafficking and secretion. Glycosylation is an important feature of biosimilar product as it has been shown that the type and degree of glycosyltion affects protein drugs treatment efficacy, vivo persistence, targeting, and immune response. In this study, N-linked glycans are released using PNGase F and are fractionated by Porous Graphitized Carbon column(SPE) for glycans extration. Quantitative permethylation of glycans involves packing of sodium hydroxide beads in microspin columns. Analytes are mixed with methyl iodide in dimethyl sulfoxide solution containg traces of water before infusing through the microreactors. The permethylated sialylated glycans were analyzed by MALDI TOF/TOF MS and MALDI QIT/TOF MS/MS.

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Nuclear Magnetic Resonance Methods to Measure Site-Specific Isotope Population of Deuterium-Enriched Solute in Natural Solvent

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충남대학교 분석과학 [1]한국기초과학지원연구원 서울서부센터

Deuterium is one of hydrogen isotopes. The presence of naturally abundant deuterium (~0.015%) in solvent is typically ignored in nuclear magnetic resonance (NMR) spectroscopic data interpretation. Here, we show a case in which the presence of naturally abundant deuterium in solvent should be considered, especially when the concentration of deuterium-enriched chemicals is varied. In this study, a simple isotope-enriched alcohol, CD3OH was prepared solutions of various concentrations which are used to measure site-specific isotope impurities in isotope-enriched samples and the natural abundance of the isotope. As the concentration of aqueous CD3OH solutions was decreased, the OD peaks in 2D NMR spectra grew relative to the CD3 peaks. Using the two different fitting methods, we confirmed that these results were caused by isotope impurity for OH groups of CD3OH and deuterium naturally present in water contributed to the OD peaks.

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Sensitivity Enhancement in SPR Sensors Based on Layer-by-Layer Self-Assembled Graphene Oxide and Reduced Graphene Oxide Layers

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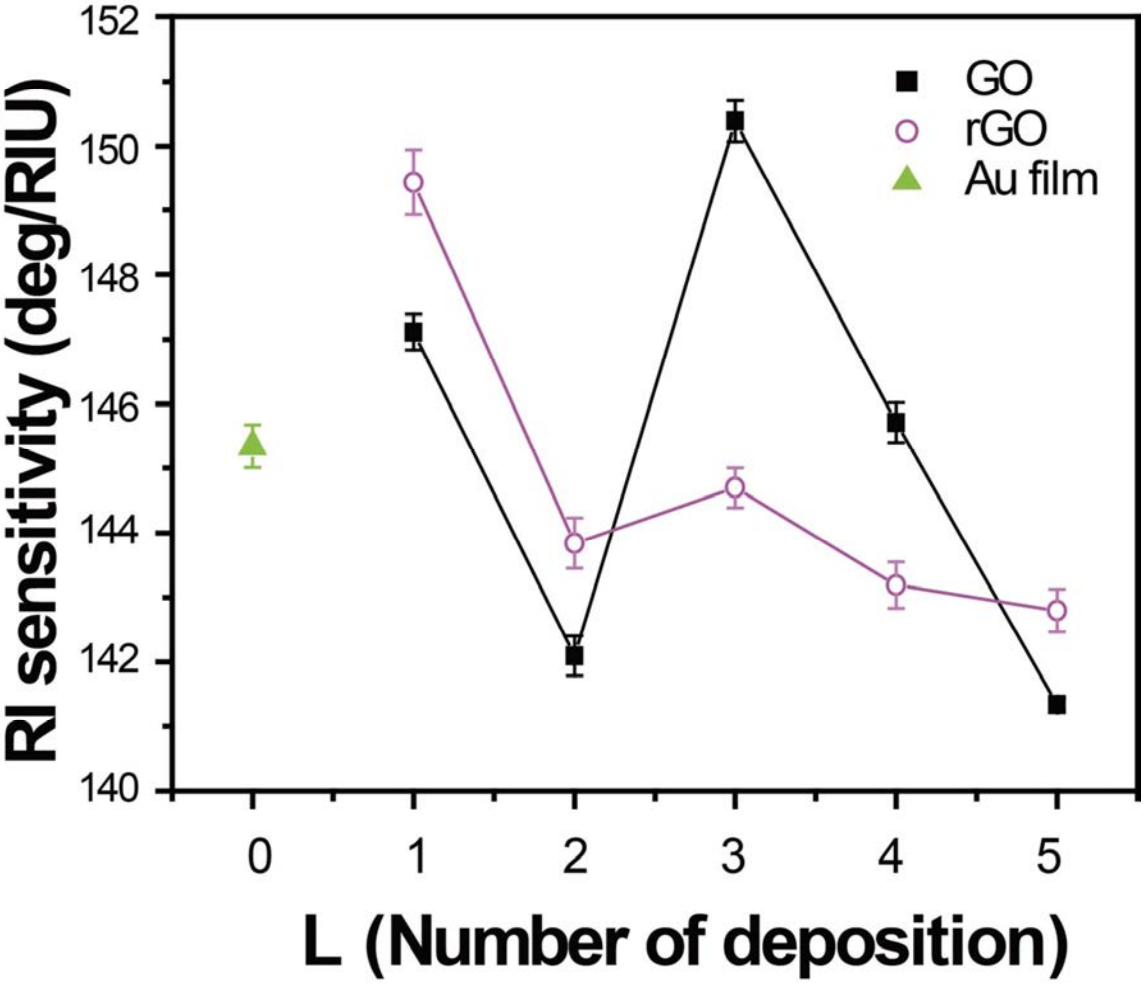
Graphene and its derivatives have been investigated extensively during the last decade because of their excellent thermal, mechanical and electric properties. Graphene also possesses very unique optical properties due to the linear dispersion relation and Dirac fermions in graphene act as massless particles. Thus these unique graphene plasmons can interact effectively with the incident photons. The use of graphene in conventional plasmonic devices has been suggested in several theoretical researches. In this work, graphene oxide (GO) and reduced graphene oxide (rGO) were introduced in SPR sensors in order to examine the coupling effect between graphene plasmons and propagating surface plasmons in Au film. GO and rGO films were deposited on Au films by layer-by-layer self-assembly method and their refractive index (RI) sensitivity was compared in SPR-based sensors. GO and rGO-deposited Au films showed different aspects in RI sensitivity: GO-deposited samples showed maximum sensitivity when the number of deposition was three while the RI sensitivity of rGO samples decreased with increasing number of layers. The biosensing activity was also performed for the graphene multilayer systems with mass sensitivity of 1.43 ng mm^{-2}.


RI sensitivity (deg/RIU)
152
150
148
146
144
142
140
0
1
2
3
4
5
L (Number of deposition)
■ GO
○ rGO
▲ Au film

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Quantitative analysis of potassium diphenylsulfone sulfonate in polycarbonate by high-performance liquid chromatography

김혜림

삼양바이오팜 분석센터

Polycarbonate(PC) is an engineering plastic that is widely used in many fields such as automobile, electrical and electronic devices and machinery. Many of these applications require a high degree of flame retardancy.As a halogen free flame retardant, potassium diphenylsulfone sulfonate(KSS) is the potassium salt of a complex of diphenyl sulfone sulfonate and diphenyl sulfone disulfonate. KSS is able to provide remarkable flame retardant performance for polycarbonate at a very low loading level, typically less than 1% by weight in a PC formulation.In this study, we have developed an high-performance liquid chromatography (HPLC) method for the quantitative analysis of KSS in PC. Chromatography was performed using Xterra C18 column with MeOH/ 10mM phosphate buffer (pH3.0) = 40:60 mobile phase at 1mL/min in isocratic condition. And wavelength was set at 235 nm. This method was shown to be a sensitive and precise tool for the quantitative determination of KSS.

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Characterization of biodegraded petroleum by comprehensive 2D gas chromatography and FT-ICR mass spectrometry

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The bioremediation method is one of the primary ways for degradation of oil spill pollutants by microorganisms. The Pseudomonas taeanensis sp. nov. MS-3 (P.taeanensis MS-3), isolated from a crude oil contaminated seashore in South Korea, has been reported as oil-degrading bacterium. In this study, the P.taeanensis MS-3 was applied to two petroleum derivatives and two crude oils. The P.taeanensis MS-3 strain was inoculated into media containing 0.3% of respective oil samples and incubated at 28℃ for 7 days on a rotary shakes at 170 rpm. The oil components from the media were extracted with toluene. The comprehensive two dimensional gas chromatography with flame ionization detector (2D-GC/FID) and atmospheric pressure photo ionization (APPI) coupled with 15T fourier transform ion cyclotron resonance mass spectrometry (15T FT-ICR MS) were employed to compare chemical composition changes as well as relative degradation rates. As a result, the alkane and ring compounds were mainly detected in extracts by 15T FT-ICR MS. The 2D-GC/FID analysis showed that the percentages of degradation for diesel, kerosene, basrah crude oil and murban crude oil are approximately 11.9 %, 31.3 %, 41.5 % and 53.4 % respectively.

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Light Emitting Diodes as a Photo Transducer in Spectrophotometry

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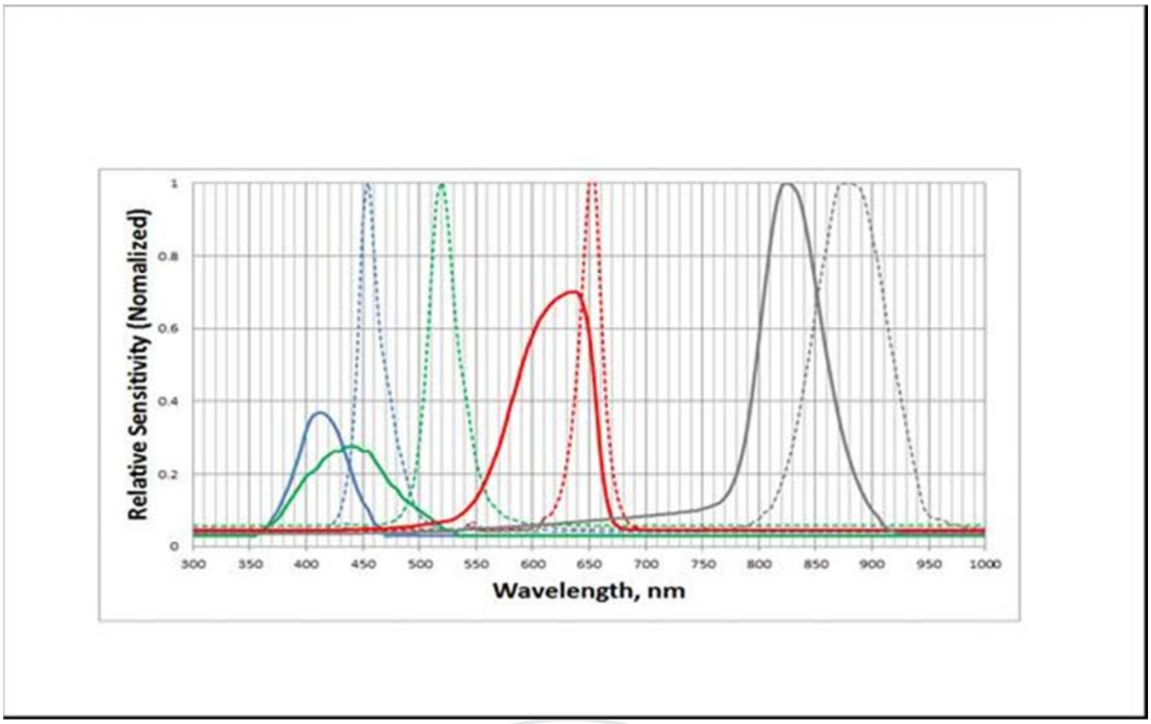
Light emitting diodes (LEDs) can be used as a photo transducer in optical measurements (i.e. absorbance and fluorescence measurements) even though they have been mostly used so far as a solid state light source in analytical chemistry. Generally speaking, a LED is sensitive to the same wavelength of light which the LED emits. Recently, Shin et al. used a pair of LEDs to be used in absorbance measurement using this principle; a red LED was a light source and the other red LED was used as a photo transducer. However, it is well known that different photo sensors showed different sensitivity to different wavelength. Therefore, It still needs to characterize LEDs in terms of relative sensitivity to the same range of wavelength (especially, IR to visible region). In this report, two pairs of LEDs (i.e. red-red LED and blue-green LED pairs) were used to analyze the mixture of two common indicator dyes (i.e. bromothymol blue and methyl orange) based on these LED characterization data. The green LED was used instead of a blue LED due to the fact that a longer wavelength emitting LED showed relatively higher sensitivity if two LEDs are sensitive somewhat to the same wavelength. Next, a red LED was used to register fluorescence of Rhodamine B which was excited by the illumination of a red LED. There was no need to use an additional optical filter in front of the detector LED due to the LED's intrinsic optical filtering capability. A calibration curve was obtained for the concentration range of 0.1 ? 10 μM.


Relative Sensitivity (Nomalized)
1
0.8
0.6
0.4
0.2
0
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
Wavelength, nm

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[발표취소] Sampling and Determination of Formaldehyde Using Solid-Phase Micro Extraction with Derivatization

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대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

발 표 취 소
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Development of Acute Oral Rat Toxicity Prediction Model with Applicability Domain Using QSAR Analysis

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(사)분자설계연구소 소재개발팀 [1](사)분자설계연구소 소재설계팀 [2]연세대학교 생명공학과

Quantitative prediction of oral toxicity study in rats studied by quantitative structure-activity relationship (QSAR) models based on the multivariate data analysis. The LD_{50} oral toxicity data of organic compounds on rats was used for modeling. 7205 LD_{50} data was collected from ChemIDplus database and E.P.A. TEST (Toxicity Estimation Software Tool) example set. The half of the entire data set was used for training the model and the rest were used for external validation set. To find optimal descriptors set, forward descriptor selection and bootstrapping internal validation was applied on the modeling. The machine learning methods such as multiple linear regression and support vector machine analyses were performed using the various molecular descriptors and consensus model of each models were used for improvement on the performance. The performance of the model evaluated by root mean square error (RMSE), mean absolute error(MAE) and squared correlation(r^2). The applicability domain(AD) of the model indicated by structural similarities in the training data set which used for modeling. The result of this model show lower error than other *in sillico* models for prediction of oral rat LD_{50} in the AD. The toxicity prediction on the computational method can be helpful on the prioritization on the toxic compounds reduce laborious task on the toxic chemical candidate.

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Identification of lipids from muscle tissue of mice using nanoflow LC-ESI-MS/MS

이종철 변슬기 문명희*

연세대학교 화학과

Responsible for various functions such as energy storage, cell signaling, and apoptosis, lipids are related with development of many different types of human diseases such as diabetes. Different types of factors cause such diseases but lack of exercise has been reported as one of the major risk factors that are correlated with many types of diseases. In this study, lipids from muscles of the lower limb of healthy mice, healthy mice under exercise, diabetic mice, and diabetic mice under exercise were investigated in order to characterize lipid species that show significant difference between healthy and diabetic mice, and changes in lipid distribution brought by exercising in order to see its effect on healthy and diabetic individuals. As each type of muscle play a different role, two types of muscle tissues, gastrocnemius and soleus, were examined. Muscle lipids were extracted from each sample using the modified Folch with MTBE/MeOH, and then the extracted lipids were identified by nanoflow liquid chromatography electrospray-ionization tandem mass spectrometry (nLC-ESI-MS/MS). A total of 291 and 299 species from gastrocnemius and soleus of healthy mice, respectively, were identified, and higher concentrations of lysophospholipids were detected in soleus than gastronecmius, whereas similar concentrations of phospholipids, neutral lipids, and sphingolipids were observed.

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Development of nanotoxicity prediction model for various silver manufactured nanoparticles

김광연* 신성은[1] 노경태[2]

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Efforts of developing toxicity prediction models for silver manufactured nanoparticles(Ag-MNPs) are introduced. Target materials were chosen with variations of size, coated materials, and the definite shapes (nanoparticles and nano-wires). With collected toxicity data both from previous literatures and public databases, filtration and scaling was performed for developing quantitative nano-toxicity relationships(QNTR). About 20 nano-descriptors mainly from quantum chemical methods were selected and evaluated for Ag-nanomaterials and its coated materials, and the featured relationships were suggested with validation. This subject is supported by Korea Institute of Toxicology (KIT) as "Foundation Construction for Evaluating Environmental Risk Assessment of Manufactured Nanomaterials".

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Analysis of volatile organic compounds with headspace in-tube microextraction/capillary electrophoresis

조성민 정두수*

서울대학교 화학부

Headspace (HS) extraction is a 3-phase extraction technique from a sample donor phase to a HS above the donor then from the HS to an acceptor phase. HS extraction is fit for volatile/semi-volatile compounds in a complex matrix. Recently, HS single drop microextraction (SDME) has been demonstrated using a drop of an acceptor phase hanging at the inlet tip of a capillary for the subsequent capillary electrophoresis (CE). However, it is difficult to hang a drop of very small volume in the HS of high temperature stably for a long extraction, and we introduced a novel and simple scheme of HS extraction, HS in-tube microextraction (ITME). Without hanging a drop, the liquid inside a separation capillary for CE is used as an acceptor phase. HS-ITME-CE was first demonstrated in the analysis of chlorophenols in wine. As a second application of HS-ITME, neutral organic pollutant such as BTEX (benzene, toluene, ethyl benzene, and xylene) is extracted from an aqueous sample to a surfactant solution inside a separation capillary. The extracts were then analyzed with a micellar electrokinetic chromatography mode of CE. At the optimal conditions, the sample were enriched to 350 on average.

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Direct Detection of Metal-binding Proteins from Blood Plasma Samples Using Chip-type Flow Field-Flow Fractionation Coupled with Inductively Coupled Plasma Mass Spectrometry

김진용 장하나[1] 임흥빈[1] 문명희*

연세대학교 화학과 [1]단국대학교 화학과

Selective analysis of metals in biological systems is an emerging research field and is important to understand the biological processes such as signal transduction, nerve transmission, and metabolic pathways. Approximately one third of all proteins and enzymes contain metal cofactors or metalloid ions in their structures, but many of the critical roles of these metal ions remain unknown. Many types of metalloproteins are reported to be potential biomarkers of diseases and as they exist in extremely low amount in biological samples, separation and detection with high sensitivity needs to be pursued in a research field of metallomics. Flow field-flow fractionation (FlFFF) is widely used to separate macromolecules, nanoparticles, micro-particles, and colloids according to their hydrodynamic size. In this study, on-line chip-type FlFFF channel coupled with inductively coupled plasma mass spectrometry (cAF4-ICP-MS) was used to profile metalloproteins from human blood samples. This hyphenated method not only separates proteins or other biological particles by size, but also on-line purification of proteins can be simultaneously achieved. Five different types of standard metalloproteins, ranging from 29 to 669 kDa, were analyzed by cAF4-ICP-MS and cAF4-UV detector, and peak shapes and their retention times were compared to validate the method of cAF4-ICP-MS. Also, human blood plasma samples were analyzed by cAF4-ICP-MS to evaluate the distribution of metalloproteins.

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발표코드: **ANAL.P-549**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Cyclosophoraose-β-Cyclodextrin Heterodimer as a Novel Complexation Agent

정다함 윤덕규 정재필[1] 정선호[2,*]

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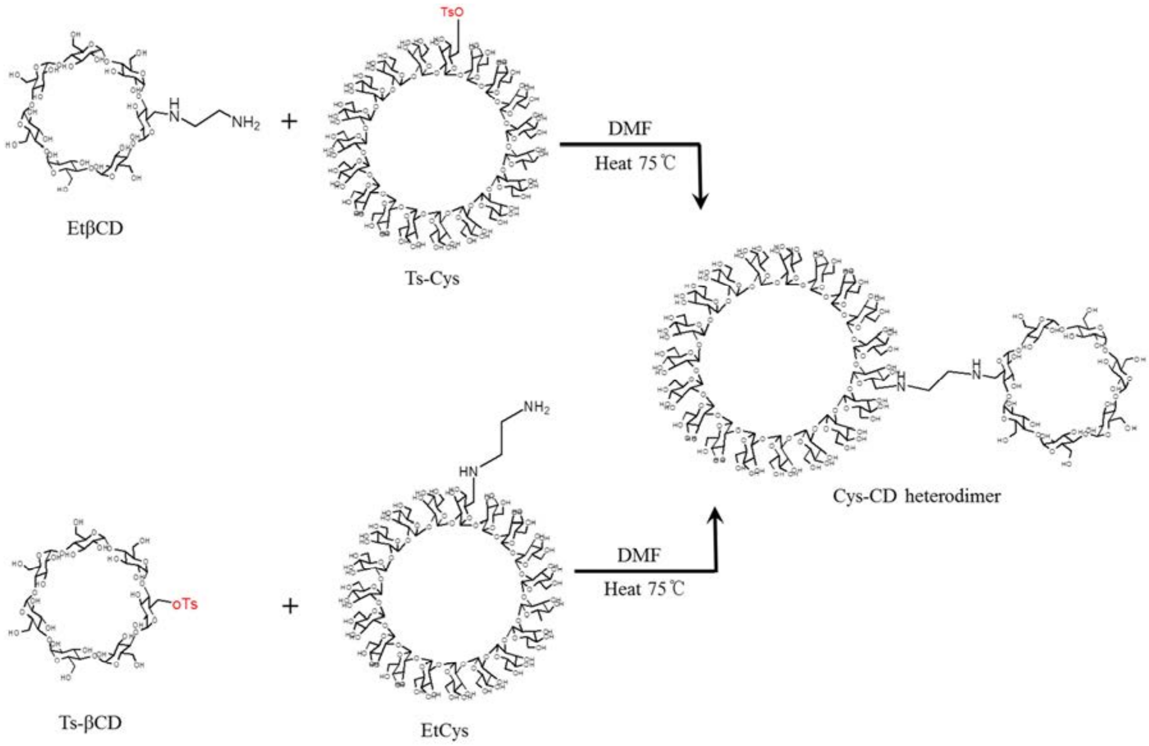
Cyclosophoraoses (Cys) produced from Rhizobium species are cyclic β-(1,2)-glucans containing between 17 and 23 glucose units, and β-Cyclodextrin (βCD) is a seven-membered cyclic β-(1,4)-glucan produced from starch by enzymatic conversion. They are known as a useful complexation agent for various application fields. In this study, the novel Cys-βCD heterodimer was synthesized by mono tosyl-Cys (Ts-Cys) reacting with mono ethylenediamine modified βCD (EtβCD) and mono ethylenediamine modified Cys (EtCys) reacting with mono tosyl-βCD (Ts-βCD). The yield of TS-Cys reacting with EtβCD is 10 times higher than Et-Cys reacting with Ts-βCD. We isolated and purified the Cys-βCD heterodimer by cationic exchange and size exclusion chromatographic techniques. Its structure was confirmed via nuclear magnetic resonance (NMR) spectroscopy and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry analysis. Since the Cys-βCD heterodimer has two different cavities or complexation ability, it is expected as an efficient host for chemo-sensors and solubility/bioavailability enhancer of natural compounds comparing with the original βCD and Cys.


TsO
EtβCD
Ts-Cys
DMF
Heat 75℃
NH2
HN
NH
Cys-CD heterodimer
oTs
Ts-βCD
EtCys
DMF
Heat 75℃

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Determination of Metallic Impurities in Buffered Oxide Etchant Solution by Using Inductively Coupled Plasma mass spectrometry(ICP-MS)

손경진 김영현 정아롱 임흥빈*

단국대학교 화학과

In this work, we studied the determination of metallic impurities in Bufferd Oxide Etchant solution using ICP-MS after matrix removal and analyte preconcentration using a carbon heating block with PFA vessels. Since it is critical to detect amounts of metal elements in the manufacturing semiconductor industry, the development of analytical methods with high sensitivity and reproducibility were urgently required. A variety of parameters (xy-position of the torch, rf power, carrier gas flow, Spray chamber temperture)were optimized to achieve the best limits of detection (LOD). Using the treatment system, the preconcentration factor of 2 was obtained. For recovery test, twenty one elements (Li, Be, Na, Mg, Al, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, As, Sr, Ag, Cd, Ba and Pb) were selected and spiked to BOE solution. Our results show that the recovery rates of twenty one elements are within the range of 64~158%. Recoveries of K, Ca and Fe were poor due to the polyatomic interference, which were measured by CID mode. Detection limits of all elements in 2% HNO3 matrix solution are less than 100 ppt in 2% HNO3 matrix solution. The use of internal standards(In) and standard addition were essential to obtain precise and accurate analytical results.

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Affinity Chromatography: Displacement Phenomena In Serial Lectin Affinity Chromatography

신지훈 조원련[1,*]

원광대학교 바이오나노화학부 [1]원광대학교 생명나노화학부

Affinity chromatography systems are becoming increasingly important as tools in the enrichment, identification, and quantification of proteins. Quantification between disease and healthy samples using affinity chromatography reveals disease-related proteins in disease biomarker discovery. However, a challenge in affinity chromatography is to capture affinity-selected proteins with reproducibility. Although all the glycoprotein species bearing a particular glycan feature are captured by an affinity column, there is no guarantee whether the same glycoproteins will appear in the next experiments with the same amount. Further disease-related proteins are frequently low abundant proteins which are easily suppressed by abundant proteins during mass analysis. The work being described here examines the utility of serial lectin affinity chromatography in understanding how to get affinity binding proteins with reproducibility and how to enrich low abundant, disease-related, and weakly bound proteins. Four serial Agarose-bound Lycopersicon esculentum lectin (LEL) affinity columns, the LEL1 → LEL2 → LEL3 → LEL4 series, were examined in order to investigate the displacement phenomena; glycoproteins with higher binding affinity displace those of lower binding affinity. The great advantage of this method is that it differentiates binding proteins to LEL according to their binding affinity. Thus serial lectin affinity chromatography (SLAC) will be a valuable tool for the recognition of displacement phenomena in affinity chromatography.

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Green synthesis of silver nanoparticles using Lotus root extract and study their antioxidant and cytotoxicity activities

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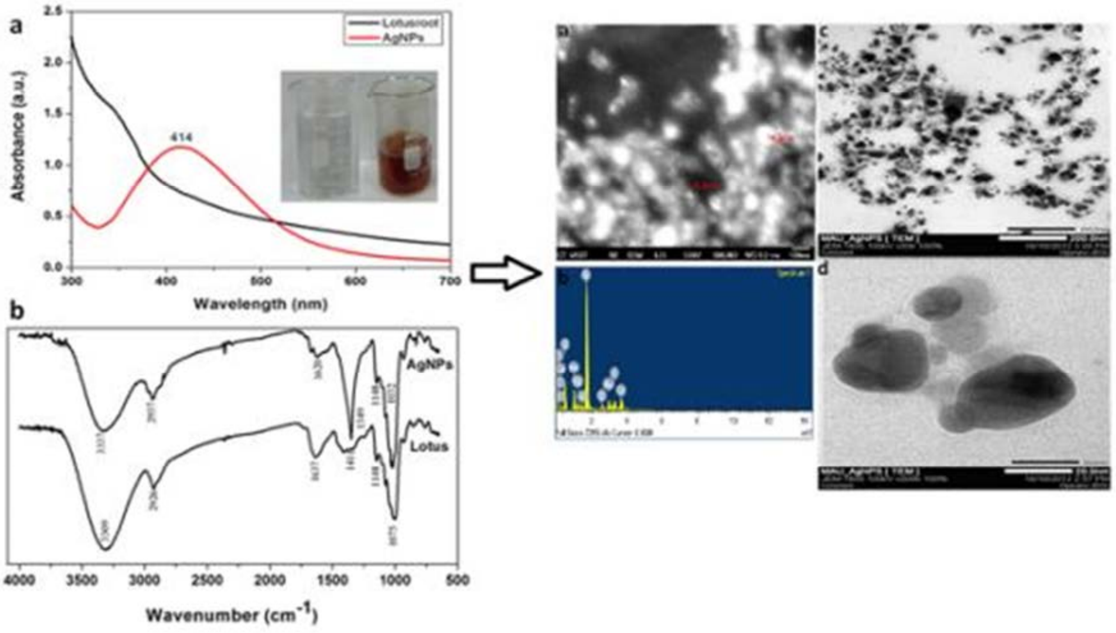
대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

In the present study, silver nanoparticles (AgNPs) with the average particle size of ~16.7nm were synthesized using eco-friendly reducing material (i.e. aqueous Nelumbo nucifera root extract). Rapid reduction results in the formation of polydispersed particles. The formation of AgNPs was characterized by surface plasmon resonance (SPR) which was determined by UV-Vis spectra (band at 412 nm), SEM-EDX, TEM and XRD. A possible mechanism involved in the reduction and stabilization of nanoparticles has been investigated using Fourier transform infrared spectroscopy (FT-IR) and Raman spectroscopy. In addition, AgNPs showed moderate antioxidant activity and excellent cytotoxicity against HeLa cell lines.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Differentiated Recognition of Structural Isomers α and β-Naphthoflavone by Synthesized β-cyclodextrin Dimers

최재민 정다함 Jae-Hyuk Yu[1] 정선호[2,*]

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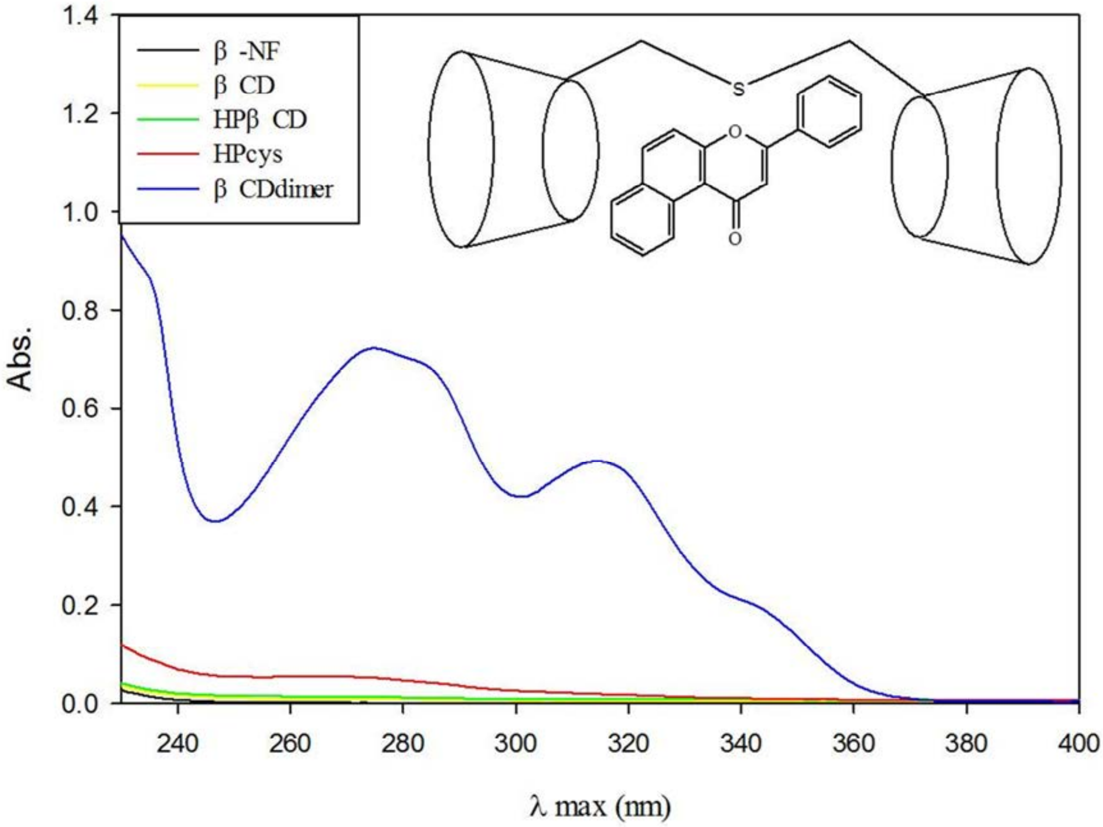
The structural isomers of α and β-naphthoflavones have distinctive functions with small structural differences. β-cyclodextrin dimers has been investigated for recognizing the structural isomer α and β-naphthoflavones. The differentiated recognizing ability of β-cyclodextrin dimers toward α and β-naphthoflavones was monitored by UV vis spectrometry. Because of the distinguished association of naphthoflavone isomers with β-cyclodextrin dimers, the solubility enhancement efficiency of two naphthoflavones by β-cyclodextrin dimers showed huge difference. In the presence of by β-cyclodextrin dimer, the solubility of α-naphthoflavones was increased 26 fold of its native solubility whereas the solubility of β-naphthoflavone dramatically increased up to 469 fold. The physicochemical properties of α and β-naphthoflavones and their carbohydrate complexes were characterized by Fourier-transform infrared spectra and differential scanning calorimetry. Scanning electron microscopy data showed the morphological structure changes of native α and β-naphthoflavones and their complex with novel carbohydrate-solubilizers. Based on these results, β-cyclodextrin dimer successfully recognizes structural isomer α and β-naphthoflavones and is also able to form an efficient complex with α and β-naphthoflavones, suggesting the potential usage of β-cyclodextrin dimer as isomer separating agent.


1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Abs.
240
260
280
300
320
340
360
380
400
λ max (nm)
β -NF
β CD
HPβ CD
HPcys
β CDdimer
S
O
O

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An investigation on the elemental speciation of As with ion chromatography coupled with inductively coupled plasma atomic emission spectrometry

박은수 최성 남상호*

목포대학교 화학과

Extraction and determination of total arsenic and arsenic species in seaweeds and seafoods were investigated. The toxic and biological effects of arsenic species depend on the different chemical forms in a sample. In this study, two kinds of separator columns were used for the separation of arsenic species in seaweeds, and the separation chromatograms were completely different for the five arsenic species. Anion separator column (AS-7 column) could not separate the five arsenic species while the other column (PRP-X100 column) separated them in seaweeds. The two columns could separate five arsenic species in standard solutions. The matrix in a seaweed made an adverse effect on the separation of the arsenic species when the AS-7 column was used.The developed method for the quantitative determination of As species included the selective extraction method, the optimization of the separation and detection method, and all the important instrumental and methodological parameters. The prevention of loss and transformation of As species was confirmed with the developed extraction and analytical method. Good reproducibility and recovery efficiency of As species with the selected extraction method were also obtained. In this study, seafoods (snow crab, red snow crab, octopus, octopus minor and squid) and seaweeds (red laver, green laver, sea tangle, sea mustard and hizikia) were investigated with the analytical method. All the samples were dried and ground to a fine powder. The main As species in seafoods was the non-toxic arsenobetain (AsB), and the highest concentration was found in the red snow crab (152 ± 4 mg/kg, dry weight). Other As species (As^{3+}, As^{5+}, monomethylarsonic acid (MMA) and dimethylarsinic acid (DMA)) were not detected in seafoods. The major As species in a hizikia was As^{5+}, and its concentration was 34.0 ± 0.4 mg/kg (dry weight). The As species (As^{3+}, As^{5+}, MMA, DMA and AsB) were not found in a green laver, sea tangle, red laver and sea mustard.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Label-Free DNAzyme-Cleaved Plasmonic Nanowire Interstice Sensor for UO_2^{2+} Detection

곽래근 김홍기[1] 김봉수*

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

Nowadays, nuclear power based on radioactivity is widely used in power plant and medical fields. However, the over-exposure of radioactivity to human beings or natural environment cause a fatal damage such as mutation and cancers. Uranium is a one of typical radioactive molecule which is widely used and formed as a UO22+ in water. Therefore, highly sensitive, selective and accurate detection of uranyl ion is very important for the estimation of health risks and environmental protection. Several uranyl ion detection methods was reported but, most of them require complicated instrument resulting in time-consuming procedure and remain a challenge with high sensitivity and selectivity, and low cost. Recently, DNA enzyme cleavage reaction has been shown to be applicable to form of metal ion. In this study, we present a sensitive and selective single nanowire on film SERS sensor for UO22+ detection that relies on DNA-zyme cleavage reaction. We expected that our Au NW SERS sensor for UO22+ detection can be employed for the practical sensing and monitoring of UO22+ in uranium-polluted environment.

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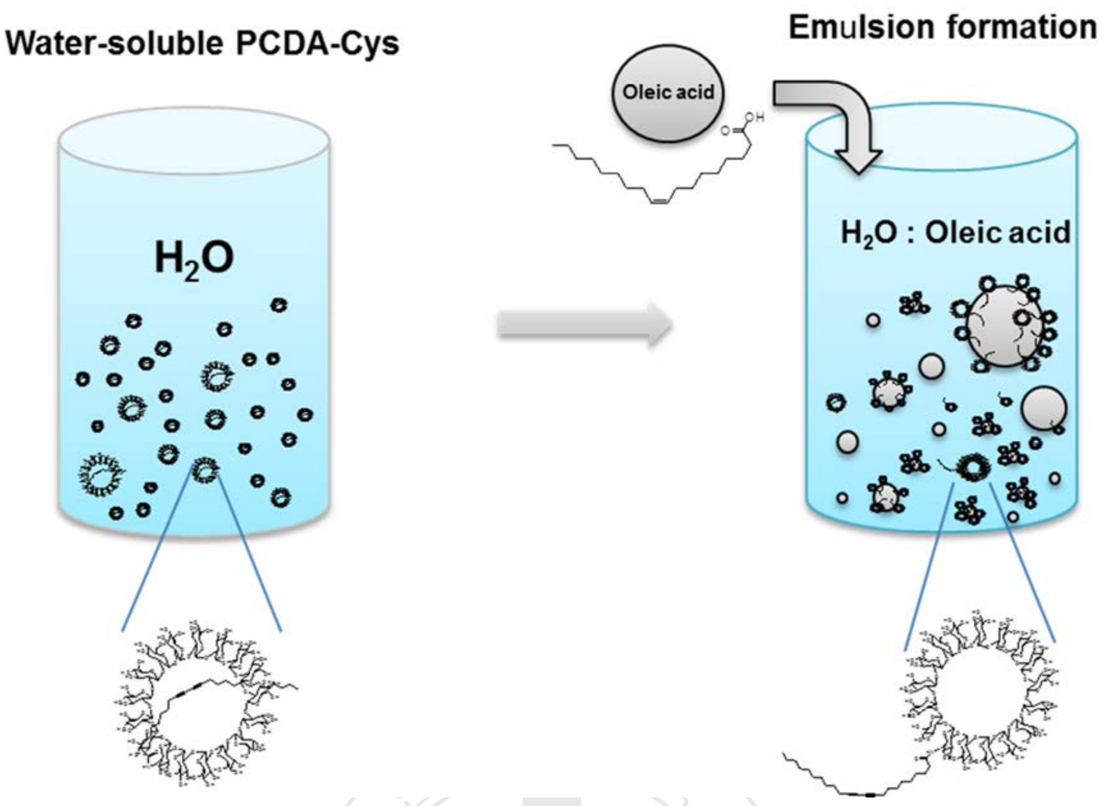
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, characterization and potential as novel surfactant of pentacosa-10,12-diynyl amidomethyl-cyclosophoraose

김환희 박경현[1] 조은애[2] 정선호[3,*]

건국대학교 생명공학 [1]건국대학교 특성화학부 [2]건국대학교 유비쿼터스정보기술연구원 [3]건국대학교 특성화학부 생명공학과

Cyclosophoraose (Cys), cyclic-(1→2)-β-D-glucans produced by *Rhizobium leguminosarum* biovar *viciae* VF-39, were modified by the *N*-hydroxysuccinimide ester of 10, 12-pentacosadiynoic acid (NHS-PCDA). The structure of PCDA-Cys was characterized using 1D, 2D nuclear magnetic resonance spectroscopy (NMR) and matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS). 2D NMR spectrum revealed that the PCDA moiety of the amphiphilic Cys was located in the cavity of Cys in water. However, the PCDA moiety is stretched out of the cavity in water and oleic acid mixture. In this condition, the potential of the PCDA-Cys as a novel emulsifier was examined through dynamic light scattering (DLS), optical microscopy, and contact angle measurement. DLS results exhibited no significant changes in the size distribution during incubation for 25 days at room temperature. Reduction of surface tension indicating the presence of surfactant reached a value of 41 mN/m at the end of 24 hours. This study demonstrates that PCDA-Cys is a candidate of emulsifying material for food, cosmetics and pharmaceutical industries.


Water-soluble PCDA-Cys
H_2O
Emulsion formation
Oleic acid
OH
O
H_2O : Oleic acid

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Determination of vanadium species by Ion Chromatography coupled with Inductively Coupled End-on-Plasma Atomic Emission Spectrometry

박은수 박민영 남상호*

목포대학교 화학과

Extraction and determination of total vanadium (V) and V species in various samples were performed. The toxic and biological effects of V species depend on the different chemical forms in a sample. Acid digestion and microwave digestion methods were investigated for the extraction of total V. Ethylenediaminetetra acetic acid (EDTA) and sulfuric acid were also studied for the extraction solvent of V species. For the separation of V (IV) and V (V), the composition and flow rate of the eluent (EDTA, Tetrabutylammonium phosphate (TBAP) and methanol) were investigated and optimized with the ion chromatography. The separated V species were detected by inductively coupled end-on-plasma atomic emission spectrometry. The stability of the V species was affected by the sample pH. The V species in a V-enriched apple was V (IV), and its concentration was 0.61 mg/kg.

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Glycopeptide Analysis of EPGs and PGIPs by Liquid Chromatography Mass Spectrometry

김상진 서현경 임재민*

창원대학교 화학과

Polygalacturonase inhibiting proteins (PGIPs) are members of the leucine rich repeat family of proteins, involved in plant defense against fungal pathogens. PGIPs exhibit a remarkable degree of specificity in terms of their ability to bind and inhibit their target molecules, the endopolygalacturonases (EPGs). This specificity has been attributed for certain EPG/PGIP combinations to differences in primary sequence, but this explanation is unable to account for the full range of binding and inhibitory activities observed. In this study, we focused on the analysis of glycopeptide of EPGs and PGIPs after incubation the glycoprotein with trypsin by liquid chromatography mass spectrometry (LC-MS^n). The recent development in mass spectrometry such as multiple dissociation techniques (CID and ETD) enables detailed structure determination of the glycopeptide. The LC-MS^n glycopeptides analysis provides glycosylation sites and site-specific glycan structural information.

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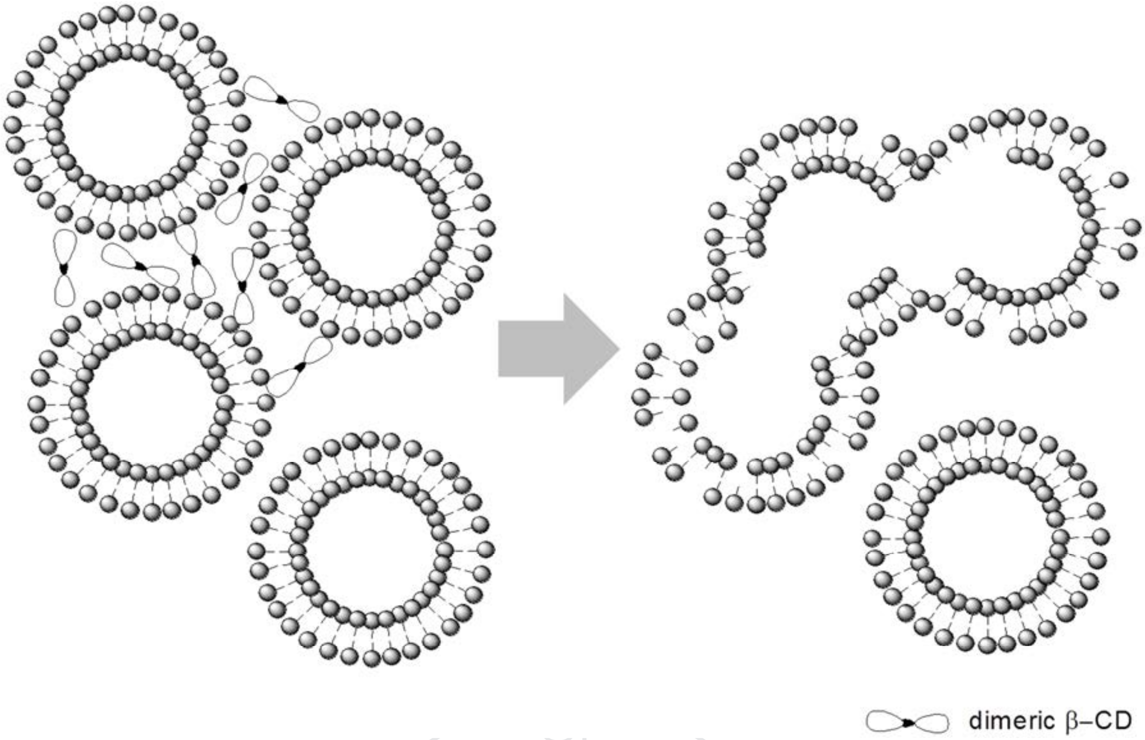
Liposome distruption by dimeric β-cyclodextrin studied with polydiacetylene colorimetric vesicles

조은애 최재민[1] 정다함[1] 전봉현[1] 정선호[2,*]

건국대학교 유비쿼터스정보기술연구원 [1]건국대학교 생명공학과 [2]건국대학교 특성화학부 생명공학과

Dimeric β-cyclodextrins (β-CD) were synthesized by the reaction of native β-CD with epichlorohydrin under basic conditions. We have investigated the effects of dimeric β-CD on the diacetylene and polydiacetylene liposomes. The vesicular diacetylene was distrupted in the presence of dimeric β-CD with the consequent inhibition of polymerization. The result might be attributed to the formation of a complex between dimeric β-CD and diacetylene liposomes, and it was clearly differentiated from that of monomeric β-CD. Furthermore, the ordered supramolecular structure of polydiacetylene was perturbed by the dimeric β-CD, which was detected from the visible color change. Finally, the morphological characteristics and size of polydiacetylene in the absence and presence of dimeric β-CD were examined using transmission electron microscopy and dynamic light scattering. The results show fused structure of size more than 200 nm along with the deformation of the vesicles, and they represent a novel phenomenon of liposome structure induced by complexation with dimeric β-CD. The evaluated physicochemical characteristics can be applied to the development of carbohydrate-based surfactants.


dimeric β-CD

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Determination of polyphenol in the fruit of chokeberry (*Aronia melanocarpa*) by using liquid chromatography-tandem mass spectrometry: overall contribution to antioxidant activity

송이 신성철*

경상대학교 화학과

Black chokeberry (*Aronia melanocarpa*) belongs to the Rosaceae family, which is native to North America. Its dark berries are similar to black currents with a very astringent flavor and have been used by Native Americans both as a food resource and as traditional medicine for treatment of the cold. Epidemiological studies have demonstrated that chokeberry provides positive effects on colorectal cancer, cardiovascular diseases, and various inflammatory conditions. The principal objective of the present study was to characterize polyphenol component in *Aronia melanocarpa* using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) with selected ion monitoring (SIM).

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In situ handwritten document analysis by using nanospray desorption electrospray ionization (nano-DESI) mass spectrometry

이광빈 차상원*

한국외국어대학교 화학과

Typical ink chemical analysis of a handwritten document includes paper sampling with a micro-punch, chemical extraction, and chromatographic or mass spectrometric analysis. Recently, mass spectrometric ionization methods such as desorption electrospray ionization (DESI), electrospray-assisted laser desorption/ionization (ELDI), and matrix-assisted laser desorption/ionization (MALDI) were utilized as in situ sampling techniques and interfaced with mass spectrometry (MS). In this study, we utilized nanospray desorption electrospray ionization (nano-DESI) MS as an in situ document ink analysis platform. Nano-DESI is one of the extractive ambient ionization methods developed by Julia Laskin in 2010. Since nano-DESI utilizes steady-state micro-liquid junction formed between two capillaries for extracting analytes, this method allows us to extract ink chemicals at a high spatial resolution and also has a potential of depth-profiling. We could get characteristic chemical profiles directly from handwritings on a paper with a homebuilt nano-DESI MS platform. In addition, we also found that nano-DESI MS has a capability of obtaining depth-dependent ink chemical profiles.

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Preparation and characterization of Nanocarbon included composite hydrogel impregnated with substituted polyaniline

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A new composite hydrogel included with nanocarbon (NC) and substituted polyaniline (S-PANI) was prepared through a sequential two step process. In the first step, NC, chitosan (CS) and polyacrylic acid (PAA) interpenetrating network (NC-CS-PAA-IPN) was prepared by the free radical grafting and cross-linking reactions among NC, CS and PAA. In the second step, S-PANI was incorporated into the micro porous channels of NC-CS-PAA-IPN through oxidative polymerization. S-PANI impregnated NC-CS-PAA-IPN composite hydrogel (NC-CS-PAA/S-PANI IPN-CHG) were characterized. Fourier transform infrared spectroscopy, scanning electron microscopy and thermogravimetry analysis were used to investigate the IPN formation, morphology and thermal stability of the NC-CS-PAA/S-PANI IPN-CHG, respectively. The NC-CS-PAA/S-PANI IPN-CHG was tested for r the removal of heavy metal ion removal from waste water.

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Synthesis of silver enriched silica-polyaniline nanocomposite via a seed mediated route

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In this work, a new seed mediated route has been developed for loading excessive silver nanoparticles (Ag NP) onto silica-polyaniline (Silica@PANI) support. Firstly, Silica@PANI support was prepared with embedded Ag NP as the seed. Subsequnetly, excessive Ag NPs were loaded onto Silica@PANI support and the Silica@PANI/Ag NP-E was synthesized. The as synthesized Silica@PANI/Ag NP-E nanocomposite was characterized by infrared spectroscopy (FT-IR), scanning electron microscopy coupled with energy dispersive X-ray system, transmission electron microscope (TEM), and X-ray photoelectron spectroscopy (XPS) measurements. In addition, Silica@PANI/Ag NP-E nanocomposite was utilized for catalytic reduction of 4-nitrophenol.

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Organic monolith frits encased in PEEK tubing with improved durability in HPLC

박신영 정원조*

인하대학교 화학과

Polymer-encased organic monolith frits were prepared as cheap frits before in our laboratory by forming organic monolith in common polymer tubing followed by cutting into slices. But previous tubing frits had critical weak point in that the monolith core was too easily detached from tubing. This study introduces a new technique which provides strong attachment of monolith to tubing inner surface. Inner surface of PEEK (Poly-ether-ether-ketone) tubing is pretreated with sulfuric acid in the presence of catalysts (vanadium oxide and sodium sulfate). After washing with water and acetone, the PEEK tubing was treated with glycidyl methacrylate (GMA). After washing, the reaction mixture of monolith (lauryl methacryltate (LMA), ethylene glycol dimethacrylate(EDMA), initiator, and porogenic solvent) was filled in the tubing and subjected to in-situ polymerization. The catalysts assisted pretreatment procedure was better in terms of monolith-tubing attachment in comparison to the pretreatment without catalysts. After slicing the tubing into many slices of frits, vortex test was carried out in order to check the durability of the frits. The frit slices were placed in a vial and an extreme shock was applied on the vial by vortex for various times. The frits made in presence of catalysts were found to be more durable. Furthermore, when the monolith-tubing was used as a chromatography column, the column prepared in the presence of catalysts resulted in better separation efficiency. In summary, catalyst-assisted sulfonation and introduction of double bonds there-on have been found useful for preparation of cheap PEEK encased monolith frits.

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Synthesis and application of C2 symmetric (R)-phenylglycinol derivatives as HPLC chiral stationary phases

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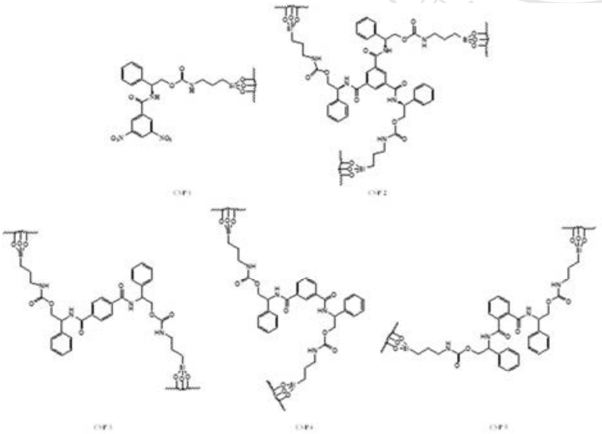
Various chiral amino alcohols, e.g. (R)-phenylglycinol, (S)-leucinol, (S)-alaninol, N-3,5-dinitrobenzoyl amide derived chiral stationary phases (CSPs) were synthesized and utilized for the resolution of various chiral analytes. As a result, (R)-phenylglycinol derived CSP (CSP 1) performed better than others1. The (R)-phenylglycinol was also used as a starting material of new C3 symmetric (R)-phenylglycinol N-1,3,5-benzenetricarboxylic acid derived chiral HPLC stationary phase (CSP 2)2,3 very recently. In this study, synthetic procedure and application of new C2 symmetric CSPs (CSP 3 ~ CSP 5) will be shown.



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Chiral separation on various modified amino alcohol derived HPLC chiral stationary phases

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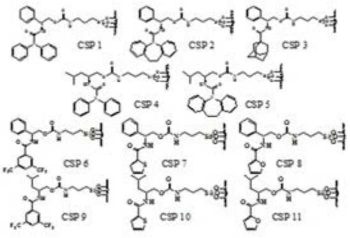
(R)-phenylglycinol and (S)-leucinol N-3,5-dinitrobenzoyl amide derived chiral stationary phases (CSPs) were used for the resolution of various chiral analytes.1-3 Very recently, (R)-phenylglycinol and (S)-leucinol derived CPSs (CSP1~5) were synthesized and used for the separation of 14 chiral analytes.4.In this study, different kinds of (R)-phenylglycinol and (S)-leucinol derived CSPs (CSP 6~11) were prepared with N-3,5-bis(trifluoromethyl)benzoyl chloride, 2-furoyl chloride, and 2- theonyl chloride instead of reported acyl chlorides. The derivatives were applied to CSPs and the CSPs were used for the resolution of various chiral samples containing chiral drugs.



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Development of SERS based point-mutated DNA detection using metal nanodendrite structure

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A point mutation is a type of serious mutation that causes the replacement of a single base nucleotide with another nucleotide of the genetic material, DNA or RNA. Because of its similarity with normal sequence, sensitive analytical method is in great demand for the detection of a point mutation. In this study, we have investigated surface enhanced Raman scattering (SERS) based sensing scheme to fulfill the necessary analytical sensitivity. We fabricated silver-gold nanodendrite structure via a simple electrochemical synthesis used it as a SERS.For the purpose, we used toehold-mediated DNA strand displacement reaction for increasing specificity of target sequence. Initially, the hybridized pair of thiol modified probe DNA (complementary to a point mutated DNA) and indicator DNA labeled with Raman dye (shorter then probe DNA) was immobilized on the surface of Ag-Au nanodendrite, thereby resulting in the increase of Raman signal due to the positioning of the Raman dye near the surface. When a target DNA was added, it pushed the indicator DNA away, so decreasing Raman intensity as a function of the concentration.In overall, the current research demonstrate sensitive and rapid detection of point mutated DNA sequence caused by Avellino corneal dystrophy using bimetallic nanodendrite SERS substrate.

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BIOCOMPATIBLE COATINGS FOR BIOANALYTICAL DEVICES

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Protein chips need to immobilize proteins that retain their native structures. Polymer coatings can be used to build up nanostructures on a protein-chip. This is generally done by synthesizing the polymer with a series of steps. Polymer coatings reported in this study were prefabricated in solution as small polymers and then assembled into a coating in a single, or a small number of steps. This reduces the time and complexity required for the device fabrication such as microfluidic systems.

Prefabricated polysuccinimide (PSI) coatings were developed as a new generation of biocompatible coatings for microfabricated analytical systems. These coatings were developed for gold and/or glass BioCD discs. Linear and branched PSIs were characterized with NMR, elemental analysis (EA), size exclusion chromatography (SEC), and AFM. These methods established that PSI coatings deposited on surfaces were usually 2-5 nm thick and very hydrophilic. This prevents non-specific binding of proteins from the surface physically and chemically.

Proteins were immobilized on inorganic surfaces in three ways: PSI coatings with biotin, protein G, or direct binding to IgG on immunological assays. Antibody immobilization and antigen detection were measured using AFM, ellipsometry (ELS), fluorescence microscopy, and interferometry. The nonspecific binding of sample proteins from the blocking coatings was confirmed to be very low through SEC development project.

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Introduction to isotope-coded carbamidomethylation-based isotope labeling for absolute quantification of serum BNP-32 using nanoLC-ESI-MS/MS

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Quantifying the amount of brain natriuretic peptide-32 (BNP-32) in human serum is significant, since BNP-32 is a crucial biomarker for diagnosis of the congestive heart failure (CHF). Nevertheless, it is still challenging in determining its quantity of the low abundant BNP-32 in serum (100 pg/mL), due to absence of a proper isotope-labeling method. To address this issue, we developed a simple and novel isotope labeling method as isotope-coded carbamidomethylation (iCCM). Carbamidomethylation (CM) with iodoacetamide (IAA) and its isotope (IAA-13C2, D2) used to block the thiol group and simultaneously lead to the mass difference of 8 Da between CM- and iCCM-labeled BNP-32. The resulting BNP-32 mixture, equally pooled, introduced to nanoLC-ESI-MS/MS to evaluate the labeling efficiency, and its relative abundance ratio for matching with the spiked mass ratio. Consequently, we found that an iCCM-based isotope labeling method is one of alternative method for quantifying targeted BNP-32 in serum with high reproducibility and labeling efficiency.

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Quantitative profiling of respiratory syncytial virus-induced N-glycoproteme using iTRAQ couple with online mHFER nLC-ESI-FT orbitrap-MS/MS

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Respiratory syncytial virus (RSV) is the leading cause of lower respiratory tract infections in infants and young children. An antiviral is available for treatment of RSV, but treatment is effective only when given early in the course of infection and presently there is no approved vaccine. RSV infection process involves the interaction between virus and host cell with N-glycosylation. Therefore, quantification of N-glycoproteome in RSV-induced sera is important task for early diagnosis. In order to quantify N-glycoproteins, we used lectin-based enrichment by means of online microbore hollow fiber enzyme reactor (mHFER)-nLC-ESI-MS/MS. For the purpose of RSV specific N-glycoproteomic profiling, RSV-infected mouse sera samples (eg. 3day and 7day) and control were tryptically digested and isotopically labeled with iTRAQ reagents. The labeled peptide from each mouse sera (eg. 3day, 7day, and control) mixed equally and pooled with lectin to form lectin-N-glycopeptide complexes. Finally, the resulting complexes introduce to mHFER-nLC-ESI-MS/MS to analysis lectin-specific N-glycopeptides. In consequence, we sucessfully quantify RSV-specific N-glycopeptides and these identified proteins may be useful to develop RSV-specific drug.

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Investigation of Korean traditional lacquer by analytical instruments

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Dendropanax morbifera is Korean traditional lacquer and it had been described in old literature. Restoration of Dendropanax lacquer is not easy because information of Dendropanax lacquer is very limited and master craftsmen become defunct. Sap collected from Dendropanax morbifera is used for lacquer. When sap is collected from Korean Dendropanax morbifera, white-colored liquid are extracted originally. They transform into yellow-colored liquid by contacting with the air and losing water. In this study, white-colored liquid and yellow-colored liquid of sap from Dendropanax morbifera were spread on the slide glass and were compared difference of their compositions. FT-IR, AFM, py-GC/MS and TOF-SIMS were used to analyze compositions of white liquid and yellow liquid and to identify the color change mechanism. Especially, AFM and TOF-SIMS were used to obtain the nanostructural information of two different kinds of sap liquid.

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Facile Synthesis and Enantioseparation on Carboxymethyl-β-CyclodextrinModified Zirconia-PAMAM Dendrimer Magnetic Microspheres

김종화 이용일*

창원대학교 화학과

Abstract The present work explores the synthesis of carboxymethyl-β-cyclodextrin modified zirconia-PAMAM dendrimermagnetic nanoparticles (Fe3O4@ZrO2@PAMAM@CMCD) and their application in selective enantioseparation of racemic drugs. The Fe3O4@ZrO2@PAMAM@CMCD magnetic nanoparticles (CMCDZPMMs) are characterized by transmission electron microscopy (TEM), X-ray Diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, thermogravimetry (TGA), elemental analysis (EA), X-ray photoelectron spectroscopy (XPS) and vibrating Sample magnetometer (VSM). As-synthesized CMCDZPMMs are applied for separation of racemic drugs and it was proposed that the functional groups at chiral center of the racemic drug molecules might interacts with hydroxyl group of CMCD and makes hydrogen bond formation resulted in selective adsorption of enantiomer. Most importantly the synthesized CMCDZPMMs have shown an excellent magnetic property that reflects in their easy separation from solution.

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Aging Effect of Ultrahigh Molecular Weight Cationic Polyacrylamide Copolymer by Frit-inlet Asymmetrical Flow Field-Flow Fractionation-Multiangle Light Scattering

우소희 문명희*

연세대학교 화학과

Polyacrylamide (PAM) is a polymer consisted of acrylamide monomer, which is highly reactive substrate in free radical polymerization and easily forms long-chain polymers. PAM is widely used in waste water treatment due to its ability to degrade by various pathways. During the degradation, molecular weight of PAM decreases and the length of the chain become shorter. Therefore, for the efficient use of PAM as a flocculant, study on molecular weight distribution and its change by degradation must be preceded.In general, synthesized polymers have a wide molecular weight distribution. Size-exclusion chromatography (SEC) is one of the most common method but it has a limited molecular weight range of separating the sample. As frit inlet asymmetrical flow field-flow fractionation (FIAF4) has no stationary phase, pressure induced on samples is minimized and sample can be separated in its intact forms. Therefore, frit-inlet FFF system can be considered as suitable method for synthesized polymers with a broad molecular weight distribution. For this reason, FIAF4 was utilized to separate cationic PAM copolymer and their absolute molecular weight was measured by multiangle light scattering (MALS).PAM samples analyzed in this research were synthesized in different time periods. Since the aged polymer experienced longer degradation process than the newly synthesized polymer, aging effect was confirmed by the change in MWD using FIAF4-MALS.

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Identification of geographical origins of coffee beans by using vibrational spectroscopic methods

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한양대학교 화학과

Coffee is one of the most consumed beverages and holds the second in the international trade market next to crude oil. So it is very crucial to have a fast and reproducible evaluation method to check for the authenticity of coffee beans. In this research, infrared and near-infrared spectroscopic methods were used as a tool for the identification of spectral features among various geographical origins and types of coffee beans. Fifty nine different coffee beans were obtained from Africa (Ethiopia, Kenya, Tanzania, etc.), Latin America (Colombia, Guatemala, Brazil, etc.), and Asia (Papua New Guinea, Indonesia). Infrared absorbance spectra of pellet samples with ground coffee bean samples and diffuse reflectance NIR spectra of coffee beans were collected. Principal component analysis (PCA) combined with linear discriminant analysis (LDA) was used for the discrimination of samples according to the types. In addition based on non-parametric method was evaluated for the same purpose. The accurate quality assurance and discrimination of geographical origins of coffee beans will be conducted in this study.

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A new phosphopeptide enrichment strategy using phospho-specific antibody combined with online-mHFER-nLC-ESI-MS/MS

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Phosphorylation, one of post-translational modifications, is well known as a key regulator implicating in cellular growth, differentiation, and signaling. However, mass spectrometry (MS)-based shotgun proteomics to identify and quantify phosphoproteome is not fully accessible yet, due to their low abundance in biological samples (e.g., sera, cells, and etc.) and low ionization efficiency during electrospray ionization (ESI). Herein, we newly introduced an enrichment strategy for phosphoproteomics by which phosphopeptides having an affinity with phospho-specific antibodies (pAbs) can be automatically isolated from ordinary peptides during online microbore hollow fiber enzyme reactor (mHFER)-nLC-ESI-MS/MS experiments. To examine the potential in phosphoproteomics, the tryptic peptides from MCF7 were mixed with pAbs, having a molecular weight of above 50 kDa, and followed by which the pAb-phosphopeptide complexs introduced into the mHFER (10 kDa in MW-cutoff) with continuous flow rate of 5 uL/min. During breakthrough run, ordinary peptides having no affinity with pAb are first waste out through membrane wall of HF. The remaining peptides bound to pAb can be simultaneously exited via online tryptic digestion in mHFER for next nLC-ESI-MS/MS run. From our experimental results, we identified total 11282 phosphorylated sites in 5673 phosphopeptides of MCF7 cell line using online mHFER-2D-nLC-ESI-MS/MS and confirmed that pAbs-based enrichment with online mHFER can be the best way for phosphoproteomics than conventional methods (e.g., IMAC, TiO2, FASP) in which the efficiency in identifying a number of phosphorylated sites is dramatically improved to be about 8-fold than conventional methods, for instance, 24, 2, and 189 phosphoylated sites for IMAC, TiO2, and FASP, respectively.

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Highly Sensitive and Selective Water-Stable FET-Based Sensors Functionalized with Cucurbit[n]uril Derivatives

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

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Applications of paper spray ionization mass spectrometry in the studies of host-guest chemistry and steroid analysis

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Paper spray ionization (PSI) method is one of the ambient ionization techniques for mass spectrometry (MS). PSI utilizes a triangular shape filer paper as a sampling base as well as an electrospray tip. PSI MS has been demonstrated as a promising tool for fast chemical screening, drug monitoring, and complex mixture fingerprinting. In this study, we applied PSI MS to understand host-guest chemistry. One of the model systems we used were complexes of cholesterol derivatives and cyclodextrins. From a series of experiments, we found that PSI MS was a very useful tool for determining binding preferences and affinities between various host and guest molecules in a very short period of time. In addition, we also performed analyses of nonderivatized sex hormones by using a homebuilt PSI MS system. We enhanced the detectability of the nonderivatized steroid ions and signal reproducibility through the optimization of the spraying solvents. After optimization, we could perform fast and reliable quantitative analyses of sex hormones which can be potentially used as a clinical screening tool for sex hormones.

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Development of home-built solid-state NMR probes for particular purposes

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The solid-state NMR has been widely used for many insoluble materials like industrial polymers and biological samples. Also solid-state NMR analysis of membrane protein on lipid bilayer or bicelle as a membrane-like environments, is especially valuable for their structure and function relationship. However, most of biological proteins on lipid bilayers have high dielectric property due to containing large amounts of lipids, water, and salts as well as probe efficiency are decreased cause of their electrical properties of lossy samples. Therefore, specific probe with high efficiency is required to study biological samples by using solid-state NMR. Development of solid-state NMR methodologies for the study of orientational information of membrane protein in bicelle could be used for the in-situ analysis of liquid crystalline materials in LCD panels as well as Li materials in Li ion batteries. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil to prevent heating by high RF power for the study with lossy samples. 1H-15N 2D SAMPI4 spectra from a single crystal and membrane proteins oriented in bicelles were successfully obtained by using these solid-state NMR probe. Also, we present a home-built 500 MHz NB 19F-13C double resonance solid-state NMR probe with a flat-square coil and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a solenoidal coil. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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NMR Structural Analysis of Antimicrobial peptides, LPcin analogs with Enhanced Activities

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Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113-135 region of Component-3 of bovine proteose-peptone PP3.LPcin was designed and modified to enhance antibacterial activity using mutation, sequence shuffling for better amphipathic characteristics. It helps to improve interacting with bacterial membranes. Three candidates were selected among 12 LPcin analogs which have better antibacterial activity than LPcin. We named them LPcin-yk1, LPcin-yk2 and LPcin-yk3 respectively. LPcin-yk1 and LPcin-yk3 has shorter amino acids at C-terminus, LPcin-yk2 has same number of amino acids but several amino acids were substituted for better amphipathic characteristics. To understand the correlation between their structures and antibacterial mechanism, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using various biophysical techniques.We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with biophysical techniques such as Ni-NTA affinity chromatography, dialysis, CNBr chemical cleavage and reversed-phase semi-prep.HPLC. To verify the purified peptides, we performed Tris-tricine PAGE, MALDI-TOF MS and CD spectrometry. In order to investigate the structures and dynamics, we use various 1D and 2D NMR techniques using micelle and bicelle samples to make membrane environments.In here, we will present not only the optimization of high-yield expression and purification, but also solution and solid-state NMR experiments to elucidate their structures. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra and PISA Wheel pattern were also underway.

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Green Sample Preparation for Determination of NSAIDs by HPLC

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Dispersive liquid-liquid microextraction (DLLME) may be utilized as a green chemistry approach to reduce the consumption of hazardous organic solvents in the chemical analysis. A simple and efficient sample preparation method was developed using DLLME prior to HPLC/UV analysis for simultaneous extraction and determination of trace amounts of Non-Steroidial Anti-Inflammatory Drugs (NSAIDs) including indoprofen, ketoprofen, naproxen, diclofenac, ibuprofen, mefenamic acid, tolfenamic acid from an aqueous sample. Optimal dispersive solvent and extraction solvent were chosen acetonitrile and chloroform, respectively, and showed increased enrichment factor (EF = 9~18) for the extraction of NSAIDs. Simultaneous chromatographic separation of seven NSAIDs by HPLC-UV/Vis system was achieved on an Eclipse XDB-C18 (4.6 mm i.d. × 150 mm length, 5 ㎛ particle size) column using isocratic elution with 0.1 % formic acid and methanol (30 :70). NSAIDs were extracted and concentrated from 5 mL of aqueous solution with pH 3.8. The volume of dispersive and extraction solvent were 1000 ㎕ and 200 ㎕, respectively. After the extraction, 5 ㎕ of extract was directly injected into the HPLC/UV system. The developed method represents a simple, rapid, environmentally friendly and inexpensive sample preparation method.

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Dimethylation vs. Acetylation in Electrospray Ionization Efficiency and Identification Integrity

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Peptide acetylation has widely been used for blocking N-terminal amines and ε-amines of lysine residues in ESI MS. For example acetylation reactions of proteolytic peptides were applied to i) chemical isotope labeling for quantitative proteomics (e.g. Terminal amine isotope labeling of substrates, TAILS), and ii) affinity tag labeling for targeted proteomics (e.g. nitroprotein proteomics). However, peptide acetylation results in the serious reduction of peptide signals during ESI ionization. This phenomenon may be related with charge neutralization form amine ($z = +1$) to amide ($z = 0$) after acetylation in a common ESI condition (e.g. 0.1 % formic acid). To overcome the signal reduction problem due to acetylation, we introduced dimethylation reaction to block amino groups on tryptic peptides keeping their positive charge after the blocking reaction. We quantitatively compared the electrospray ionization efficiency and identification integrity of dimethylation and acetylation in tryptic BSA and ischemia sample. Peptide dimethylation showed higher ESI RI (relative intensity) than peptide acetylation in tryptic BSA (up to 375 times enhancement). In addition peptide dimethylation reduced the bias of identification rate by chemical modification in ischemia sample (RID integrity = No peptides ending with Arg/No. peptides ending with Lys = 2.96 (?0.11), 0.75 (?0.05) for acetylated and dimethylated sample, cf. RID integrity = 1.01 (?0.04) for intact sample). These results suggest that dimethylation of tryptic peptides be a more efficient and less biased blocking method than acetylation for ESI-MS/MS.

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The Separation of Plant Hormones by NanoLC-ESI-MS

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Plant hormones act as necessary roles in regulating and controlling numerous aspects of plant growth, development, and response to stimulation. Each class of plant hormones has characteristic biological effects at trace concentrations, and most plant hormones are involved in many different processes on the growth and development. Therefore, we chose through plant hormones and identified by nano liquid chromatography electrospray mass spectrometry (LC-ESI-MS). In order to optimize, chromatographic conditions such as gradient, a component of solvent, ratios of solvent, flow rate, etc also carried out. Among plant hormones, specially, methyl jasmonate is consisted to four stereoisomers which regulate a wide range of physiological processes. Previous researchers have reported to methods of chiral in methyl jasmonate that used to separate using GC, LC and mass spectrometry. When the separation of sample that was mixed plant hormones, we try to separate chiral compounds. In this case, nano LC column made packing materials which were synthesis in our laboratory.

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Synthesis and Characterization of Si-CNFs composites by Chemical Vapor Depositon based on Ni-Cu catalysts

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Carbon based materials have been attracted and studied in the field of Li secondary battery, because of chemical stability and conductivity properties. Many researchers have attempted to enhance the efficiency of Li secondary battery. In this study, we have synthesized carbon nanofibers(CNFs) and Si-CNFs composites by Chemical Vapor Deposition(CVD) using Ni and Cu co-catalysts. First of all, we synthesized catalysts by co-precipitation method using Ni and Cu nitrates. Carbon nanofibers have then been synthesized by Chemical Vapor Deposition using Ni and Cu catalysts (according to molar ratio of Ni and Cu). Finally, we have also prepared Si-CNF composites by CVD method, after we have mixed catalysts (molar ratio of Ni and Cu was 8:2) with Si particles using ball milling. The physicochemical properties of the grown carbon nanofibers were investigated with Scanning electron microscopy(SEM), Energy dispersive spectroscopy(EDS), X-ray Diffraction(XRD), BET, Raman spectroscopy, and X-ray photoelectron spectroscopy(XPS). The electrochemical properties and the capacitance of the anodic materials, fabricated with CNFs and Si-CNFs composite in Li secondary batteries, were investigated by galvanostatic charge-discharge and cyclic voltammetry.

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Investigating the Optimized Ag Nanorod Array Fabrication Conditions for SERS Applications

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The Ag nanorod array fabricated by oblique angle deposition (OAD) is widely used as SERS (Surface Enhanced Raman Spectroscopy) substrate due to its several advantages such as high reproducibility, uniformity, large SERS active area as well as high Raman signal enhancement. In a previous KCS conference, our research group reported the fabrication of Ag nanorods by OAD technique and obtained the SERS signal with an enhancement factor of ~ 10^7. In this experiment, thermal evaporation was used for Ag nanorods growth instead of e-beam. The substrate temperature during the Ag evaporation is one of critical factors for fabrication of well aligned Ag nanorods. In this presentation, profound investigations were carried out to find critical factors affecting the Ag nanorod array formation. Various condition parameters, such as deposition angle, deposition rate, source-to-substrate distance and deposition thickness during the evaporation process were investigated. The relationship between Ag nanorod morphology and SERS signal intensity were presented. Ag nanorod morphologies resulted from different Ag evaporation conditions were characterized by field emission-scanning electron microscopy (FE-SEM). The SERS signal intensity was found to improve as the deposition angle, source-to-substrate distance and deposition thickness were optimized. The results obtained in this investigation will be of great use in designing improved Ag nanorods array substrates for SERS applications.

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Comparative study on optimization of sample preparation procedure in GC-MS quantification of organotin compounds

이종한

LG하우시스 연구소

Ever since the discovery of their excellent versatility in early 20th century, organotin compounds, such as tributyltin(TBT), dibutyltin(DBT), monobutyltin(MBT), and triphenyltin(TPhT), have been widely used not only as antifoulant or insecticide, but also as heat stabilizer for PVC, wood preservative, or catalyst for synthetic resins. However, it has been figured out that those organotin compounds induce imposex phenomena towards various marine lives and a high level of regulation has been imposed on the usage of the organotin complexes. In General, current determination and quantification method for the organotin complexes within various forms of samples based on gas chromatography-mass spectrometry (GC-MS) which is followed by inevitable and tedious sequential steps of extraction and derivatization to impart non-polar and volatile characteristics on organotin compounds. To maximize cost and time efficiency for determination of those compounds, herein, we conducted comparative study between conventional and modified preparation sequence on organotin complexes (TBT, DBT, MBT, and TPhT) by intentional omission of required reagent and/or chemical environment or combine discrete steps. Effectiveness of those modifications is evaluated by the comparison of the recovery rate of the organotin complexes.

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Development of a volatile component sensitive colorimetric chemosensor for determination of fruits ripeness

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A naked-eye detective chemosensor has been a major concern of many application fields due to the simplicity, favorable performance, selectivity, and low cost. In smart packaging fields for agricultural food products, chemosensor aids consumer with communication as a marketing tool and an offer to the consumer with the great easy of use and time-saving convenience for the final purchasing decision.Most of the post-harvest fruits have emitted the volatile components, such as ethylene, acetaldehyde, and alcohol etc. Ethylene is one of the critical gas molecules participating in ripen, storage, and circulation of fruits and agricultural products. Apple and Kiwi are the representative climatic fruits which emit the ethylene gas and other volatile components during storage. To fabricate the ethylene sensitive colorimetric indicator (ECI), the color-changing material representing the selectivity of ethylene was synthesized by the reaction of bathophananthroline ligands and palladium chloride under chloroform. An acetaldehyde sensitive colorimetric indicator (ACI) was prepared by coating the bromophenol blue on the barium sulfate-coated paper. ACI showed the bleached color change from blue to light blue under the exposure of acetaldehyde vapor. ECI deposited by the synthesized palladium complex showed the proper selectivity of ethylene giving rise to color change from beige to dark brown, the irreversible detection without recovering its original color, and stability in exposure of air and humidity. This reflected that ECI fabricated by doping the synthesized palladium complex was applicable to the ripeness sensor of the agricultural products.

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SERS-based aptasensor for sensitive trace analysis of Bisphenol A in drinking water

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Bisphenol A (BPA) is a commonly used material for epoxy resin and polycarbonate in plastic industries. BPA is currently regarded as an endocrine disrupting chemical (EDC) that is potentially estrogenic. Thus, fast and sensitive detection of BPA in drinking water is important. In this study, we report a surface-enhanced Raman scattering (SERS)-based aptasensor platform for the ultrasensitive detection of BPA in water. This technique involves the synthesis of double strand DNA-embedded Au/Ag core-shell nanoparticles. In the presence of BPA, Cy3-labeled DNA amtamers were released from the nanoparticles causing a decrease in the SERS signal intensity. Quantitative analysis of BPA was performed by calculating the Raman peak intensity of Cy3 at 1,590 cm^{-1}. This proposed aptamer-conjugated nanoparticles showed its applicability for detecting BPA in simple, selective and quantitative manner.

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Early diagnostics of prostate cancer by the sensitive SERS detection of mRNA PCA3 marker in urine

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We report a new SERS-based DNA-RNA hybridization assay platform for PCA3, a long non-coding mRNA, specifically overexpressed in prostate cancer. Here, one antisense oliginucleotide (ASO)-conjugated magnetic bead and the other ASO-conjugated hollow gold nanosphere (HGN) were utilized as supporting substrate and SERS-active probe, respectively. Label-free target PCA3 was captured by the sequence-specific hybridizations by two ASOs immobilized on each metal surface. In this work, PCA3 hybridizations could be detected without PCR amplification because the SERS signal intensity is very high. According to our assay data, the limit of detection was estimated to be 1 fM for PCA3. Consequently, this SERS-based PCA3 assay is expected to be a promising tool for early diagnosis of prostate cancer in urine.

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Early diagnosis of prostate cancer by simultaneous detection of two PSA biomarmers using SERS-based immunoassay

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Prostate specific antigen (PSA) is a 30 kDa serine protease. PSA in blood exists in multiple forms: free or complex with the protease inhibitors a1-antichymotrypsin (ACT). Total PSA is a combination of both free and PSA/ACT complex. Numerous studies showed that the clinical accuracy of the PSA determination can be improved by measuring the ratio of either free-PSA or PSA/ACT in relation to total PSA. Enzyme-linked immunosorbent assay (ELISA) and photoluminescence bioassays have been widely used for the quantitative analysis of PSA in clinical laboratory. However, those techniques have some technical drawbacks such as poor signal-to-noise ratio, limit of detection and simultaneous multiplex detection capability. Thus, scientists and medical doctors are still concerned about the ways to improve the PSA immunoassay test for the precise diagnosis of prostate cancer. In this work, a novel SERS-based immunoassay platform using gold nanoparticles and magnetic beads has been developed for highly sensitive detection of dual PSA markers. Here, XRITC- and MGITC-labelled gold nanoparticles have been used as SERS nanotags for dual PSA marker assay. On the other hand, magnetic beads have been used as supporting substrates for the high-density loading of immunocomplexes. This SERS-based technique provides a new immunoassay platform for fast and sensitive diagnosis of prostate cancer.

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Surafce renewable nano-Iridium oxide composite pH electrode

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A practical surafce renewable nano-Iridium oxide polymeric composite electrode was prepared by incorporating nano iridium oxide particles in PMMA matrix. The iridium oxide nanoparticles were prepared by the hydrolysis of $(NH_4)_2IrCl_6$ and were then dispersed in acetone containing PMMA. The suspension of the nano-iridium oxide and PMMA was precipitated into water and then pressure-molded to disk-type nano-iridium oxide composite electrode material. The nano-iridium oxide served as an active pH sensing material as well as an electrical conductor. The electrodes showed highly improved pH response characteristics. The electrode showed excellent linear response between pH 3-11 with a slope of -59.7 mV/pH (R = 0.9999) and fast response time of $t_{90}< 2$ s. An average slope of -58.8 ± 0.2 mV/pH and E°intercept of 657.8 ± 1.3 mV vs. 3M Ag/AgCl were observed steadily for a month without appreciable deactivation. Less porous and hydrophobic surface of the PMMA composite electrode minimized equilibration time resulting in the fast response. The electrode can be stored in deionized water or even in air after uses. The electrode surface can be renewed reproducibly by simple polishing whenever contaminated or deactivated. Therefore the lifetime of the electrode was extended greatly.

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Quantitative analysis of diaquat in drinking water using SERS-based microdroplet sensor

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We present a fast and sensitive trace analysis of diaquat dibromide monohydrate (DQ) in water using a surface-enhanced Raman scattering (SERS)-based microdroplet (MD) sensor. This sensor is composed of two compartments, the first being for droplet generation for fresh silver nanoparticle (AgNP) synthesis, and the second for droplet merging for SERS detection. AgNPs were grown in droplets, and then each droplet was synchronously merged with another droplet containing DQ for SERS detection. This microdroplet system prevented memory effects caused by the precipitation of nanoparticle aggregates on channel walls because the droplets were isolated by oil phase. The limit of detection (LOD) of DQ in water was determined to be below 5 nM, which satisfies the maximum contaminant level defined by the United States EPA. This SERS-based integrated sensing system is expected to be useful as an in-the-field sensing platform for fast and reproducible trace analysis of environmental pollutants in water.

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The study for MALDI-MS spectrum interpretation for polymer reaction

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polymer 반응 초기에 다양한 형태의 prepolymer 가 생성된다. 이 생성물들은 일정한 간격의 분자량 변화를 보여주기 때문에 반응경로에 따라 생성되는 여러 종류의 polymer 에 대한 분자량 예측이 가능하다. 본 연구는 예측 되는 모든 경로에 대한 분자량 변화를 추적하여, 다양한 경로로 진행되는 polymer 생성 반응에 대한 반응 경로 및 반응 생성물에 대한 체계적인 해석 방법을 확립하려는 시도이다.

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Synthesis and size characterization of silica nanoparticles using Asymmetrical Flow Field-Flow Fractionation (AF4): Large-scale synthesis

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Silica nanoparticles are used widely in various fields such as food, medical, and biological industries. The particle size is one of important parameters that determines characteristics (and thus their applicability) of the silica nanoparticles. Accurate sizing technique is thus required for quality control in synthesis of silica nanoparticles. Various techniques have been used for size characterization of nanoparticles including dynamic light scattering (DLS), electron microscopy (transmission electron microscopy (TEM) and scanning electron microscope (SEM)), and field-flow fractionation (FFF). Unlike others, FFF provides size-based separation of colloidal particles. In FFF, retention time is directly related with particle size, and thus a FFF elution profile can be converted to size distribution directly. It has been shown that FFF is useful for separation of particles ranging in size from a few nm up to about 100 μm. Synthesis of silica nanoparticles having narrow size distributions is not trivial as there are various parameters affecting the characteristics of the synthesized silica nanoparticles. In this study, silica nanoparticles were synthesized by emulsion polymerization by mixing ethanol with ammonium hydroxide, and tetra ethyl orthosilicate (TEOS) at room temperature. And then the asymmetrical flow FFF (AF4), a member of FFF family, was employed for size characterization of the silica particles. The AF4 results were compared with those obtained from SEM and DLS. First, the synthesis was performed in a smaller scale (about 175 mL), where the effect on the particle size distribution (PSD) of various parameters were systematically investigated. Then the scale was enlarged to about 2 L. It was observed that, as the purity of TEOS or ethanol increases, the size of the silica particles tended to decrease, while, as the purity of ammonium hydroxide increases, the size of silica nanoparticles tended to increase. Results suggest AF4 is a useful

tool for fast and accurate determination of the size distribution of particles of various types including silica nanoparticles.

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Au Nanowire SERS Platform for Telomerase Activity Detection

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Human telomere acts as biological clock, consisting of TTA GGG repeats at the end of the chromosomes. During cell division, this telomere is shortened, which can cause the fusion with neighboring chromosomes. However, telomerase replenish shortened telomere by adding telomeric repeats (TTA GGG)n. Due to the high expression level of telomerase in tumor cells, telomerase is an attractive tumor biomarker and a potential target for cancer therapy. Developing the robust sensor platform for the measurement of telomerase activity is desired in cancer diagnosis and therapy. Many researchers have explored the newly designed sensor for sensitive and reproducible telomerase activity detection. Especially, surface-enhanced Raman scattering (SERS) has been considered as a highly sensitive and robust optical analysis technique for biomolecule detection. Herein, we fabricated noble metal nanowire SERS platform for telomerase activity detection. An ultrasensitive and highly-reproducible sensing was possible by using our novel SERS platform. We anticipate that our SERS sensor has the great potential in practical cancer diagnosis.

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Size analysis of metal-oxide nanoparticle using Field-Flow Fractionation

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Metal nanoparticles are becoming increasingly popular for treatment of contaminated soil and groundwater. It is known that the aggregation of metal nanoparticles is affected by the environmental condition. Thus, in order to understand behavior of metal nanoparticles in environment, stability of the particles needs to be studied. Field-flow fractionation (FFF) is a family of analytical separation techniques that can be applied for separation and characterization of various types of nanoparticles. FFF have some potential advantages over chromatographic techniques. Separation in FFF is achieved solely through the interaction of the sample components with an external physical field. There is no stationary phase. This allows us to avoid variety of problems caused by non-specific interaction between the sample components and the column-packing materials. Also the accessible range of information is broad, and often complimentary when various members of FFF family are employed together, so that even complex systems with broad size distributions, heterogeneous mixtures or strongly interacting systems can be analyzed. In this study, metal nanoparticles of various types were analyzed using various techniques including asymmetrical flow FFF (AsFlFFF), sedimentation FFF (SdFFF), and dynamic light scattering (DLS). In FFF, strength of the external field and flow rate were optimized for FFF analysis. Also the behavior of the metal nanoparticles was systematically investigated as a function of the type of dispersing agent and the ionic strength of the medium.

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Molecular characterization of butadiene rubber using size-exclusion chromatography and thermal field-flow fractionation/multi-angle light scattering

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Rubber has a significant role in tire industry, which tries to attain a better compromise between the wear and rolling resistance, and ice and wet grip properties of tire tread compounds. Butadiene rubber (BR) is used widely in tire tread compounds, hoses, and conveyor belts. Molecular weight (MW) and gel content are important parameters of polymers as they influence the physical, mechanical, and rheological properties of the polymers. Small difference in low or high MW fractions can result in significant differences in end use properties. Thus the molecular weight distribution (MWD) of a polymer is one of important parameters in quality control, monitoring of product stability, reclaiming off-spec material, and development of new materials.Thermal field-flow fractionation (ThFFF) is a polymer separation technique whose operation is controlled by the thermal diffusion coefficient, D_T, a basic transport parameter describing the movement of a matter under a temperature gradient. ThFFF is useful for MW-based separation and molecular characterization of various types of polymers. ThFFF channel is open (unpacked), and is particularly useful for separation of polymers of high MW that are susceptible to shear degradation or those containing microgel. ThFFF can provide separation of microgels from the soluble species.Size exclusion chromatography (SEC) is a particularly valuable tool in the measurement of the molecular weights and molecular weight distributions of polymers.Online-coupling of ThFFF with a multi angle light scattering (MALS) and a concentration detector such as refractive index (RI) or UV/VIS detector yields the molar mass and root-mean-square (RMS) radius (R_g) of each ThFFF slice, and thus the conformational information of the molecules. In this study, ThFFF coupled online with a MALS and a RI detector (ThFFF-MALS-RI) was employed for molecular characterization BR’s from various sources. ThFFF provided a good separation of the microgel particles from the soluble polymers with enhanced sensitivity by MALS for the microgel particles. ThFFF results were compared with those from SEC. Results suggest ThFFF-MALS-RI is a powerful tool for analysis of various types of microgel-containing polymeric materials.

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Characterization of egg yolk plasma using asymmetrical flow field-flow fractionation coupled with multiple detectors

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In this study, the capability of asymmetrical flow field-flow fractionation (AF4) coupled online with a UV/VIS, quasi-elastic light scattering (QELS), multiangle light scattering (MALS) and fluorescence (FS) detectors (AF4-UV/VIS-QELS-MALS-FS) was evaluated for separation and characterization of egg yolk plasma. AF4 provided gentle separation of the major components of the egg yolk plasma such as free proteins, low density lipoproteins (LDL) and their aggregates, according to their hydrodynamic sizes. Free proteins were completely separated from LDL by a programmed AF4 analysis, where the cross-flow was gradually reduced during a run. For each component, QELS and MALS yielded hydrodynamic radius (R_h) and radius of gyration (R_g) , respectively, allowing study on conformation (e.g., shape) of each component based on the ratio, R_g/R_h. The R_g/R_h data were confirmed by Cryo-transmission electron microscopy (Cryo-TEM) images of collected AF4 fractions. The R_g/R_h results indicated that LDL has spherical shape, while larger aggregates have swollen micro-gel structure. Elution of LDL was confirmed by staining with a fluorescent dye, Nile red. Collected fractions of free proteins were further characterized using a sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE). Results suggested that the absence of Ca^{2+} leads to aggregation, while the presence of Ca^{2+} leads to bindings of proteins. It was shown that AF4-UV/VIS-QELS-MALS-FS is a gentle and useful tool for analysis of egg yolk plasma.

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Molecular size-based separation of starch molecules and physical characterization using Asymmetrical Flow Field-Flow Fractionation (AsFlFFF)

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Starch is a mixture of two α-glucans, amylose and amylopectin, containing α-(1,4) linkages. Amylose (AMY) molecule are essentially linear, while amylopectin (AMP) molecules are branched with 5-6% alpha-(1,6) linkages. Usually AMY and AMP are different in physical properties such as molar masses, radius of gyration (R_g) and hydrodynamic radius (R_h).The rheological and functional properties of starches are influenced by various factors including the molecular size, molar mass distribution, the concentration ratio of AMY to AMP, and the branching characteristics of AMP.Field-flow fractionation (FFF) is a family of separation techniques capable of providing separation and characterization of macromolecules or particles ranging in size from 1nm up to about 100μm. Among the members of FFF family, asymmetrical flow field-flow fractionation (AsFlFFF) is especially suited to analytical separation of bio-colloidal particles. AsFlFFF can provide separation of AMY and AMP, allowing quantitative analysis of the two components, and when coupled with detectors such as multi-angle light scattering (MALS) and refractive index (RI), it can provide the absolute weight-average molar mass (Mw) without the need for calibration.In this study, AsFlFFF conditions were optimized for separation of AMY and AMP and physical characterization of starches in potato and amaranth.

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Analysis of macromolecules in beer by flow field-flow fractionation coupled with multiangle light scattering (FlFFF-MALS)

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Beer is a complex mixture of various types of macromolecules including proteins and polysaccharides. There is an increasing demand for in-depth and accurate analysis of the macromolecules in beer. Macromolecules in beer are derived as a result of brewing that involves various modifications of proteins and polysaccharides of barley seeds. It is known that properties of proteinaceous molecules are related to the mechanism of formation and foam stability. Presence of some proteinaceous molecules results in a formation of haze. The presence of polysaccharides with high molar mass tends to increase viscosity and turbidity of beer.In this study, three types of beer were prepared using the mashing process. The capability of FlFFF coupledd online with multiangle light scattering (FlFFF-MALS) for determination of molar mass distributioni and quantitative analysis of macromolecules in beers were investigated. Also the beer components were identified by enzymatic treatment. The results reveal that FlFFF-MALS may become a useful tool for monitoring of the change in the macromolecular composition of beer during the mashing processes.

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Importance of hydrophobic introduction between Phe 45 and Phe18 in Structure of *Enterococcus faecalis* Acyl Carrier Protein

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Fatty acid synthesis is essential for cell growth and viability. The Acyl Carrier Protein (ACP) is a key element in the biosynthesis of fatty acids being responsible for the acyl group shuttling and delivery within a series of related enzymes.*Enterococcus faecalis* (*E. faecalis*) is a Gram-positive, commensal bacterium inhabiting the gastrointestinal tracts of humans and other mammals. *E. faecalis* can cause life-threatening infections in humans, especially in the hospital environment. *E. faecalis* can withstand oxidative stress, dry condition, and extremes of temperature and pH. In this study, structures of *Ef*-ACP as well as thermal stabilities of *Ef*-ACP were investigated. CD experiments showed that melting temperature of *Ef*-ACP is 78°C, which is much higher than that of *E.coli* ACP (68°C). We determined the solution structure of *Ef*-ACP. The overall structure consists of four α-helices (helix I (3-17), helix II (39-53), helix III (59-64), helix IV (68-78)) connected by three loops. Phe45 in *Ef*-ACP has stacking interactions with His17 and Phe18, which are essential for the thermal stability of *Ef*-ACP. Stacking interactions between Phe45and and Phe18 contribute to the thermal stability of *Ef*-ACP by stacking interactions and they block the path into the alternate binding cavity of *Ef*-ACP which accommodate the growing acyl chain. Spin relaxation experiments werer performed and the dynamics of *Ef*-ACP will be discussed. This study will be helpful to understand the specific recognition mechanisms between *Ef*-ACP and functionally different enzyme partners in fatty acid synthesis pathway.

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Fibril formation by I26P or S20G mutant of fusion proteins (chaperone-L23-hIAPP)

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The 37-residue protein, human iset amyloid polypeptide (hIAPP) misfolds and forms aggregates within the pancreas of Type II diabete patients. In order to regulate the aggregation process of misfolded proteins into toxic oligomers, we have constructed recombinant fusion plasmids with chaperone domains (FKBP, FKBPIF, F36V, F36VIF and SlyD*) and amyloid proteins, hIAPP with a linker of 23 amino acids (H6-chaperone-L23-hIAPP). In the previous study, FKBPIF (or F36VIF) chaperone proteins exhibit the accelerated amyloid fibril formation among chaperone proteins when fused. In this study we applied the I26P or S20G mutant of chaperone-L23-hIAPP fusion proteins, which were overexpressed by IPTG in E.coli and further purified by Ni2+- affinity chromatography. We have measured thioflavin T (ThT) fluorescence to address the role of I26P or S20G mutant in regulating the rate of amyloid fibril formation.

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Expression and purification of the 37-residue human islet amyloid polypeptide (hIAPP)

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The pathogenesis of type Ⅱ diabetes is associated with the aggregation of the 37-residue human islet amyloid polypeptide (hIAPP) into cytotoxic β sheet and α-synuclein(α-syn) aggregates and fibrils. We want to use hIAPP because of hIAPP's fibril formation rate faster than SYN's. However, disadvantage of hIAPP that expensive price and small amount may limit the study. So, we created a new plasmid to obtain only hIAPP separately in a special expression system.The new plasmid connected UBQ, TEV protease cleavage, INTEIN in pTXB1 vector. Fusion proteins were overexpressed by IPTG in E.coli and further purified by Ni+2-affinity chromatography. And then cut the each all connection point and get pure hIAPP by using Size Exclusion Chromatography (SEC) column.

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Evaluation of herbicide binding site residues in *Mycobacterium tuberculosis* Acetohydroxyacid synthase through site-directed mutagenesis

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Acetohydroxyacid synthase (AHAS) is a thiamin diphosphate (ThDP)- and flavin adenine dinucleotide (FAD)-dependent plant and microbial enzyme that catalyzes the first common step in the biosynthesis of essential amino acids such as leucine, isoleucine and valine. This enzyme has been suggested as the target for several classes of herbicides or anti-bacterials. In this study, the residues (R318, A146, Q148, M512, and V513) of the catalytic subunit in *Mycobacterium tuberculosis* acetohydroxyacid synthase (MTB AHAS) were selected, and the possible role was evaluated by site-directed mutagenesis. The residues in *Mycobacterium tuberculosis* acetohydroxyacid synthase (MTB AHAS) are found to be conserved with *Arabidopsis thaliana* acetohydroxyacid synthase (AtAHAS) and occupy the herbicide binding site in AtAHAS. The variant enzymes were characterized with respect to kinetic parameters and sensitivity against herbicides. The site-directed mutagenesis has affected significantly the catalytic activity and lowered inhibition property (IC50) against herbicides (Chlorimuron Ethyl, C.E). Furthermore, the binding energy was also much affected in molecular docking analysis with herbicide (C.E). This result suggested that the conserved residues play an important role for binding of herbicide in MTB AHAS.

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나노입자를 이용한 광열치료제 개발

조헌호 김성경 윤형준 허진 반창일*

포항공과대학교(POSTECH) 화학과

Nanoparticles have gained wide attention due to their potential in medicine, such as molecular imaging, immunization, and targeted therapy. Gold nanoparticles, offering facile synthesis and biocompatibility, have been applied for a variety of therapeutics, especially in cancer therapy. Gold nanostars, which feature tunable plasmon bands in the near-infrared (NIR) tissue optical window, have potential for in vivo imaging and therapeutic applications. In this work, a powerful photothermal probe that can selectively and effectively target both types of prostate cancer cells was designed. Using this system, we achieved remarkable results.

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A myriad of dynamics appear throughout the Escherichia coli ACP, reflecting their functional plasticity

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Acyl carrier protein (ACP) is at the main system responsible for fatty acid biosynthesis and the acyl chain distribution found in membrane lipids. Acyl carrier protein from E.coli (EcACP) is a small, soluble acidic protein. The structure of EcACP has been solved by NMR spectroscopy. The overall structure of E. coli ACP consists of four α-helices connected by three loops. In the presence of divalent cation, apo-ACP shows only one conformation, while holo-ACP shows two sets of resonances, suggesting that two conformers are in dynamic equilibrium. To study the thermal stability of EcACP, we measured melting temperatures using circular dichroism (CD) spectroscopy. Since ACP is highly acidic, binding of divalent metal ion can stabilize the folding of ACP. However, there are no differences of secondary structures of EcACP with or without metal ions, whereas EcACP without metal ion has lower melting temperature compared to ACP with metal ion. In order to understand the fundamentals of thermal stabilities of EcACP, we performed multidimensional heteronuclear NMR experiments and completed the backbone resonance assignment and side chain assignment. From the assignment, it is found that there are two metal binding sites, one near Asp31 and Asp35, the other near Glu47 and Asp56.

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1H, 13C and 15N NMR assignments of the protein backbone of bovine angiogenin

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Angiogenesis is a complex process to form new blood vessel, which is critical for cell reproduction, developement and wound repair under normal condition. This process includes endothelial cell proliferation, migration and membrane degradation. A variety of pathological conditions are also dependent on angiogenesis. For that reason angiogenesis is crucial for the growth of tumors. It is angiogenic molecules that is a member of the pancreatic ribonuclease superfamily and is overexpressed in many cancers. Angiogenin is one of the angiogenic factors and a influential inducer of blood vessel formation. 1H, 13C and 15N NMR assignments of the protein backbone of bovine angiogenin were performed using the 3 dimensional NMR experiments. We acquired 3D NMR spectra and assigned all the backbone chemical shifts including Cα, Cβ, and HN of angiogenin. Computational docking studies of angiogenin also showed that flavonoids are docked well with angiogenin. These findings should prove to be useful in the design of more effective and specific angiogenin antagonists

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A colorimetric aptasensor for the detection of biomarkers using cationic surfactant and gold nanoparticles

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Scientists have been trying to develop a simple, rapid and accurate diagnostic method. Gold nanoparticle (AuNP)-based colorimetry have received attention since it does not require any special instruments and can be observed easily with the naked eye. Among others, assay procedures based on the non-crosslinking aggregation mechanism of AuNPs are convenient and cost effective due to the absence of the elaborate and expensive synthesis of ligand-modified AuNPs. In this study, we report a new label-free biosensor to detect biomarkers, based on the interaction among the aptamer, cationic surfactant and AuNPs. A cationic surfactant aggregates AuNPs in controllable sizes and colors via its competitive binding to aptamers. It can be possible to observe the color changes of the AuNPs solutions from red to blue, which depends on the concentration of biomarker. Using the aptasensor, biomarkers were sensitively detected. The specificity of the aptasensor was also evaluated using several other human proteins. Additionally, the biomarker was successfully detected in the human serum sample. Therefore, the proposed aptasensor might be used as a powerful diagnostic tool.

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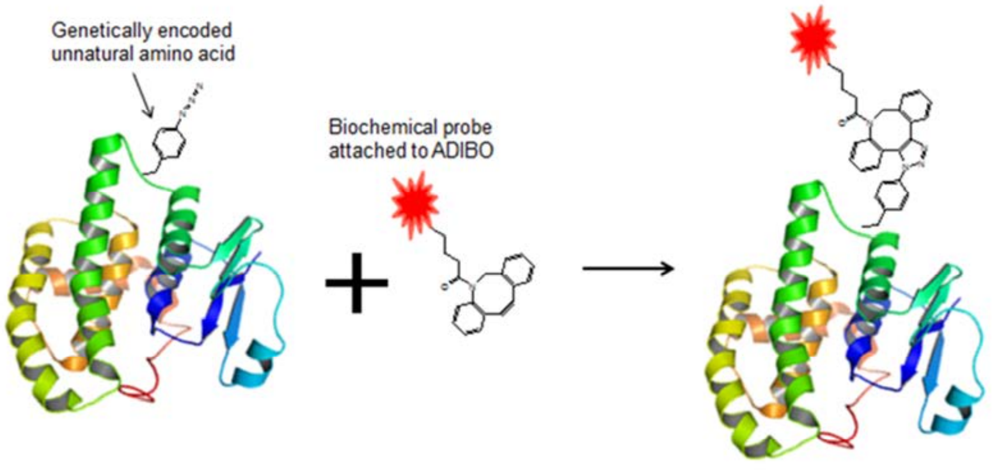
Site-specific protein conjugation by copper-free click reaction

이현수* <u>고우석</u>

서강대학교 화학과

There are currently many methods available for labeling proteins in order to study their structure and function. However, the utility of these methods is hampered by low efficiency, slow reaction rates, non-biocompatible reaction conditions, large-sized labeling groups, and the requirement of specific side chains such as cysteine or lysine. In this study, a simple and efficient method for protein labeling was developed, in which an azide-containing amino acid was introduced into a protein and conjugated to a labeling reagent by strain-promoted azide-alkyne cycloaddition (SPAAC). This method allowed us to label proteins and antibody fragments by simply mixing a protein and a labeling reagent in physiological conditions with a labeling yield of approximately 80% in 120 min. Because the genetic incorporation of the azide-containing amino acid can be generally applied to any protein and the SPAAC reaction is highly specific, this method should prove useful for labeling and analyzing proteins.



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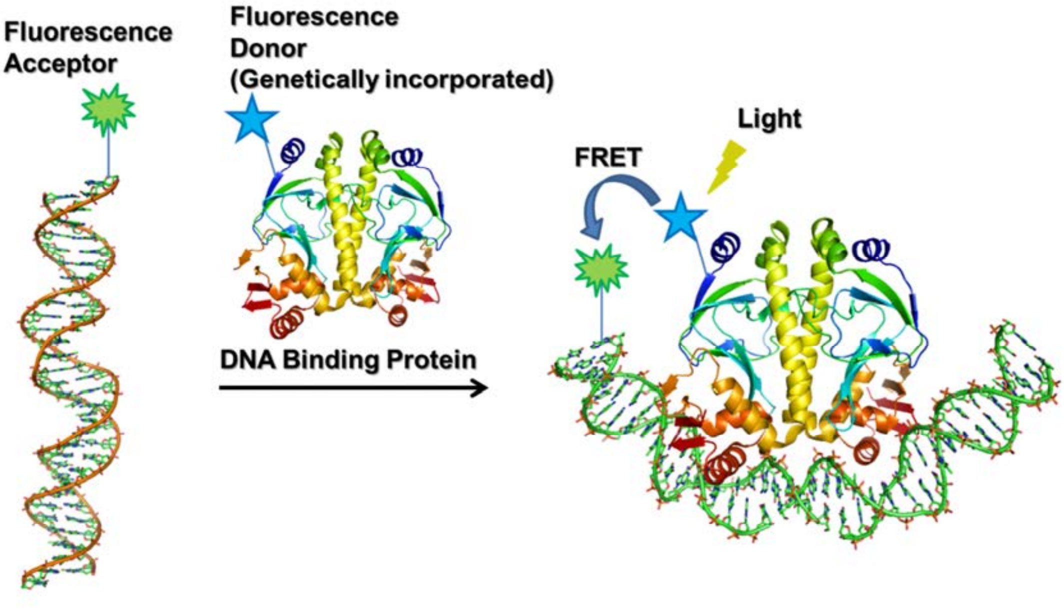
FRET-based analysis of protein-nucleic acid interactions by genetically incorporating a fluorescent amino acid

이현수* 강희진

서강대학교 화학과

Protein-nucleic acid interaction is an important process in many biological phenomena. In this study, a fluorescence resonance energy transfer (FRET)-based protein-DNA binding assay has been developed in which a fluorescent amino acid is genetically incorporated into a DNA binding protein. A coumarin-containing amino acid was incorporated into a DNA binding protein, and the mutant protein specifically produced a FRET signal upon binding to its cognate DNA labeled with a fluorophore. The protein-DNA interactions were then measured under equilibrium conditions. This method is advantageous for studying protein-nucleic acid interactions because it is technically easy and applicable to any nucleic acid binding protein.



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금 나노입자 및 고분자-압타센서를 이용한 표적 단백질 검출The colorimetric detection of target protein based on aptamer-polymer system with gold nanoparticles

윤형준 조헌호 김성경 허진 반창일*

포항공과대학교(POSTECH) 화학과

The development of a detection method for target protein is important to the biological diagnosis of human diseases. We have developed simple detection method which is based on the affinity of pL1 aptamer against family of pLDH (Malaria specific biomarkers), such as Plasmodium vivax lactate dehydrogenase (PvLDH) and Plasmodium falciparum lactate dehydrogenase (PfLDH). Using the pL1 aptamer, partner polymer and gold nanoparticles, the development of a colorimetric detection technique of pLDH species was possible. Also, the developed aptasensor has high selectivity for the pLDH family over other non-targeting proteins. Furthermore, we proved that the aptasensor is effective for malaria diagnosis by analysis of target protein pLDH from blood samples of the malaria patient. In conclusion, the developed system with pL1 aptamer, which is molecular sensor for pLDH, could make an effective diagnosis of malaria possible.

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The effect of extein pI values on the kinetics of split-Npu intein mediated protein trans-splicing reaction

김다희 권영은*

동국대학교 의생명공학과

Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. As the PTS became a useful tool for various biological studies, it is important to understand the factors that affect the kinetics of the PTS. For this study, we have chosen Npu DnaE intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate the effect of extein pI's on the PTS kinetics, we prepared multiple pairs of split-inteins that carry exteins of various pI's. We observed accelerated reaction rates as the pI's of N exteins increase. In case of various C intein pairs, we observed accelerated reaction rates as the pI's of C intein flanking sequence decrease. This result provides a good guideline in designing efficient PTS.

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Dicer Nuclease Promoted Production of Let7a-1 MicroRNA Is Enhanced in the Presence of Tryptophan Containing Amphiphilic Peptides

현순실 유재훈*

서울대학교 화학교육과

Members of a library of Trp containing amphiphilic peptides were synthesized and screened for their ability to bind to pre-miRNA targets. Two of this family, the peptide Ac-WKKLLKWLKKLLKLAG-NH2 (2b) and Ac-WKKLLKWLKKLLDabLAG-NH2 (4b) were found to have nanomolar binding affinities against pre-let7a-1. Peptides 2b and 4b cause an increase in the in vitro Dicer promoted cleavage of pre-let7a-1. This observation was confirmed using a cell-based assay, the results of which show that up to a 50% increase in Dicer activity takes place. Enhanced expressions of let7a-1 promoted by the peptides result in specific reductions of the target mRNAs. The results of a microarray study show that lower amount of fluctuating genes are generated in the presence of 2b or 4b in contrast to that caused by exogenous delivery of let7a-1. Because peptides 2b and 4b promote enhanced formation of mature let7a-1 only at the endogenous miRNA level, it specifically controls genes related to let7a-1.

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Ubiquitin folding and electrostatic interactions

박순호

강릉원주대학교 치의학과

The contribution of electrostatic interactions to protein folding reaction was studied by using mutant ubiquitin with lysine to alanine mutation at residue position 29. Based on the three dimensional structure of ubiquitin, lysine 29 is located close to negatively charged glutamate 16 and aspartate 21. Thus the native state of ubiquitin is considered to be stabilized by the electrostatic interactions between these residues. The equilibrium unfolding experiment showed that the native stability was decreased by about ~20% upon mutation. This observation indicates lysine 29 indeed forms electrostatic interactions with nearby residues. Folding kinetics measurements using stopped-flow device and quantitative analysis of kinetics data indicate that ubiquitin folds from unfolded state to native state via intermediate state. This intermediate state forms immediately after initiation of folding and the native state forms relatively slowly from this intermediate state. Furthermore this folding intermediate was destabilized considerably upon mutation. These observations indicate that electrostatic interactions can form early stage of ubiquitin folding and hence lead the folding reaction.

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Functional Expression of a Cystine-rich Peptide (Paralichthys olivaceus β -defensin) in Escherichia coli periplasm

곽동건

부산대학교 화학과

In the present study, a peptide β-defensin, isolated from the teleost, P. olivaceus, was recombinant expressed in E. coli periplasm. The antimicrobial peptide contains six cysteine residues, that the terms of disulfide bridge pairing determines the activity of the peptide. To further verify the characterization of β-defensin, its functional expression is urgent. Here, we showed that the β-defensin could be functionally expressed in the periplasmic area of E.coli by jointing a mini-tag (Y) in the N-terminal of peptide. The DNA sequences of β-defensin and Y-tag were cloned into pQE30 vector by PCR technology, together with a six-histindine tag and a factor x recognition site. Recombinant fusion protein was expressed in E.coli strain M15[pREP4], and purified by Ni2+-column.

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Functional expression of Carassius auratus cytochrome P4501A in a novel Shewanella oneidensis expression system and its application to degradation of benzo[a]pyrene

김서현

부산대학교 화학과

Cytochrome P4501A (CYP1A) in fish has attracted an increasing interest because of its important roles in the metabolic activation of certain xenobiotics such as aromatic hydrocarbons. CYPs are reported to be expressed in yeast, insect cells and Escherichia coli, but are critical for high-level expression. Besides, this study found that the purification of recombinant goldfish CYP1A would result in a loss of enzyme activity. Because large quantities of functional CYP1A are required, it is necessary to find a suitable host with high-level expression. In the present study, a novel expression system using Shewanella oneidensis was established successfully for the production of goldfish CYP1A. A signal peptide in the expression vector leads to the high-level expression in the periplasmic space of Shewanella. The recombinant CYP1A in Shewanella reached up to 1μmol per liter of culture, and showed the typical P450 hemoprotein spectra. An ethoxyresorufin O-deethylase assay revealed the amount of functional proteins in Shewanella to be almost ten times more than those in other expression systems. These results indicate the possible application of periplasmic fractions to obtain sufficient quantities of functional CYP1A for further studies.

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Exogenous Human Proteasomes Facilitated Degradation of Overexpressed Proteins through Clathrin-Mediated Endocytosis by Mesoporous Silica Nanoparticles

한동훈 이민재*

경희대학교 응용화학과

The 26S proteasome is 2.5 MDa holoenzymes that degrade ultimately pathogenic proteins involved in various types of disease. We report here that exogenous proteasomes delivered by mesoporous silica nanoparticles (MSN) delay the formation of aggregates of tau proteins, hallmark pathogen of Alzheimer’s disease (AD), which were caused by the overexpression. His-tagged human proteasomes that were non-covalently loaded onto MSN modified with Ni-NTA moieties (MSNPN) were directly delivered into cells through clathrin-mediated endocytosis without cytotoxicity, and its proteolytic activities still retained after endosome escape. The delivered human proteasomes degraded excessive tau proteins which were overexpressed and aggregation-prone in cultured cell models. The level of endogenous tau proteins wasn’t altered by exogenous human proteasomes. The exogenous proteasomes not only predominantly targeted ubiquitin-independent proteasomal substrate like a GFP-odc but also it induced rapid turnover of tau proteins. The inhibition effect of exogenous proteasomes was significant against the overexpressed tau- and ROS-induced cytotoxicity in cells. Accordingly, our results suggest that the delay of formation of tau aggregates was attributed by the proteolytic activities of exogenous proteasomes which might preferentially degrade the proteotoxic overexpressing tau proteins.

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Mutation in the Core Particle Enhances Mammalian Proteasome Activity by Open-Gate

최원훈 이민재*

경희대학교 응용화학과

The proteasome core particle (CP) has the substrate translocation channel that is topologically blocked by the N-terminal of the α3 subunits when it is in the closed form. For substrate degradation, the gate of CP channels is opened upon association with the regulatory particle (RP, PA200) or other proteasome activators (PA26, PA28). Here we show that deletion of the N-terminal tails of the α3 subunits (α3-ΔN) disrupt the gate of mammalian proteasomes without affecting their structural stability. Relieved from the autoinhibitory status, purified α3-ΔN proteasomes showed enhanced proteasome activity in vitro as measured by both small fluorogenic peptide substrates and polyubiquitinated Sic1 (Ub-Sic1). Degradation of overexpressed proteasome substrates, including tau and?α-synuclein, was significantly facilitated in the cells which stably express α3-ΔN proteasomes. Moreover, these cells showed significantly promoted cell survival against proteotoxic stress caused by overexpressed tau and reactive oxygen species (ROS). Direct delivery of exogenous α3-ΔN proteasomes by Mesoporous Silica Nanparticle into cultured cells resulted in significantly decreased levels of tau aggregates. From these, it is reasonable that the CP gated regulates substrates degradation in mammalian proteasomes. Opening the gate through deleting the N-terminus tail of α3 may be an effective strategy to increase proteasome activity and to reduce levels of abnormally overexpressed proteins in cells.

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Docosahexaenoic acid Affects Proteasome Activity Through Oxidative Modification of Proteins

신승균 이민재*

경희대학교 응용화학과

Docosahexaenoic acid (DHA), a member of ?-3 polyunsaturated fatty acids (PUFAs), is widely recognized to have broad health benefits, including anti-cancer effects. DHA in cells, however, may undergo various oxidative modifications and functions as key substrates to generate reactive oxygen species (ROS) and harmful, oxidized proteins. The proteasomes is the major cellular machinery that degrades not only ubiquitin (Ub)-conjugated proteins but also misfolded, damaged, and oxidized proteins. Here we show that DHA may indirectly inhibit proteasome activity through generating excess amounts of oxidized proteins in cells. Sic1 proteins treated with DHA, but not unmodified sic1 or DHA alone, significantly reduced suc-LLVY-AMC hydrolysis activity of purified proteasomes. Cells treated with DHA were less efficient in degrading overexpressed proteasome substrates including aB-crystallin and tau. These effects of DHA were reversed by N-acetylcysteine (NAC), which significantly reduced the levels of aggregates forms of tau. These data demonstrate that increased ROS levels induced by DHA may have pathological implication in various proteotoxic diseases, including age-related macular degeneration (AMD) and Alzheimer’s disease (AD).

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Improved Tau Degradation by USP14 Aptamersvia Elevated Proteasome Activity

김지현 이민재[*]

경희대학교 응용화학과

The ubiquitin-proteasome system (UPS) is the primary degradation mechanism for intracellular proteins, including regulatory proteins of signal transduction pathways, transcription factors, and many proteotoxic proteins with aggregation-prone structures. Synthetically, UPS output has been reported to be downregulated in various neurodegenerative disorders, and enhancement of proteasome activity was proven to be beneficial in many related disease models. Through the ubiquitin (Ub)-chain trimming function of USP14, a proteasome-associated deubiquitinating (DUB) enzyme, the proteasome functions under tonic inhibitory conditions is suggested for recent evidence. Here we show identification of specific RNA aptamers targeting USP14 which significantly inhibited DUB activity of USP14 using an *in vitro* selection process. Nucleotide sequences of these non-cytotoxic USP14 aptamers contain conserved GGAGG motifs, followed by G-rich sequences, and are expected to have similar secondary structures. Selected RNA aptamers efficiently elevated proteasomal activity, as measured by both small fluorogenic peptide substrates and polyubiquitinated Sic1 (Ub-Sic1) proteins. In addition, proteasomal degradation of tau proteins was significantly enhanced in the presence of USP14 aptamers both *in vitro* and in cultured cells. Thus, our study ensures inhibitory USP14 aptamers as promising tools to enhance proteasome activity and facilitate proteotoxic protein degradation to protect cells under various neurodegenerative stresses.

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A Novel Blood Brain Barrier-Permeable Arg/N-end Rule Inhibitor Can Perturb theGPCR Signaling Pathway

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경희대학교 응용화학과

In eukaryotes, the N-end rule pathway consists of two branches, the Arg/N-end rule pathway and the Ac/N-end rule pathway. In the Arg/N-end rule pathway, unacetylated N-terminal destabilizing residues function as essential determinants of protein degradation signals (N-degron). Here, we show that a neurostimulant, para-chloroamphetamine (PCA), specifically inhibits the Arg/N-end rule pathway, delaying the degradation of its artificial and physiological substrates, including regulators of G protein signaling 4 (RGS4), not only in vitro and in cultured cells but also in the mice brains. In silico computational analysis indicated that PCA strongly interacts with both UBR box and ClpS box, which bind to type 1 and type 2 N-degrons, respectively. Consistent with the role of RGS4 in G protein signaling, treatment with PCA impaired the activations of GPCR downstream effectors in HeLa cells as well as in phenocopying ATE1-null mutants. In addition, levels of pathological C-terminal fragments of TDP43 bearing N-degrons (Arg208-TDP25) were significantly elevated in the presence of PCA. Thus, our study identifies PCA as a potential tool to understand and modulate various pathological processes regulated by the Arg/N-end rule pathway, including neurodegenerative processes in FTLD-U and ALS.

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Genetic variations in the CLU and PICALM genes are associated with Alzheimer's disease in Koreans patients

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단국대학교 화학과 [1]단국대학교 자연과학대학

Alzheimer's disease (AD), characterized with progressive cognitive impairments, is the most common form of dementia in an aging population. AD is pathologically defined as neuronal loss, the accumulation of neurofibrillary tangles and extracellular amyloid plaques in the brain.Clusterin (CLU)gene is an apolipoprotein. The functions of CLU protein are apoptosis, complement regulation, lipid transport, membrane protection, and cell-cell interactions. CLU expression is reported to increase amyloid plaques in affected by cerebrospinal fluid of AD case.phosphatidylinositol binding clathrin assembly protein (PICALM) gene encodes a protein involved in clathrin assembly. PICALM gene is expressed in neurons. PICALM plays an essential role in regulation of synaptic vesicle in brains. Also, several studies reported that mediated Aβ generation may influence accumulation of Aβ in AD brains.Recently, genome wide associated studies (GWAS) suggested that polymorphisms of CLU and PICALM genes were significantly associated with risk of AD. In this study, we investigated the association between two AD related genes and risk of AD in Korean patients using PCR-RFLP and statistical analysis.

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Investigation of Multidrug-Resistant Mycobacterium tuberculosis isolates from Korean TB patients

최지영 조민호 김진호 문명진 최영훈 장원철[1,*]

단국대학교 화학과 [1]단국대학교 자연과학대학

Tuberculosis (TB) remains one of the most prevalent contagious diseases in worldwide. According to the World Health Organization (WHO), there were estimated 8.6 million new TB cases in the world and 1.3 million deaths in 2012. New TB cases and Multidrug-resistant tuberculosis (MDR-TB) cases are reported 39,545 and 1,212, respectively in Korea and that show the highest incidence of tuberculosis among participating OECD countries. MDR-TB is defined as resistant to both isoniazid (INH) and rifampin (RIF). MDR-TB reduces efficiency of treatment with anti-TB drug leads to higher mortality. Traditional culture-based diagnostics of testing for drug resistance are too slow as patients undergoing treatment. Recently several studies reported that mutation of the rpoB (516, 526 and 531 codon) and katG 315 codon leads to resistance of RIF and INH, respectively.In this study, The M. tuberculosis strains were isolated from at the TB patients between August 2011 and July 2012 provided at the Dankook University hospital. We assessed the frequencies of MDR-TB in three-hundred Korean TB patients by PCR-sequencing.

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Adsorption and Antioxidant Activity of Vinca Alkaloids in Vinca Minor Extract

이향렬

한국교통대학교 생명공학과

The adsorption and antioxidant activities of Alkaloids of Vinca Minor L. was isolated and studied. The effect of solvents for alkaloids extraction was investigated. The amount of hydrophilic alkaloids such as glycosides was found to increase by hot water extraction method whereas hydrophobic alkaloids such as vincamine were isolated much more by ethanol extraction. Vinca alkaloid compounds including vincamine from Vinca minor L. have been isolated and characterized for their spectrophotometric analysis. Extracts with Ethanol and hot water were tested against the DPPH (2,2-diphneyl-1-picryl-hydrzayl-hydrate) free-radical to investigate their antioxidant activity. Cytotoxic properties of those extracts have also been investigated with HaCaT cell (human ketatinocyte cell), HT-29 cell (human colorectal adenocarcinoma cell) and Raw cell, showing no significant cytotoxic effects. We also measured the ROS using dichlorofluorescin deacetate(DCFDA), a popular fluorescence-based probe for reactive oxygen species detection. The result showed that the increasement of reactive oxygen species formation in HaCaT and HT-29 cell lines.

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Modulation of hepatic metabolites by calorie restriction

민순기 정선희 류도현 황금숙[1,*]

성균관대학교 화학과 [1]한국기초과학지원연구원 통합대사체연구그룹

Obesity, whose prevalence is increasing rapidly worldwide, is recognized as a risk factor for diabetes, cardiovascular disease, nonalcoholic fatty liver disease (NFLD), and renal disease. To investigate metabolite changes by caloric restriction in obesity mice, we performed metabolic profiling of liver tissues of mice. In this study, we used one obese model; db/db mutant mouse. The db/db mouse is a model of obesity and diabetes wherein leptin receptor activity is deficient because the mice are homozygous for a point mutation in the gene for the leptin receptor. db/db mice were divided two groups; non-calorie restriction and calorie restriction(2g/day) for 12 weeks. Then, we applied metabolic profiling based on ultra-performance liquid chromatography/quadrupole time-of flight mass spectrometry (UPLC/Q-TOF MS) and nuclear magnetic resonance (NMR) to find metabolite changes between calorie restriction (CR) and non-calorie restriction (NCR) in db/db mice. Each multivariate statistical analysis with the MS and NMR data of liver tissue extracts showed clear metabolic differences between CR and NCR groups in mice model. This study identified features of hepatic metabolites of calorie restricted mice and demonstrated that MS and NMR based approach are a useful tool to investigate the metabolite changes by caloric restriction.

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A naphthalimide-based Cu(II) ensemble for the detection of cyanide ions

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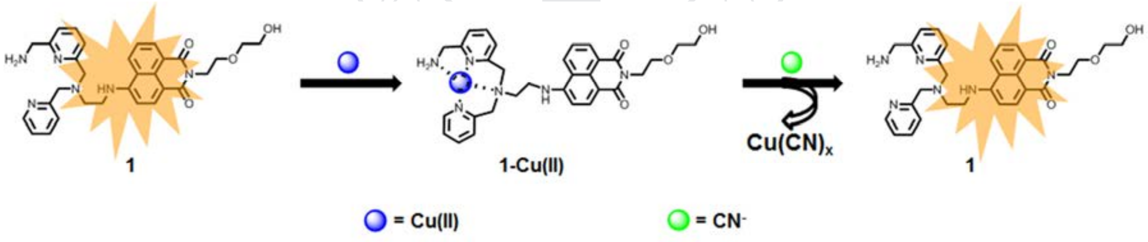
A novel fluorescent probe 1 based on naphthalimide was designed and synthesized. The binding behavior of 1-Cu(II) ensemble prepared *in situ* has investigated toward various anions by UV-vis and fluorescence spectroscopy. Among various anions tested, 1-Cu(II) ensemble shows selective and sensitive response towards cyanide ion in aqueous solution.



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1H-NMR-based metabolomics study of obesity prone and obesity resistant mice in response to a high fat diet

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성균관대학교 화학과 [1]한국기초과학지원연구원 통합대사체연구그룹

Obesity has increased dramatically in recent years and become a serious health problem. One of the issue in obesity is individual differences in responses to a high fat diets. Therefore, it is interesting to characterize metabolic responses of the individuals to high fat diet (HFD) and to find out what cause two distinct phenotypes, obesity-prone and obesity-resistant. In the present study, we performed metabolic profiling in three different groups of mice; normal diet (ND), fed a normal diet; obesity-prone (HFD-OP), fed a HFD and showed the higher weight gain; obesity-resistant HFD-OR), fed a HFD but showed the lower weight gain compared to HFD-OP. We analyzed mouse liver tissue extracts using proton nuclear magnetic resonance spectroscopy (1H-NMR) to compare the metabolic patterns among the ND, HFD-OP, and HFD-OR groups. Multivariate statistical analysis showed a clear differentiation among three groups (HFD-OP, HFD-OR and Normal diet, ND). Notably, HFD-OR group was closer to ND group than HFD-OP group. The major metabolites contributed to the discrimination among groups included choline, glycine, hydroxybutylate, hypoxanthine, mannose, tyrosine, valine, and xanthine. In conclusion, this study demonstrated that 1H NMR based metabolic profiling with multivariate analysis can be useful approach to understand the metabolic differences in response to high fat diet and correlations between metabolic profile and weight gain.

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In vitro vesicle fusion assay for investigating the pathogenesis of β-amyloid/α-synuclein co-aggregates on SNARE-dependent vesicle fusion

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Alzheimer’s disease (AD) and Parkinson’s disease (PD) are caused by β-amyloid (Aβ) and α-synuclein (αS), respectively. Ample evidence suggests that these two pathogenic proteins are closely linked and have a synergistic effect on eliciting neurodegenerative disorders. However, the pathophysiological consequences of Aβ and αS co-existence are still elusive. Here, we show that large-sized αS oligomers, which are normally difficult to form, are readily generated by Aβ42-seeding and that these oligomers efficiently hamper neuronal SNARE-mediated vesicle fusion. The direct binding of the Aβ-seeded αS oligomers to the N-terminal domain of synaptobrevin-2, a vesicular SNARE protein, is responsible for the inhibition of fusion. In contrast, large-sized Aβ42 oligomers (or aggregates) or the products of αS incubated without Aβ42 have no effect on vesicle fusion. These results are confirmed by examining PC12 cell exocytosis. Our results suggest that Aβ and αS cooperate to escalate the production of toxic oligomers, whose main toxicity is the inhibition of vesicle fusion and consequently prompts synaptic dysfunction.

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Chemical probe-based biosensing endoplasmic reticulum stress

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경희대학교 동서의학대학원 [1]고려대학교 화학과

Endoplasmic reticulum stress (ER stress) is a strong basis in understanding pathogenesis of various human diseases. Here, we summarize our recent results from confocal microscopy-based biosensing of various ER stress models by tunicamycin, brefeldin A, and palmitic acid-insult.

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Graphene-enhanced cardiomyogenic differentiation of human embryonic stem cells

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Graphene has drawn attention as a substrate for stem cell culture and been reported to stimulate differentiation of multipotent adult stem cells. However, its effect on differentiation of pluripotent embryonic stem cells (ESCs) has not been reported yet. Here, we report that graphene enhances cardiomyogenic differentiation of human ESCs (hESCs). Large-area graphene on glass coverslips was prepared by the chemical vapor deposition method. Vitronectin (VN) coating on the graphene was required for a high viability of hESCs cultured on the graphene. hESCs were cultured on either VN-coated glass (glass group) or VN-coated graphene (graphene group) for 21 days. The cells were also cultured on Matrigel-coated glass (Matrigel group), which is a substrate for the conventional, directed cardiomyogenic differentiation systems. Culture on graphene promoted expression of genes involved in stepwise differentiation into mesodermal and endodermal lineage cells and, in turn, cardiomyogenic differentiation as compared to culture on glass or Matrigel. In addition, culture on graphene enhanced the gene expression of cardiac-specific extracellular matrices. The enhanced cardiomyogenic differentiation was, at least in part, due to enhanced hESC adhesion and the upregulation of extracellular signal-regulated kinases signaling. Graphene could aid to develop stem cell therapies for ischemic heart diseases by enhancing the cardiomyogenic differentiation of hESCs.

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Apolipoprotein A-I mimic peptides with Cys mutation can enhance cholesterol efflux from macrophage

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Apolipoprotein A-I mimetic 4F (DWFKAFYDKVAEKFKEAF) is an amphipathic α-helical peptide with hydrophilic and hydrophobic spheres. Both spheres make intermolecular interactions with another molecule of the same peptide or with cholesterol/ester, forming high density lipoprotein-cholesterol (HDL-C) like particle. A variety of amphipathic peptides has been designed and synthesized as mimicry of 4F by substitution of the most important amino acids to unnatural amino acids both in hydrophilic and hydrophobic spheres. These variants were screened for a mimicry of apoA-? using HDL-C induced cholesterol efflux. A new peptide (2s) with naphthylalanine moiety among these variants showed more than 5-fold improved cholesterol efflux than that of the reference peptide, 4F. We further prepared a series of mutated peptides from 2s sequence. The cysteine-containing analogues of the descendent peptides showed better cholesterol efflux and anti-inflammatory activities relative to 2s. Taken together, we developed improved apo-AI mimetic peptides than the parent 4F or 2s. The improved peptide could be used as a potential therapeutic for releasing risks of atherosclerosis.

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Engineered split- Npu intein mediated protein trans-splicing reaction and cross-reactivities

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동국대학교 의생명공학과

Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. While the PTS became a useful tool for various biological studies, the difficulties associated with the synthesis of 40mer peptide became a drawback in its applications. Here we have generated several engineered split-inteins by shifting the split-site of naturally split-inteins to new positions. We utilized Npu DnaE Intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate how the lengths of N and C intein affect the PTS kinetics, we prepared multiple pairs of split-inteins that consist of various lengths of N and C-inteins. The kinetics of reaction between each engineered pairs and the cross-reactivities were studied. As a result, we found that the mixed pair of split-inteins (native C-intein(w35Ic) and engineered N-intein(e123In)) mediated faster PTS compared to wild type pair of split intein. We also observed The pair of engineered split inteins mediated PTS with decent reaction kinetics (t1/2~ 17 mins). These findings enables faster labeling reaction based on split intein mediated PTS as well as more practical approach by making the synthesis of C-intein easier. This result provides a good guide-line for designing efficient PTS.

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Auxotroph Rescue with Biocompatible Reactions

이윤미

광운대학교 화학과

The non-enzymatic chemical transformation that is biocompatible can rescue the growth of auxotrophic E.coli strains by providing essential metabolites. We applied Ru-catalyzed allyloxycarbonyl (Alloc) deprotection in the presence of the microorganisms to the release of p-aminobenzoic acid (PABA), which is a precursor to folic acid for cell growth. By generating PABA through the non-enzymatic reaction, PABA auxothrophs were able to grow in M9 glycerol minimal medium.

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Structure ensemble based virtual screening discovered new inhibitors of tyrosinase

최준혁 지준구*

경북대학교 약학과

Tyrosinase participates in two distinct reactions, the hydroxylation of L-Tyrosine to L-DOPA and the subsequent conversion of L-DOPA to L-Dopaquinone, in producing melanin in melanocyte. Central roles of melanin in melanocyte have attracted attentions from pharmaceutical and cosmetic companies for developing therapeutic and cosmetic agents by inhibiting the function of tyrosinase. Here we report new inhibitors of mushroom tyrosinase that were predicted by computational methods and confirmed by enzymatic and biophysical assays. In order to enhance the performance of virtual screening, molecular dynamics simulation first produced an ensemble of 10,000 trajectories. Second, we chose a structure that revealed the optimal receiver operating characteristic curve with the known direct binders and their physicochemically matched decoys. Third, high-throughput virtual screening was performed against small molecule library that consists of about 400,000 commercially available molecules. Fourth, we purchased top 60 molecules and tested their inhibitory activities. The extended assays with the analogues of the molecules that showed activities followed. In total, about 30 new inhibitors of tyrosinase were discovered. Several compounds showed much stronger activities than the known tyrosinase inhibitors of arbutin, hydroquinone and kojic acid, having IC50 values in nM range.

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Molecular dynamics simulation studies of oncogenic K-Ras mutants at the positions of Gly12 and Gly13

이승주 지준구*

경북대학교 약학과

One of the most mutated proteins in cancer is Ras. For instance, about 50 % colorectal cancers harbor mutated K-Ras, one of three Ras isoforms. Mutations in K-Ras occur most frequently at the position of Gly12, followed by Gly13 and Gln61. Oncogenic mutants interrupt ther instrinsic GTP hydrolyzing activities of K-Ras, resulting in constitutive activations of K-Ras, resulting in constitutive activations of K-Ras and subsequent downstream signals. Since K-Ras is closely related with the resistance to anticancer drugs, identifying the existences and types of K-Ras mutants in cancer patients become necessary for personalized medicine. To investigate the possible relations between the K-Ras mutants and the types of cancers, a series of molecular dynamcis simulations have been performed with the K-Ras mutant at the position of Gly12 and Gly13. We will discuss the quantitative motional differences in the mutants.

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Surface Modification of Conjugated Polymer Nanoparticles (Pdot) using PS-binding Peptides for Bioimaging

박성준 이윤식*

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Aromatic dialdehydes and diacetonitriles can be transformed into highly fluorescent conjugated polymer nanoparticles (Pdot), through in situ colloidal Knoevenagel polymerization. Their bright fluorescence in the near-infrared region gave viable in vivo imaging capacity, which was proven by sentinel lymph node mapping. However due to their lack of functional groups, further in vivo application has been hardly achieved. To overcome this problem, polystyrene (PS)-binding peptides were used to modify the surface of Pdots. The cyano vinylene-based polymers forming the Pdots interacted with the PS-binding peptides at the surface by π-π stacking and van der Waals force. Using the functional groups of the peptide, bio-friendly functionalization was carried out and their in vitro/ in vivo performance was studied.

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Identification of Natural Product Inhibitors for CDC25 Phosphatases

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Cell division cycle 25 (Cdc25) homologs are dual specificity phosphatases that dephosphorylate both a serine/threonine and a tyrosine side chain of protein substrates. Cdc25 phosphatases also play a critical role in the cell cycle progression by activating kinase of Cdk/cyclin complexes. The human Cdc25 family are composed of three members: Cdc25A, B, and C. Overexpression of Cdc25s results in cell cycle progression, which causes head, colon, and breast cancers. In addition, high expression level of the proteins has been implied to correlate with either a poor prognosis or aggressiveness of tumor. Consequently, discovery of selective Cdc25s inhibitors may be a starting point to develop anticancer therapy. We have screened 658 member of purified natural compounds for inhibition of purified Cdc25s to identify hit compounds for each enzyme. Furthermore, we determined IC_{50} and K_i values of the hits for the enzyme inhibition, and proposed the inhibitor-binding pockets on the enzymes through docking simulation.

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Identification of a Potent Inhibitor of Human Vaccinia-H1 Related (VHR) Phosphatase from Natural Product

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동국대학교 화학과

Human vaccinia-H1 related (VHR) phosphatase, encoded by DUSP3 gene, is one of the smallest known phosphatases regulate phosphorylation of proteins relevant to human diseases. Especially, VHR has been reported as having both tumor suppressive and oncogenic properties, suggesting that identification of its selective inhibitors expected potential anticancer drugs. We screened natural product library for VHR inhibition to identify hit compounds. Furthermore, kinetic evaluation of the hit compounds identified a potent competitive inhibitor with nM Ki.

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Traceless and site-specific fluorescent labeling of membrane anchored proteins in live cells

이의연 권영은*

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The understanding of protein interaction and cellular dynamics is an important step to get insight of biological processes. Therefore, a recent life science research has increasing demands on studying physiological events on the molecular level in real-time. For this purpose, live cell imaging using fluorescent proteins (FPs) has been widely utilized to visualize target proteins under a microscopy by constructing fusion proteins. However, several limitations of FPs, such as slow maturation kinetics or issues with photo-stability under laser illumination, have led researchers to examine new technologies beyond FP-based imaging. In this study, we have utilized Npu DnaE split-intein mediated protein trans-splicing (PTS) reaction for site-specific fluorescent labeling of cell surface proteins. Trans-splicing reaction is a self-processing reaction and can be used to introduce various synthetic probes to target proteins. We prepared a model cell surface protein fused to N-terminal fragment of Npu DnaE intein and a C-terminal fragment of Npu DnaE intein fused to a fluorescent probe. Here, we adopted an engineered Npu intein. The engineered C-intein is considerably shorter compared to wild-type C-inteins, to make the preparation of C-intein becomes easier and to make this approach more practical. We demonstrated that engineered Npu intein mediated labeling reaction is comparable to wild-type Npu intein. No external energy was required for the labeling reaction. This approach can be used for dual color labeling systems by using orthogonal split-inteins and will lead to new methologies that investigate protein localization, transportation, and cell signaling.

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Coupling of spectral shift with spin state equilibrium in the inhibition of rice allene oxide synthase-1 by imidazole

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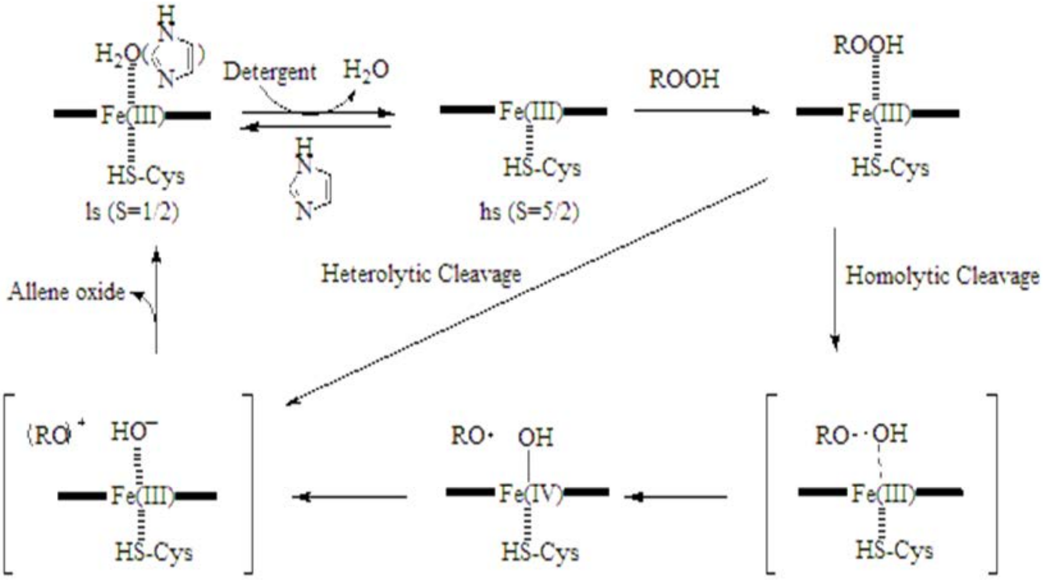
Allene oxide synthase (AOS) is a member of cytochrome P450 subfamily (CYP74) and plays an important role in octadecaoind pathway and defense signaling in plants. CYP74 enzymes are non-classical cytochrome P450 in which molecular oxygen and NADPH-dependent P450 reductase are not required for the catalytic turn over. Instead, CYP74 family enzymes use a hydroperoxide group both as the activated oxygen donor and as a source of reducing equivalents. AOS can utilize 13(S)-hydroperoxyoctadecadi(tri)enoic acid (13(S)-HPOD(T)E) or 9(S)-hydroperoxyoctadecadi(tri)enoic acid (9(S)-HPOD(T)E) as a substrate depending on the specificity, which is converted into the corresponding allene oxide, 12,13-epoxy-9,11-octadecadienoic acid (12,13-EOD(T)) or 9,10-epoxy-10,12,(15)-octadecadi(tri)enoic acid (9,10-EOD(T)). In this study, biochemical and spectroscopic properties of rice allene oxide synthase-1 were characterized. UV-Visible spectral analysis of native OsAOS1 revealed a Soret maximum at 393 nm, which shifted to 424 upon binding of OsAOS1 to imidazole, which were correlated with inhibition of OsAOS1 activity. we analyzed spin state population of OsAOS1 by EPR and compared with the spectral shift induced by imidazole. Our results provide evidences that the imidazole ligand binds to iron(III) as the sixth ligand (distal position) and drives the spin state equilibrium toward low spin state of iron(III) in OsAOS1. The possible dehydration mechanism of OsAOS1 is proposed.


H
N
H_2O
N
Detergent
H_2O
Fe(III)
HS-Cys
ls (S=1/2)
H
N
N
Fe(III)
HS-Cys
hs (S=5/2)
ROOH
ROOH
Fe(III)
HS-Cys
Allene oxide
Heterolytic Cleavage
Homolytic Cleavage
(RO)⁺
HO⁻
Fe(III)
HS-Cys
RO·
OH
Fe(IV)
HS-Cys
RO··OH
Fe(III)
HS-Cys

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Plasmid DNA as a reference molecule for Detection of Genetically Modified Rice with SYBR Green1 Dye using Real-Time Quantitative PCR

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Owing to the policy of GMO Labeling, method for quantitative detection of GMO have to developed and improved. Presently Real-time PCR is one of the suitable method for GMO detection and estimation of transgene copy number. The purpose of our study was to developed novel standard plasmid as a reference molecule for detection of GM rice. Two exogenous target DNA fragments overexpressing the Allen Oxide Cyclase gene and one endogenous fragment of Sucrose Phosphate Synthase gene are present in this plasmid. three primers were designed for each of the exogenous and endogenous DNA fragments with two primers for the former DNA fragment and one for later one, these were tested by qualitative PCR. The specificity of these primers were further checked by generating Melting curve analysis using Real-time quantitative PCR. Standard curve was established by both plasmid DNA and genomic DNA to compare the two types of DNA calibrators using SYBR Green 1 and comparing result showed that the plasmid DNA is suitable as reference molecule. Therefore it is concluded that plasmid DNA can be used instead of genomic DNA as reference molecule.

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SPECIFIC INTRODUCTION OF A GLUTAMINE RESIDUE OF AN ALPHA-HELICAL ANTIMICROBIAL PEPTIDE CONVERTS ITS MEMBRANE DISRUPTING TO CELL PENETRATING ABILITY ELUCIDATED BY METHOTREXATED-CONJUGATED HEMOLYTIC ACTIVITY

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서울대학교 화학교육과

Antimicrobial peptides (AMPs) are results of innate immune response of most of all living creatures against pathogens. Membrane disruption by the AMPs is a major mode of action for pathogen death, but translocation of AMPs followed by modulation of internal targets might be other causes for the pathogen death. While those cell disrupting and cell penetrating characters might exist simultaneously in natural AMPs, we tried to convert cell disrupting to the cell penetrating character by systematic mutations of a model LK peptide that possesses antimicrobial activity. For this purpose, methotrexate (MTX) was conjugated to the N-terminus of the mutant peptides and hemolytic toxicity of the resulting MTX-conjugated peptides were observed and compared with non-conjugated peptides in human red blood cells. Indeed, a specific MTX-conjugated Gln mutation (MTX-L8Q) gave 16-fold improved hemolytic toxicity relative to non-conjugated mutant. It was verified the cell penetrating ability of L8Q accompanies with no observable membrane disruption. Encouraged by these results, we applied this approach to naturally occurring amphipathic AMPs and confirmed the possibility that Gln mutation could be one of strategies for converting cell disrupting to cell penetrating character.

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DESIGN AND SYNTHESIS OF AMPHIPATHIC A-HELICAL MODLE PEPTIDES TO OPTIMIZE CELL-PENETRATING PROPERTIES

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Some a-helical amphipathic peptides with hydrophobic and cationic residues in hydrophilic face have unique properties such as antimicrobial activity and the cell penetrating ability. Especially, a model LK and KLA peptides have been known as widely used mitochondrial and microbial membrane targeting. We also observed KLA and LK peptides have some cell penetrating ability. Recent results of our laboratory demonstrated that formation of dimer α-helical bundles with these model peptides have unusually high cell penetrating abilities. Too optimize cell penetrating ability, we further changed various aspects of model peptides, such as sequences, length of amino acids, portion of cationic residues, sizes of hydrophobic residues at hydrophobic face. Results of experiments suggests that the length, the portion of cationic residues, the size of hydrophobic residues of the monomeric peptides affect significantly on the penetrating ability, while the orientation (parallel or anti-parallel) of dimers or consequences of peptide do not. More potent cell penetrating peptides could be designed and synthesized by applying these newly observed knowledge.

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Detergent-dependent oligomerization and coupling of spectral shift with spin state equilibrium in rice allene oxide synthase-1

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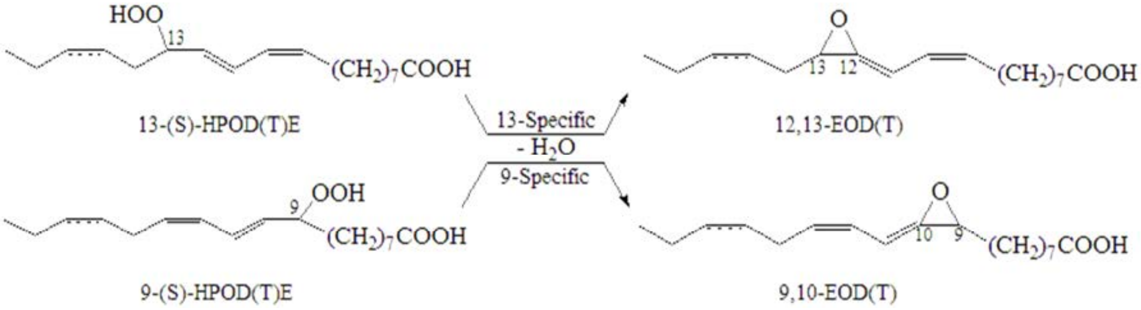
Allene oxide synthase (AOS) is a member of the cytochrome P450 subfamily 74 and converts fatty acid hydroperoxides into unstable fatty acid epoxides, which can be metabolized to 12-oxophytodienoic acid and subsequently undergoes reduction and β-oxidation to yield JA. In this study, biochemical and spectroscopic properties of rice allene oxide synthase-1 were characterized. OsAOS1 without any putative chloroplast targeting sequence was localized in chloroplast and showed steterospecific conversion of 9 and 13 di(tri)enoic hydrperoxy fatty acids. Oligomeric state of OsAOS1 was confirmed by cross-linking experiments. UV-Visible spectral analysis of native OsAOS1 revealed a Soret maximum at 393 nm, which shifted to 424 upon binding of OsAOS1 to imidazole, which were correlated with inhibition of OsAOS1 activity. F92L point mutation enhanced HPL activity and spectral shifts of Soret maximum were observed with P430A and F92L/P430A mutants. We analyzed spin state population of OsAOS1 by EPR and compared with the spectral shift induced by imidazole. Our results suggest that detergent-dependent oligomeric state of OsAOS1 is an important factor for the regulation of its catalytic efficiency and provide evidences that the imidazole ligand binds to iron(III) as the sixth ligand (distal position) and drives the spin state equilibrium toward low spin state of iron(III) in OsAOS1.



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Natural Product inhibitors selective to Slingshot (SSH) protein tyrosine phosphatase (PTP) family

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Protein tyrosine phosphatases (PTPs) play an important role in regulating protein tyrosine phosphorylation. Protein phosphatase slingshot (SSH) homologs are members of dual specificity protein phosphatase (DUSP), consisting of three members, SSH-1, -2 and -3. SSHs dephosphorylate cofilin to cause actin reorganization, resulting in increased cell migration. In addition, dysfunction of cofilin has been known to cause neurodegenerative diseases and vascular diseases. Consequently, the inhibitors of SSHs may be used as potential therapeutics for the diseases described above. Therefore, we screened 658 natural compounds for SSH inhibition by in vitro enzyme assay using 6, 8-difluoro-4-methylumberlliferyl phosphate (DiFMUP) as a fluorescent substrate, identifying inhibitors selective to SSHs over the other PTPs.

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Development of a single chain antibody that specific to homocysteine

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Homocysteine is an amino acid containing a free thiol moiety. The level of homocysteine in plasma relates to cardiovascular and Alzheimer's diseases, and the measurement of homocysteine is important for diagnosis of such diseases. However, selective and efficient detection of homocysteine is difficult due to the interference of structurely similar compounds such as cysteine and glutathione. To develop a selective detection method, we synthesized an adduct of homocysteine and a coumarin-derivative, and screened M13 library displaying single chain antibody (scFv). After 4 round of biopanning, a scFv clone which is specific to the sing M13 an single chain antibody specific to homocysteine-coumarin adduct was identified. The purified scFv showed specific binding homocysteine-coumarin adduct not to cysteine-coumarin adduct. This scFv will be used for an efficient and selective detection of homocysteine in plasma.

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Expression and Structural Studies of FAS1 Domains of Human Periostin, an Extracellular Matrix Protein Involved in Cancer Metastasis and Chronic Allergic Inflammatory Diseases

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Periostin, a component of the extracellular matrix expressed by fibroblasts in normal tissues and stroma of primary tumor, is associated with asthma, chronic allergic inflammation and metastatic colony formation. The four internal repeat fasciclin I (FAS1) domains of periostin play an important role in cell adhesion and tumor metastasis by binding with integrins. At the N-terminus, periostin has a cysteine-rich EMILIN (EMI) domain involved in protein-protein interactions. We successfully refolded EMI domain having a correct three intramolecular disulfide bonds in a proper redox buffer condition. The gene of the FAS1 domains of human periostin were systemically constructed and their expression were tested using *E. coli* expression system. Although all FAS1 domains were well expressed, but only FAS1_II and IV were soluble fractions after cell lysis. The structural characteristics of FAS1 domains studied by circular dichroism (CD) and nuclear magnetic resonance (NMR) spectroscopy. CD studies clearly showed that FAS1_II and IV domains were composed of α-helix and β-sheet structure, which is consistent with a previously determined FAS1 domain from *Drosophila melanogaster*. NMR studies showed that FAS1_II and IV domains are well folded. We obtained backbone resonance assignment of FAS1_IV domain of human periostin using triple resonance NMR spectroscopy : HNCA, HN(CO)CA, HNCACB, CBCA(CO)NH. These results suggest that human periostin domain especially FAS1_IV is good target for further biochemical and structural studies.

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The new strategy to identify protein interaction between cobB and acetyl-CoA synthetase in *Escherichia coli*, based on the photocrosslinking chemistry

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고려대학교 화학과

Recently, acetylation on protein lysine residue in prokaryotes is found that occurs broadly as much as in eukaryotes. This protein acetylation has the effects on many cellular phenomenon including transcription, translation, and protein-protein interactions especially gene transcription regulation. However, the mechanism of this protein acetylation and deacetylation in prokaryotes is not fully understood. The numerous acetylation sites and acetylated proteins in prokaryotes have been revealed by using MS analysis. By contrast, the information about deacetylation mechanism is little known. Up to the present, studies on the identification of unknown substrates interacting with cobB, a solely known deacetylase in *Escherichia coli,* are still challenged. Thus, we hope to demonstrate the possibility of photocrosslinking method for identification of unknown cobB substrates. Herein, we develop a photocrosslinking method for photocrosslinkage between cobB and Acetyl-CoA Synthetase based on the genetic incorporation of unnatural amino acid into cobB, thereby proofing the possibility and utility of photocrosslinking approaches.

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A thiol-reactive rosamine derivative inhibits tau aggregation by blocking tau intermolecular disulfide bond formation

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The primary function of tau is to promote and stabilize microtubule assembly in neuronal axons. When pathologically modified, tau dissociates from microtubules and become insoluble aggregates called neurofibrillary tangles (NFTs). The NFTs are made up of paired helical filaments (PHFs) that constitute the defining characteristics of Alzheimer's disease, Parkinson's disease and many other neurodegenerative disorders collectively called tauopathies. The PHFs are consisted of aggregated tau. Tau aggregation is a multistep process with diverse intermediate stages. To become a susceptible intermediate for aggregation, tau protein undergoes a series of post-translational modifications. Among diverse modifications, oxidation state of the protein has been shown significant role to influence tau aggregation tendency. Full length human tau contains two cysteine residues (Cys291 and Cys322) in its amino acid. These cysteines can form both intra- and inter-molecular disulfide bonds. During in vitro tau aggregation, tau-tau disulfide-linked dimers form first that serve as the seeds for higher order aggregates. So, intermolecular disulfide linkage is important in the generation of tau aggregates. Here we envision that prevention of tau disulfide bond formation with a small molecule would inhibit the generation of tau aggregates. We have tested a bunch of chemical compounds for their ability to inhibit the assembly of tau into aggregated filaments in vitro. The exclusive criteria of our tested compounds are the thiol reactivity and they also possess the fluorescence properties. In particular, two novel compounds were proved effective in the inhibition of tau filament formation with IC50 values in the low micromolar range. Therefore, this finding provides a new strategy for inhibiting tau aggregation by targeting tau intermolecular disulfide cross-links.

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Identification of natural product inhibitors for protein-tyrosine phosphatase non-receptor type 1 (PTP1B)

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동국대학교 화학과

The relevance of the PTPs in diverse pathophysiology has made them interesting targets for new classes of drugs. PTP1B is a member of protein tyrosine phosphatase (PTP) superfamily. Among PTPs, PTP1B has emerged as the best-validated drug target. Since PTP1B is a negative regulator of the insulin signaling pathway it is considered as a promising therapeutic target for treatment of type 2 diabetes. Natural compounds, by themselves, can make full use of the promising drugs as well as lead compounds for developing drugs. We screened 658 natural products to identify selective inhibitors for PTP1B.The selected natural products were further characterized by enzyme kinetics.

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Nanomolar inhibition of HIV-1 transcription using dimeric alpha-helical cell-penetrating peptides

장상목 현순실 김서연 이연[1,*] 유재훈[*]

서울대학교 화학교육과 [1]서울대학교 화학부

We constructed dimeric alpha-helical peptide bundles based on leucines (L) and lysines (K) for both efficient cell penetration and inhibition of Tat-TAR interaction. The LK dimers can nearly quantitatively penetrate into eukaryotic cells and effectively inhibit the elongation of the TAR transcript at low nanomolar concentrations. The effective inhibition of HIV-1 replication strongly suggests that the LK dimer has the strong potential as an anti-HIV-1 drug.

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A graphene oxide based platform for detection of mutant fusion DNA using quencher-free fluorescent DNA probe and polymerase chain reaction

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Graphene oxide (GO) has been applied in diverse biomedical areas as a versatile material for sensors. GO preferentially binds to single-stranded DNA (ssDNA) over double-stranded DNA (dsDNA) and quenches fluorescence when the fluorophore stays close to GO surface. In this study, we developed a simple and efficient method for detection of mutant fusion gene using fluorescent probe DNA and polymerase chain reaction. Bcr-Abl fusion gene that causes Chronic Myeloid Leukemia (CML) was used as a model system for detection of mutant gene. In our designed system for mutant gene detection, GO quenches the fluorescent probe DNA and Taq polymerase degrades the probe DNA due to its 5′-end nuclease activity. When the Bcr-Abl mutant gene is present, PCR amplification of Bcr-Abl results in degradation of the fluorescent probe DNA annealed to the Bcr-Abl amplicon. In the absence of Bcr-Abl, the fluorescent ssDNA probe remains intact due to the absence of amplification. Addition of GO to each reaction solution gave rise to different fluorescence signal; enhanced fluorescence with degraded probe DNA in Bcr-Abl (+), and quenched fluorescence with ssDNA adsorbed onto GO in Bcr-Abl (-). We observed fluorescence signal difference between Bcr-Abl positive and negative cells, and the fluorescence signal was quantitatively correlated with composition of these cells. Thus, our detection system can be applicable as quantitative assay for primary diagnosis as well as monitoring therapeutic responses by measuring the expression level of Bcr-Abl fusion gene in leukemia patients.

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Cellular responses by particulate matter in human respiratory epithelial cells

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Particulate matter (PM) is one of the most common ambient air pollutants, which is derived from diesel engine, wildfires, yellow dust, and other combustion sources. In general, size of the PM determines the negative effect on human health. Recently, PM-caused risks of damaging respiratory organs including lung disease are increasing every year. Autophagy and apoptosis are cellular responses to nutritional deficiencies and/or degradation of dysfunctional proteins, which is necessary for maintaining of cellular homeostasis. Previous studies have reported that PM-induced autophagy and apoptosis has been considered as an important molecular mechanism of PM-mediated cytotoxicity in lung cancer epithelial cells. In this study, we investigated effect of particulate matter (PM2.5) on cellular responses in human respiratory epithelial primary cells. The epithelial cells showed decrease of cell viability when exposed to PM in a time and dose dependent manner. In addition to onset of autophagy via increase of LC-3 (microtubule-associated protein light chain-3) puncta, PM treatment increases expression of inflammatory cytokine, tumor necrosis factor-α (TNF- α) in human respiratory epithelial primary cells. Thus, inflammation response as well as autophagosome formation were induced for survival of respiratory epithelial primary cells under challenge of PM.

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Detection of single nucleotide polymorphisms with DNAzyme and graphene oxide

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Single nucleotide polymorphisms (SNPs) are caused by DNA sequences containing a single different nucleotide, which are often related with disease and drug efficiency to each individual. Therefore, a method of SNP detection is needed for the diagnosis of SNP-related diseases and the prescription of personalized medicine. In this study, we report a novel assay for detection of SNPs using graphene oxide (GO), DNAzyme (Dz), and fluorescent labeled DNA (F-DNA). GO has a high affinity to single strand nucleic acid with a fluorescence quenching near the GO surface, whereas it shows a weak affinity for the double stranded nucleic acids. Dz is a catalytic oligodeoxyribonucleotide that can cleave phosphodiester bonds in the target RNA. As a model system, we used a fragment of ABL RNA (45 mer) containing a point mutation (T315I) in ABL gene of BCR-ABL mutant chimeric gene that causes chronic myeloid leukemia (CML). The T315I point mutation results in drug (imatinib mesylate) resistance with no other alternative regimens. In our SNP detection system, Dz specifically cleaved T315I mutant ABL RNA and generated pieces of RNA. RNA/F-DNA duplexes were then formed by adding F-DNA that can anneal to a cleaved product of T315I mutant RNA. GO was then added to the reaction solution, and the fluorescence of these RNA/F-DNA duplexes generated from the T315I mutant RNA was not quenched by GO. However, the ABL RNA lacking the SNP (i.e. wild type ABL RNA) was not cleaved by Dz, and RNA/F-DNA duplexes were subsequently formed as partial duplexes with single stranded portions. The fluorescence of the partial duplex RNA/F-DNA was adsorbed onto GO with significant fluorescence quenching. We confirmed appreciable fluorescence differences between T315I mutant RNA and ABL wild type RNA, using the fluorescence quenching GO-based SNP detection, which will be applicable for the detection of SNPs in RNA with simplicity, sensitivity, and selectivity.

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Comparison of delivery efficiency of doxorubicin intercalated in RNA aptamer and the one encapsulated in RNA aptamer-conjugated liposome

백시은 김동은*

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Combination of drug delivery and specific targeting has potentials for treating cancer diseases. To achieve this goal, specific ligands targeting cancer cells and bioconjugate vehicles for drug delivery are necessary. Liposomes are one of successful drug-delivery materials because they can reduce toxicity and enhance stable drug delivery by encapsulation of drugs. They are composed of a lipid bilayer, which can fuse with the cell membrane. Aptamers are single-stranded nucleic acid that can bind to target molecules with high affinity and specificity. RNA aptamer has been used as drug delivery material targeting the tumor, in which anti-cancer drug was intercalated in aptamer. For example, prostate cancer cells expressing prostate-specific membrane antigen (PSMA) have been targeted for specific delivery of doxorubicin (Dox) with PSMA RNA aptamer. In our study, we compared two methods for Dox delivery to the PSMA (+) cancer cells, which are intercalation of Dox into the aptamer (Apt-Dox) and encapsulation of Dox in the aptamer-conjugated liposome (termed as “aptamosome”). Based on results regarding specificity and Dox delivery efficiency toward PSMA(+) cancer cells, aptamosomes encapsulating Dox (Apm-Dox) was superior to Apt-Dox. Thus, we demonstrated that anti-cancer drug Dox is safely encapsulated in the aptamosome which specifically targets the PSMA(+) prostate cancer cells.

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Alleviation of capsular formation on the silicone implant inserted in rats by biomembrane-mimic coating

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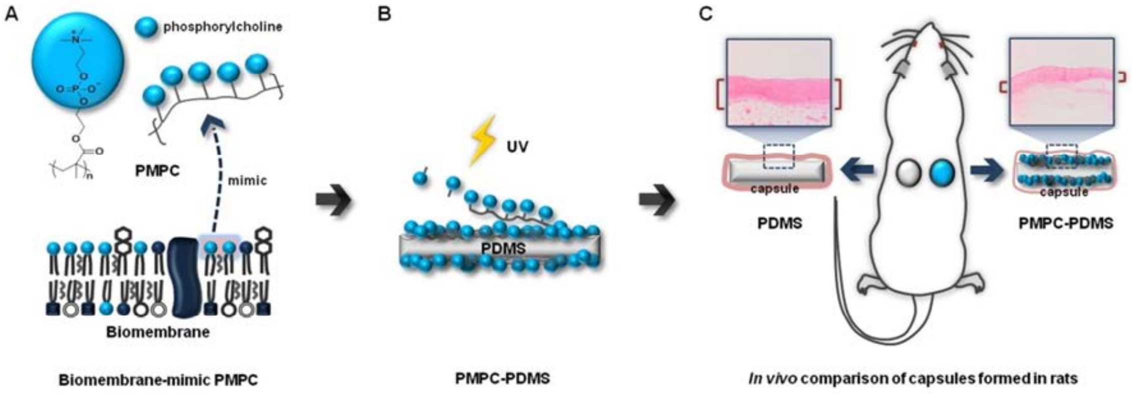
Silicone implants are popularly used in breast augmentation and reconstruction surgeries, but limited biocompatibility induces severe side effects such as capsular contracture, an excessive foreign body reaction forming a tight and hard fibrous capsule around the implant. This study examined the effects of biomembrane-mimic surface coating of silicone implants to the capsular formation. Covalently attached biomembrane-mimic polymer, poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC), prevented nonspecific protein adsorption and fibroblast adhesion on the silicone surface. More importantly, in vivo capsule formation around the PMPC-grafted silicone implant in rats represented significantly thinner capsules, lower collagen density, and more regular collagen alignment than bare silicone implant. The decrease of α-smooth muscle actin also supported the alleviation of capsular formation by the biomembrane-mimic coating. Decrease of inflammation-related cells, myeloperoxidase, and transforming growth factor-β showed reduced inflammation in the capsular tissue. The biomembrane-mimic coating of silicone implants will have a high potential to prevent capsular contracture and to develop biocompatible materials for various biomedical applications.



Biomembrane-mimic PMPC

PMPC-PDMS

In vivo comparison of capsules formed in rats

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Technical Developments of Correlative Microscopy using Transient Receptor Potential Canonical (TRPC) 4 and Quantum dot in vivo

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The trasient receptor potential (TRP) channel family is a class of Ca2+ permeable channels. TRPC4 is a member of the transient receptor potential canonical channels. This protein forms a non-selective calcium-permeable cation channel that is activated by Gq-coupled receptors and tyrosine kinases, and plays a role in multiple processes including endothelial permeability, vasodilation, neurotransmitter release and cell proliferation. Although the extensive studies on the function of TRPC4 have been reported so far, the mechanisms of Calcium sensing and signaling through the transmembrane region are remains elusive. We have shows that with the use of immunohistochemistry, Quantum dot express TRPC4 at the cell membrane. By confocal imaging and Cryo-electron microscopy, we detected localization and changes of a few fluorescence signals upon binding of the Calcium in cells of TRPC4. These results may provide valuable insights for the further structural study of transmembrane domain of TRPC to elucidate the activation mechanism. Therefore, further structural studies of TRPC4 in cells with various labeling strategies and Cryo-electron tomography (CryoET) allows 3D visualization of cellular will be needed.Furthermore, to enable imaging of frozenhydrated and fluorescently labeled biological specimens on EM grids, we have developed a homebuilt cryo-fluorescence light microscopy stage. This allows direct correlation between two sets of imaging data, optical imaging and electron imaging. The correlative approach detailed here will be valuable for broader applications in cell biology, such as cell signaling, membrane receptor trafficking, and many other dynamic cellular processes.

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A Medusa-Like β-cyclodextrin with Maleic Anhydride Derivatives, A Potential Carrier for pH-Sensitive DrugRelease

박으뜸 이연[1,*]

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We developed a new pH-sensitive drug delivery carrier based on β-cyclodextrin (β-CD) and 1-methyl-2-(2'-carboxyethyl) maleic anhydrides (MCM). To optimize pH-sensitivity for controlled drug release, we synthesizedfive maleic acid amide derivatives (maleic, citraconic, cis-aconitic, 2-(2’-carboxyethyl) maleic, MCM) maleic acidamide), and compared their degradability for the development of pH-sensitive biomaterials with tailored kinetics of therelease of drugs. Based on these results, we selected MCM and the primary hydroxyl groups of β-CD weresuccessfully attached to MCM residues to produce a medusa-like β-CD-MCM. The MCM residue was conjugated withcephradine (CP) with high efficiency (>90%). More importantly, β-CD-MCM-CP responded to the small pH drop from7.4 to 5.5 and released greater than 80% of the drugs within 0.5 h at pH 5.5. In addition, the inclusion complexbetween β-CD-MCM-CP and the adamantane derivative was formed by simple mixing to show the possibility ofintroducing multi-functionality. Based on these results, β-CD-MCM can target weakly acidic tissues or organelles, suchas tumours, inflammatory tissues, abscesses, or endosomes, and be easily modified with various functional moieties,such as ligands for cell binding or penetration, enabling more efficient and specific drug delivery.

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PTM-orchestrated regulation of tau aggregation

임성수 김도희[1] 김윤경*

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Microtubule-associated protein tau is abnormally hyperphosphorylated and aggregated into neurofibrillary tangles (NFTs) in multiple neurodegenerative disorders including Alzheimer's disease (AD). It has become apparent that the hyperphosphorylation of tau plays a crucial role in the aggregation process. Therefore, the strategies to reduce tau phosphorylation are important therapeutic target to cure tauopathies. The glycosylation stand out as a potent therapeutic target to prevent tau pathology. The O-linked N-acetylglucosamine (O-GlcNAc) posttranslational modification of tau has been shown to be reciprocal to its phosphorylation; increasing O-GlcNAc leads to reductions in tau phosphorylation. O-GlcNAc glycosylation regulated phosphorylation of tau in a site-specific manner both in vitro and in vivo. By protection of tau phosphorylation site, O-GlcNAc glycosylation negatively regulated tau phosphorylation. Though its pathological importance in tau pathology, the mechanism of tau modifications are not clear. Here, we focus on understanding the balance between phosphorylation and glycosylation of the tau protein, which is implicated in tau aggregation process in neurodegenerative disease are intimately linked.

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Classification of bacteria using ESI lipid spectra

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Identification of bacteria has been performed with GC-MS by obtaining fatty acid methyl ester (FAME) spectra and statistical treatment. Though FAME can be used successfully for identifying bacteria, recent development of ionization method leads us to use higher mass molecule since recording large molecular weight became easy. So, there has been attempt to identify bacteria using lipid profile using electrospray ionization (ESI), low temperature plasma (LTP), and so on. ESI is a technique used in mass spectrometry to produce ions using an electrospray in which a high voltage is applied to a liquid to create an aerosol. It is especially useful in producing ions from macromolecules because it overcomes the propensity of these molecules to fragment when ionized. The ESI spray requires little or no sample preparation prior to analysis and thus allows the sample to be examined rapidly in a near native state. In this study, four bacteria are cultivated 12 hr and 24 hr in LB agar plate. The bacteria are harvested with 1.5ml PBS. PBS was removed after mild centrifugation. Harvested samples were resuspended with 100% MeOH and directly analyzed by ESI-MS. The positive and the negative ion mode mass spectra were recorded for each bacterial sample with a scan range of 100?1400 m?z. The spectra obtained with both methods are compared with each other including the different culture duration. The plates are cultivated for each bacterium and their spectral patterns are analyzed by principal component analysis (PCA). The feasibility of identifying bacteria with lipid spectra and its field application is discussed.

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Facile Microscale Radiosynthesis of [^{18}F]-3’-deoxy-3’-fluorothymidine

김희권

전북대학교 의학전문대학원/핵의학교실

[^{18}F]-3’-deoxy-3’-fluorothymidine ([^{18}F]FLT) is a compound used in junction with positron emission tomography (PET) to study the cellular proliferation of tumors. Despite the recent studies done on the radiosyntheses PET probes on miniaturized devices, there have yet to be studies conducted on [^{18}F]FLT. We have studied miscroscale-level radiosynthetic conditions by examining several microscale reactions that produced a high radiochemical yield of [^{18}F]FLT. Synthesis of [^{18}F]FLT was done using 3-N-Boc-5′-O-dimethoxytrityl-3′-O-nosyl-thymidine on a microchip, and crude purification was done using the cartridge method. Through the analysis of several effects on the radio-synthetic reaction, [^{18}F]FLT was successfully prepared with a radiochemical yield of 71% and the product showed purity greater than 99%. These results suggest that our method can be adopted as a new guideline for a more rapid and efficient method of synthesizing [^{18}F]FLT.

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Novel and Facile Preparations of [^{18}F]-Flouromisonidazole([^{18}F]-FMISO) for Hypoxia Imaging Agents

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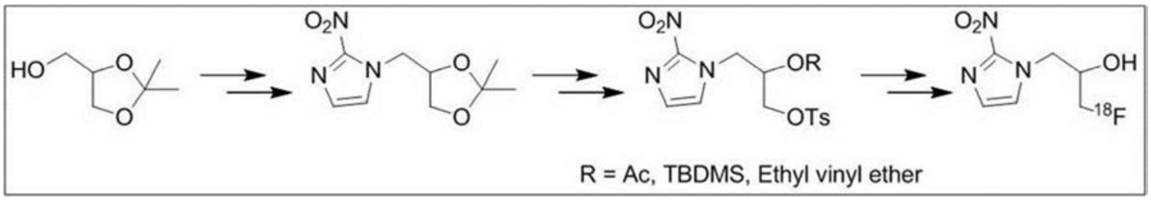
전북대학교 의과학과 [1]전북대학교 의학전문대학원/핵의학교실

Hypoxia is a decreased oxygenation condition in tissues. Many tumors are related with hypoxia due to oxygen deficiency. In order to detect hypoxia, [^{18}F]-Flouromisonidazole([^{18}F]-FMISO), a hypoxia imaging marker, is commonly used in Positron Emission Tomography(PET). This study was focused on development of new synthesis processes for the [^{18}F]-FMISO. The synthesis started with an inexpensive starting material, (2,2-dimethyl-1,3-dioxolan-4-yl)methanol. And two different one-pot syntheses were employed for the preparations of the [^{18}F]-FMISO precursors which contain three leaving groups; tert-butyldimethylsilyl(TBDMS) group, acetyl(Ac) group, and ethyl vinyl ether group. And then new [^{18}F]-FMISO precursors was used to synthesize [^{18}F]-FMISO via treatment of K2.2.2., K2CO3 and ^{18}F, followed by hydrolysis with HCl. These new synthetic routes provide alternative choices for the hypoxia imaging marker.



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Relationship between the boiling point of the solvent(Tetrahydronaphthalene, Anisole, Chloroform) for tips-pentacene and the electrical character of OTFT device

조영재

현대로템 산업설비제어기술팀

To investigate the relation between the boiling point of the solvent I wrote this paper. I studied 3 kinds of OTFT units which are made by using Tetrahydronaphthalene, Anisole and Chloroform as a solvent for tips-pentacene. By observing how each tips-pentacene is crystallized when I used a different kinds of solvent, I could find the relationship among the boiling point, crystalliztion characteristic. Futher, I could find the reletionship between a crystalliztion characteristic and a electrical characteristic of the OTFT through an analysis of the output curve and transfer curve for each OTFT unit

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Synthesis of 1*H*-benzo[*g*]indazole derivatives from Morita-Baylis-Hillman adducts: propargyl-allenyl isomerization and 6π-electrocyclization involving two aromatic π-bonds

임진우 유진 김재녕*

전남대학교 화학과

The indazole nucleus is pharmaceutically important and constitutes the key subunit in many drug substances with a broad range of pharmacological activities. Thus numerous synthetic methods of indazole derivatives are known. However, there have been reported a few reports on the synthesis of tricyclic angular 1*H*-benzo[*g*]indazoles, and most of the syntheses required a multi-step process. In these contexts, we developed an efficient synthetic process of 1*H*-benzo[*g*]indazoles from readily available Morita-Baylis-Hillman (MBH) bromides. The synthesis of 1*H*-benzo[*g*]indazoles was carried out from MBH bromide *via* a sequential copper-catalyzed alkynylation, one-pot synthesis of pyrazole, propargyl-allenyl isomerization, and a 6π-electrocyclization involving two aromatic π-bonds and an allenyl π-bond.

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Synthesis of 3-(γ,δ-disubstituted)alkylidene-2-oxindoles from isatins by Wittig reaction with Morita-Baylis-Hillman bromides

문혜란 임진우[1] 김재녕[1,*]

전남대학교 자연과학대학 화학과 [1]전남대학교 화학과

The 3-alkylidene-2-oxindole ring system represents a key substructure found in many biologically important compounds. Thus, further functionalizations of the 3-alkylidene moiety including an extension of the conjugation with C=C bond have received much attention. In these contests, various 3-(γ,δ-disubstituted)alkylidene-2-oxindoles have been synthesized by the Wittig reaction between isatins and the phosphorous ylide derived *in-situ* from the Morita-Baylis-Hillman bromides. Further studies on the chemical transformations of prepared compounds will be presented including 6π-electrocyclization and the reaction with Lawesson's reagent.

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Facile one-pot synthesis of 1,3,5-trisubstituted pyrazoles from α,β-enones

유진 문혜란[1] 김재녕*

전남대학교 화학과 [1]전남대학교 자연과학대학 화학과

1,3,5-Trisubstituted pyrazolines are important heterocyclic compounds which can be prepared from substituted hydrazines and α,β-enones. The oxidation of these pyrazolines provides the corresponding pyrazoles, which are known to possess diverse biological activities. A direct synthesis of 1,3,5-trisubstituted pyrazoles from α,β-enones has also been reported; however, most of them suffer from low yield and/or harsh reaction conditions. Thus, an efficient and practical one-pot synthetic procedure of 1,3,5-trisubstituted pyrazoles is highly required until now. In these contexts, we developed a practical and efficient one-pot synthesis of 1,3,5-trisubstituted pyrazoles from α,β-enones and arylhydrazine hydrochlorides. The pyrazoles were formed *via* a tandem formation of the corresponding pyrazolines and an acid-catalyzed aerobic oxidation process.

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Synthesis of pyrazolo[4,3-*c*]quinolines from Morita-Baylis-Hillman adduct of 2-bromobenzaldehydes

유진 문혜란[1] 김재녕*

전남대학교 화학과 [1]전남대학교 자연과학대학 화학과

Pyrazolo[4,3-*c*]quinoline derivatives have received much attention due to their wide pharmaceutical and biological activities including $GABA_A$ receptor modulators and interleukin inhibitors. Thus, the synthesis of pyrazolo[4,3-*c*]quinoline derivatives has been studied extensively. Among the synthetic methods, condensation of 3-acylquinolin-4-ones with appropriate hydrazine derivatives and S_NAr type cyclization of 4-haloquinolines have been used most frequently. In addition, other methods have also been reported involving the use of Cu-catalyzed *N*-arylations or [3+2] cycloaddition of azomethine ylide as a key step. In this context, we developed a new synthetic procedure of pyrazolo[4,3-*c*]quinoline derivatives. The synthesis has been carried out from the Morita-Baylis-Hillman bromide of 2-bromobenzaldehyde and methyl vinyl ketone *via* the sequential introduction of tosylamide, condensation with *N*-substituted hydrazines, conversion to pyrazoles, Cu-assisted intramolecular *N*-arylation, and the final elimination of *p*-toluenesulfinic acid.

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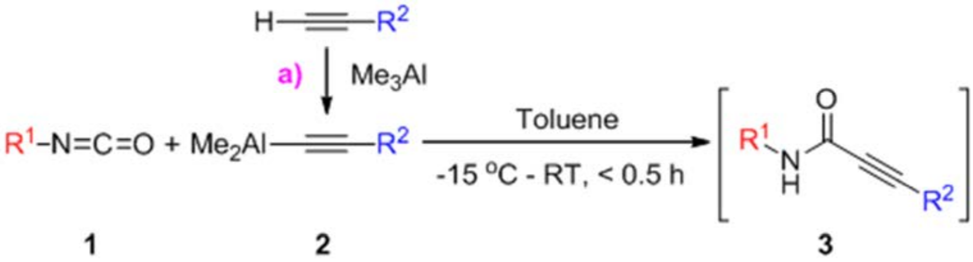
Synthesis of propiolamides from isocyanates and alkynyldimethylaluminum prepared from terminal alkynes and trimethylaluminum

정성수 이상협*

대구가톨릭대학교 생명화학과

As a part of ongoing program on the development of novel synthetic methods in organic synthesis, we report herein an efficient procedure for the synthesis of N-substituted propiolamides from isocyanates using alkynyldimethylaluminum reagents. To verify the functional group tolerance, a variety of isocyanate substrates were reacted with alkynyldimethylaluminum reagents derived from wide range of terminal alkynes to provide desired products in excellent yield.



a) Toluene, 60 °C, 6-10 h

R^1 = alkyl, aryl(with various functional groups), benzyl, benzoyl, allyl, naphtyl
R^2 = (cyclic)alkyl, aryl, heteroaryl

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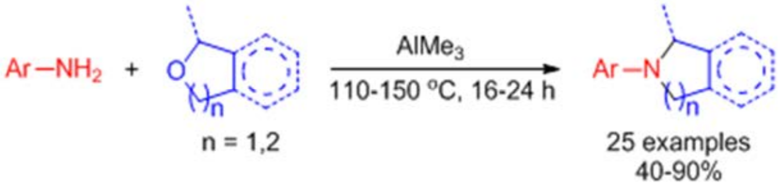
Synthesis of N-aryl azacycles from corresponding oxacycles using aluminum-amides prepared from arylamines and trimethylaluminum

이상협

대구가톨릭대학교 생명화학과

Synthesis of N-aryl substituted, five- and six-membered azacycloalkanes, isoindolines and tetrahydroisoquinolines, has been described. In this synthesis, cyclic ethers (n = 1, 2) were treated with dimethylaluminumamide reagents, derived from a range of aryl amines and trimethylaluminum, to afford the corresponding azacycles in good yields.



Balaji L. Korbad and Sang-Hyeup Lee;
Chem. Commun. (DOI: 10.1039/C4CC04111A)

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Synthesis of N,N-disubstituted 3-amino-1,4-diynes and 3-amino-1-ynes : Addition of alkynyldimethylaluminum reagent to formamides and N,O-acetals

이상협

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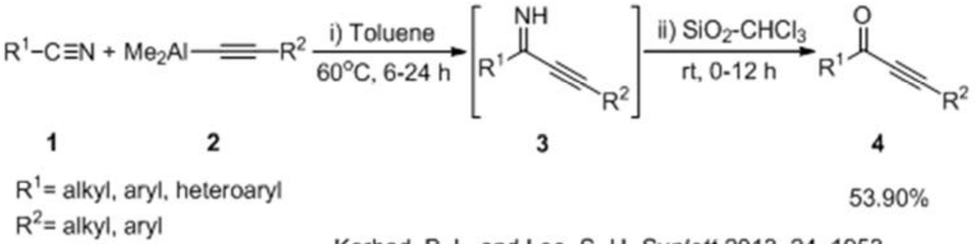
Organoaluminum reagents have proven as remarkable reagents in organic synthesis due to their inherent reactivity, wide range of applicability, low cost and commercial availability. Organoaluminum compounds can easily react with various heteroatoms in organic molecules, particularly with oxygen and nitrogen, even with carbon to form a strong coordinate complex (1:1). Micouin et al. has developed the alkynyldimethylaluminum reagent from the reaction of alkynes with trimethylaluminum using a catalytic amount of Et3N. We have utilized alkynylaluminum reagents for the synthesis of α,β-alkynyl ketones 3-(N,N-Disubstituted Amino)-1,4-diynes and 1-ynes.

Balaji L. Korbad and S.-H. Lee
Eur. J. Org. Chem. (DOI: 10.1002/ejoc.201402464)



Korbad, B. L. and Lee, S.-H. *Synlett* 2013, 24, 1953

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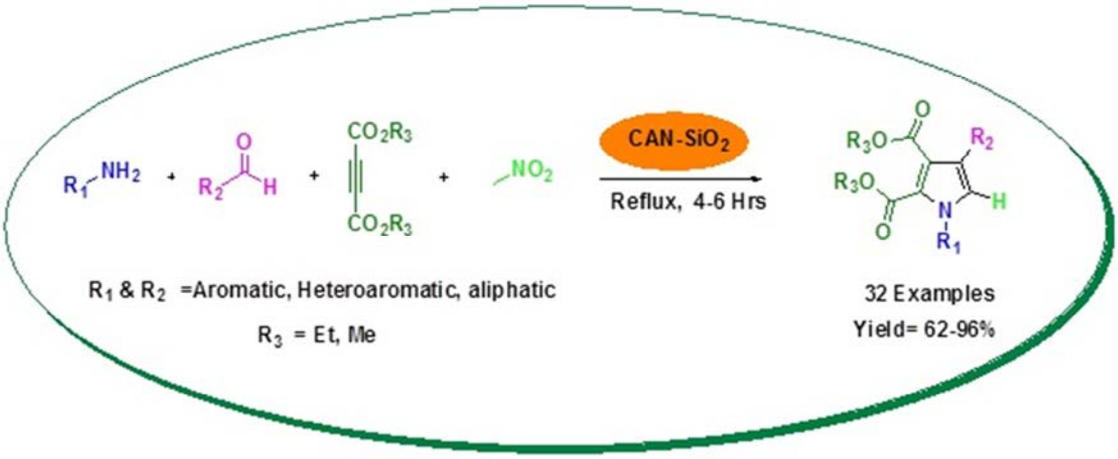
CAN:SiO2 -the most efficient catalyst for the four-component reaction for the synthesis of tetrasubstituted pyrroles

Atar Amol Balu 정연태*

부경대학교 이미지시스템공학과

An efficient, and expeditious method has been developed for the synthesis of tetrasubstituted pyrroles via a four component, one-pot cyclocondensation reaction of amines, aldehydes, dialkyl acetylenedicarboxylates and nitroalkanes using silica supported ceric ammonium nitrate as heterogeneous catalyst for the first time. Reusable silica supported ceric ammonium nitrate was found to be a highly efficient and renewable heterogeneous catalyst for the rapid and convenient synthesis of tetrasubstituted pyrroles derivatives. The advantageous features of this novel methodology are high atom-economy, operational simplicity, shorter reaction time, convergence, and facile automation.



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발표분야: 유기화학

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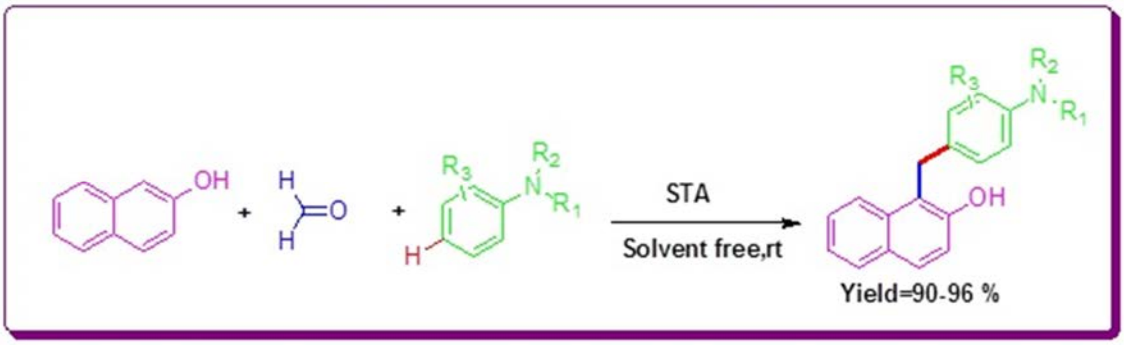
Silica tungstic acid (STA): A green catalyst for the synthesis of diarylmethanes via a one-pot, three-component reaction under solvent free condition

ShindeVijayVilas 정연태*

부경대학교 이미지시스템공학과

A cost-effective and eco-friendly synthesis of diarylmethanes derivatives has been developed through the Mannich type Friedel?Crafts addition reaction of tertiary aromatic amine formaldehydes with β-naphthol/ indole using silica supported tungstic acid (STA) as a recyclable heterogeneous acid catalyst in solvent free condition. Here we proposed two schemes using same catalyst. Effect of different solvents and comparison of silica supported tungstic acid with different acid catalysts have also been studied.



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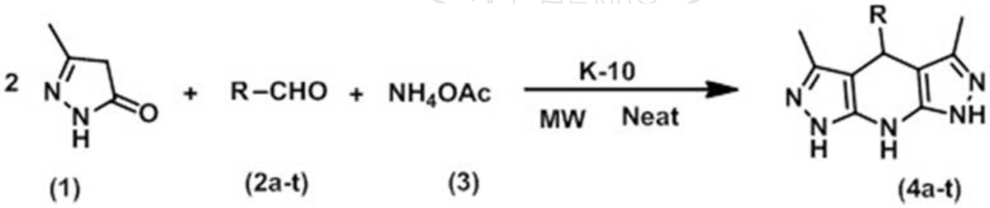
발표종류: 포스터, 발표일시: 수 16:00~19:00

Montmorillonite (K-10): An efficient catalyst for the synthesis of tetrahydrodipyrazolo[3,4-b:4',3'-e]pyridines under microwave irradiation

Mudumala Veeranarayana Reddy 정연태*

부경대학교 이미지시스템공학과

An efficient, rapid, and green synthesis of tetrahydrodipyrazolo[3,4-b:4',3'-e]pyridines has been accomplished under solvent-free conditions by the reaction of 3-methyl-1H-pyrazol-5(4H)-one, aldehydes and ammonium acetate. This approach exploits the synthetic potential of microwave irradiation and Montmorillonite K-10 combination and offers many advantages, such as excellent product yields, shorter reaction time, reusable catalyst, easy isolation of products, and environmentally benign reaction conditions.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-673**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Counter Cation on thermal stability and solubility property of Cy3 Dye

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부경대학교 이미지시스템공학과

In this research, we prepared some Cy3 dyes with different counter cation in order to check thermal stability and solubility property, which are important properties of dyes for LCD color filter. These compounds showed maximum absorption wavelength (λmax) in the range of 549 - 555 nm in UV/Vis spectrum and red color. Solubility characteristics and thermal stability of those were dependent on the structure of counter cation. The solubility property and thermal stability of Cy3 dye with ethyl counter cation aer better than those of Cy3 dyes with the other counter cation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Amine Functionalized Metal-Organic Frameworks

정수연 하현빈 박수정 함형우 김민*

충북대학교 화학과

금속-유기 골격체(Metal-Organic Framework, MOF)는 금속 이온 또는 단위체에 유기 리간드가 반복적으로 결합하여 형성하는 유기-무기 혼성의 성질을 가지는 다공성 구조체이다. MOF 는 자체의 빈 공간과 낮은 밀도 때문에 기체 저장 및 수송, 분자 수송, 촉매 등 여러 분야에서 높은 관심을 받고 있다. 또한 MOF 는 유기 리간드 부분을 포함하고 있기 때문에, 기존에 알려진 다양한 종류의 다공성 구조체 (예: 제올라이트, 활성탄소 메조포러스 실리카 등)에 비하여 작용기 및 성질 조절이 용이하다는 장점을 가지고 있다. 본 발표에서는 기존에 알려져 있는 아민기가 도입 된 MOF 의 성질을 비교 연구하기 위하여 차수가 조절 된 아민이 도입 된 리간드의 합성과 MOF 의 합성을 논의하고자 한다.

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발표코드: **ORGN.P-675**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Cobalt Catalyzed Rearrangement of Aldoximes into Amides

김세은 장원석 김영조* 김민*

충북대학교 화학과

아마이드는 우리 생체내의 단백질을 이루는 중요 결합 중에 하나로, 공업 화학과 고분자 화학에서도 다양하게 사용되는 화학 결합이다. 아마이드의 공업적 규모 대량 합성은 옥심의 재배열 반응의 일종인 Beckmann 재배열 반응을 통하여 주로 수행되고 있다. 하지만 전통적인 Beckmann 재배열 반응은 강한 산과 높은 온도를 필요로 하고 산의 사용에 따른 부수물이 다량 발생한다는 단점을 가지고 있다. 이러한 Beckmann 반응의 단점을 극복하기 위하여, 새로운 재배열 반응의 연구가 최근 이루어지고 있다. 특히 후전이금속을 촉매로 사용한 옥심의 재배열 반응은 강산을 사용하던 기존의 방법보다 더 낮은 온도와 온화한 조건에서 수행가능하고 반응 부수물이 적어지는 긍정적인 효과가 보고되어있다. 본 발표에서는 현재까지 알려진 재배열 반응의 촉매들인 루테늄, 로듐 등의 금속보다 가격이 저렴하고 대량 생산에의 적용이 상대적으로 수월한 코발트 촉매를 사용하는 옥심의 재배열 반응을 다루고자 한다. 특별히, 간단한 리간드 조절로 같은 시작 물질에서부터 다른 종류의 생성물을 합성할 수 있는 새로운 선택성에 대하여 이야기 하고자 한다.

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발표코드: **ORGN.P-676**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

새로운 인계 촉매계를 이용한 탄소-질소 결합 형성 교차 짝지음 반응에 대한 연구

김소한 장원석 김민* 김영조*

충북대학교 화학과

팔라듐 촉매는 할로젠화 아릴의 탄소-할로젠 결합의 활성화와 아민의 질소-수소결합의 활성화를 통하여 새로운 탄소-질소결합을 형성하는 반응을 잘 수행하는 것으로 알려져 있다. 현재까지 팔라듐과 함께 사용할 수 있는 여러 종류의, 뛰어난 활성을 보이는 촉매계가 보고되었음에도 불구하고, 새로운 반응성과 높은 선택성을 위하여 지속적인 신규촉매에 대한연구가 필요하다. 이에 본 연구실에서는 새로운 인계화합물을 팔라듐과 함께 사용하면, 상대적으로 반응성이 낮은 염화아릴과 다양한 아민의 교차 짝지음 반응에 효과적인 촉매계로 쓰일 수 있음을 보이고자 한다.

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발표코드: **ORGN.P-677**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

새로운 인계 촉매계를 이용한 염화아릴과다양한 나이트릴의 알파-아릴화 반응에 대한 연구

김소한 장원석 김민* 김영조*

충북대학교 화학과

팔라듐촉매를 이용한 아릴화반응은 탄소-할로젠결합을 활성화시켜서 새로운탄소-탄소결합을 형성하는, 유기분자의 기본골격을 형성하는데 다양하게 사용되는 중요한 유기반응 중에 하나이다. 전통적으로 할로젠화 아릴화합물 중에서 브로모와 아이오도그룹이 주로 사용되어 왔지만, 최근들어 염화아릴을사용하는 반응에서 팔라듐과 인계촉매계 조합이 촉매활성이 보여진다고 알려져있다. 이에 본 연구실 에서는 새로운 인계화합물을 합성하고 이를 이용하여 염화아릴과 다양한 나이트릴의 알파-아릴화 반응에 효과적인 촉매계로쓰일 수 있음을 증명하고자 한다.

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발표코드: **ORGN.P-678**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Cobalt-catalyzed Dehydration of Aldoximes into Nitriles

장원석 김세은 김영조* 김민*

충북대학교 화학과

나이트릴 작용기는 탄소와 질소의 삼중결합으로 이루어진 작용기로 여러 종류의 유기 반응을 통하여 아민, 아마이드, 카복실산 등으로 변환될 수 있는 중요한 합성 중간체이다. 이런 나이트릴 작용기를 도입하는 방법으로는 나이트릴기 자체를 치환하는 방법이나 탈수 반응을 통한 삼중 결합의 형성이 주로 사용되고 있다. 전통적으로 탈수 반응은 강한 산 조건에서 가열을 통하여 수행되는 것이 사용되고 있으나, 근래에 들어서 전이금속촉매를 이용한 보다 온화한 조건에서의 탈수 반응 수행이 다양하게 연구되고 있다.본 발표에서는 전이금속 중 상대적으로 가격이 저렴하고, 안정성이 높아서 쉽게 다를 수 있는 코발트를 촉매로 활용하여 옥심의 탈수 반응을 진행한 연구 결과를 발표하고자 한다. 특히, 새로운 형태의 리간드를 도입하여 합성된 코발트 촉매의 구조를 단결정 구조 분석을 통하여 밝히고, 이를 이용한 효과적인 옥심의 나이트릴 전환 반응에 대하여 논의 할 것이다.

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발표코드: **ORGN.P-679**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Synthesis of Triphenylanimes through Copper-catalyzed N-Arylation

김동해 유광호 김영조* 김민*

충북대학교 화학과

헤테로고리 화합물은 약학과 전합성에서 매우 중요한 기본 골격으로, 근래에 들어서 헤테로 고리 화합물의 다양한 작용기 도입 및 새로운 결합 형성 반응이 연구되어지고 있다. 특히 상대적으로 산성도가 높은 헤테로 원자 바로 옆의 탄소-수소 결합은 높은 반응성 때문에 다양한 반응에 이용되고 있다. 새로운 탄소-탄소 결합 형성을 위하여 주로 팔라듐과 로듐 등의 후전이금속을 이용한 조건이 개발되었고, 상대적으로 가격이 저렴한 구리 등도 반응의 개발에 다양하게 이용되어지고 있다. 본 발표에서는 기존에 알려진 구리 촉매에 의한 헤테로 고리 화합물의 탄소-수소 결합 활성화를 통한 탄소-탄소 결합 형성 반응을 변형하여, 새로운 형태의 고리 열림 질소-아릴화 반응을 연구한 결과를 발표하고자 한다.

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발표코드: **ORGN.P-680**

발표분야: 유기화학

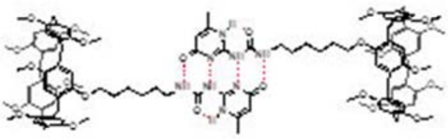
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembled supramolecular structures based on copillar[5]arene and four-way cationic porphyrin derivatives

이재철 백경수* 박연실

숭실대학교 화학과

Copillare[5]arene with ureidopyrimidinone moiety 1 exists as a dimer 1_2 in nonpolar solvent and can self-assemble into various supramolecular structures with guests which enable cationic-π interactions. The new four-way tetra-cationic porphyrin guest 2 are designed and synthesized. The characteristics of this four-way self-assembled supramolecular structure will be presented.



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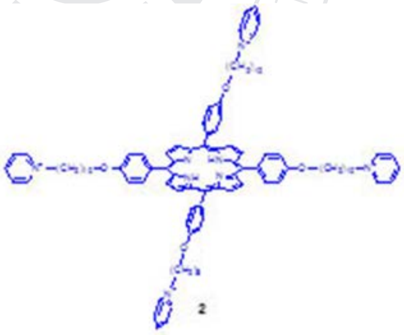

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일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-681**

발표분야: 유기화학

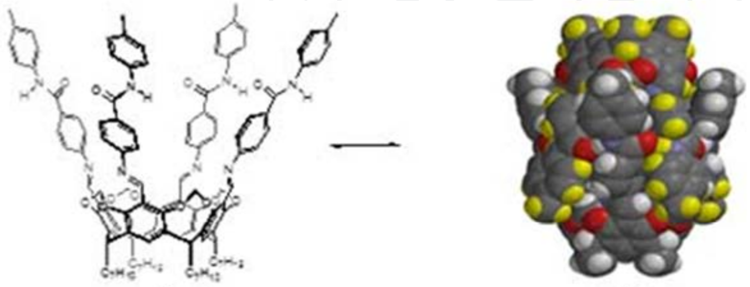
발표종류: 포스터, 발표일시: 수 16:00~19:00

New molecular capsule with an extended inner cavity

김조원 백경수* 박연실

숭실대학교 화학과

A new molecular capsule with an extended inner cavity was developed by the introduction of four *N-p-*tolylbenzamide moieties on the upper rim of a imino-cavitand based on resorcin[4]arene. Cavitand 1 having four amides could self-assemble into molecular capsule 1_2 through the eight intermolecular amide C=O???N-H hydrogen bonds when suitable guests are present in noncompeting solvent. The synthesis and characteristics of molecular capsule 1_2 will be presented.



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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-682**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective fluorescence sensing of aromatic carboxylic acids based on *N*-alkylanthracene derivatives

Anup Pandith 김보연 김홍석*

경북대학교 응용화학과

The recognition of aromatic carboxylic acids with different architectures is not well known. In relation to this, imidazole as a binding motif is investigated. A series of anthracene-based imidazole receptors for aromatic carboxylic acids sensing were prepared and investigated. The preorganization of sensors allowed three-point binding with aromatic carboxylic acids through multiple hydrogen-bonding interaction with amino N-H group and imidazole moiety. The sensing ability of receptor 2 toward various SA derivatives has been examined by UV-vis and fluorescence spectroscopy.

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발표코드: **ORGN.P-683**

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Pyrenesulfonyl imidazolium derivative as selective CN$^-$ ion sensor in aqueous media

Ashwani Kumar Anup Pandith 김홍석*

경북대학교 응용화학과

N-Imidazolpropyl pyrenesulfonamide 1 and its dimidazolium salt (2) have been synthesized for the sensing of anions and found to be selective and sensitive toward CN$^-$ ion in PBS-EtOH (5:95, pH = 7.4) solution. The sensing ability of these probes 1 and 2 toward CN$^-$ ion has been examined by UV-vis, fluorescence, and NMR spectroscopy. The lowest detection limit for the estimation of cyanide ions is 0.5 μM (13 ppb), which is lower than the permissible limit by WHO for drinking water.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Zn^{2+} and $H_2PO_4^-$ selective fluorogenic sensors based on thiazole-sulfonamides

안미란 김보연 김홍석*

경북대학교 응용화학과

The developments of turn-on fluorescent probes have attracted attention. Previously, the synthesis and Zn^{2+}, Cu^{2+}, Ga^{3+} and Al^{3+} sensing properties of several thiazole based chemosensors were reported. New highly selective fluorescent thiazole-sulfoamide derivatives were synthesized and investigated for the quantification of zinc and dihydrogen phosphate ions in ethanol.

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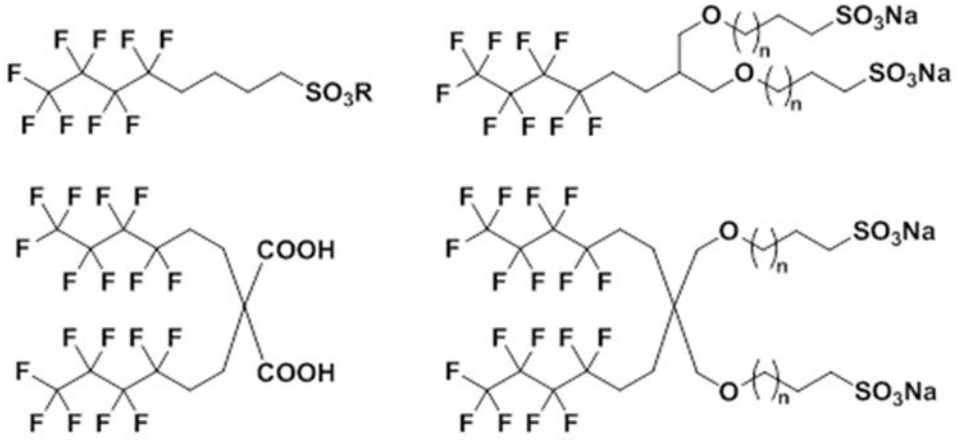
Synthesis and properties of new PFOS alternatives

Vijay kumar chirumarrysridhar 고요한 신동수*

창원대학교 화학과

Perfluorooctanesulfonic acid (PFOS) and perfluorooctanecarboxylic acid (PFOA) are well known surfactants and are key ingredients in many stain repellents, paints and fire fighting foam industries. On the other hand PFOS related substances are toxic towards health and environment due to its non-biodegradability. The perfluoroalkyl chain can be substituted with hemifluoro alkyl chain to gain biodegradable substances. In this purpose, we used fluorous alkyliodides coupled to ethyl vinylsulfonate in presence of Zn/CuI in ionic liquids as well as in formamide to obtain ethylperfluoroalkylsulfonate. Simultaneously, we have synthesized di-sulfonates starting from hemifluorinated alkylhalide to avail monoalkyl and dialkyl derivatives. The biodegradability and surface tension reduction properties were also measured.



R = Li, Na, K, Et_4N^+, $Me_2(C_{10}H_{21})_2N^+$ etc.
n = 1, 2

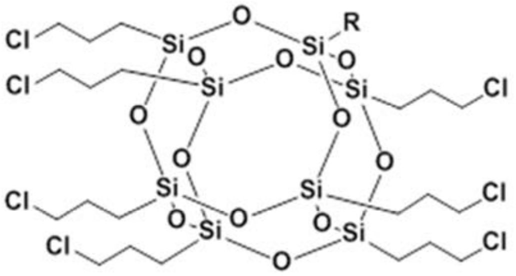
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-686**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and derivatives of hepta(3-chloropropyl)-tricycloheptasiloxane trisodium silanolate

Vijay kumar kumar deepak 신동수*

창원대학교 화학과

Incompletely condensed silsesquioxanes (trisilanols or trisilanolate-T7) having one silicon atom short of T8 cube are of great importance due to the presence of a reactive trisilanolate or trisilanol site and are used as excellent platforms for synthesizing new hybrid materials. However, trisilanols reported in the literature are dreadfully limited and have all seven unreactive organic moieties except heptaphenyl trisilanol (7Ph-T7-(OH)3). Thus, synthesis of trisilanols with seven reactive organic groups is a promising task in the design of hybrid materials with high-performance in several applications. Here, we report the first synthesis of incompletely condensed (with seven reactive groups) POSS, hepta(3-chloropropyl)-tricycloheptasiloxane trisodium silanolate (7Cl-T7-(ONa)3 in gram scale. The reactivity of the chloride functional groups in 7Cl-T8-R makes it an attractive synthetic platform on which to build new compounds for inorganic and organic derivatives of POSS molecules.


Cl
Cl
Cl
Cl
Si
Si
Si
Si
Si
Si
Si
Si
O
R
Cl
Cl
Cl
Cl

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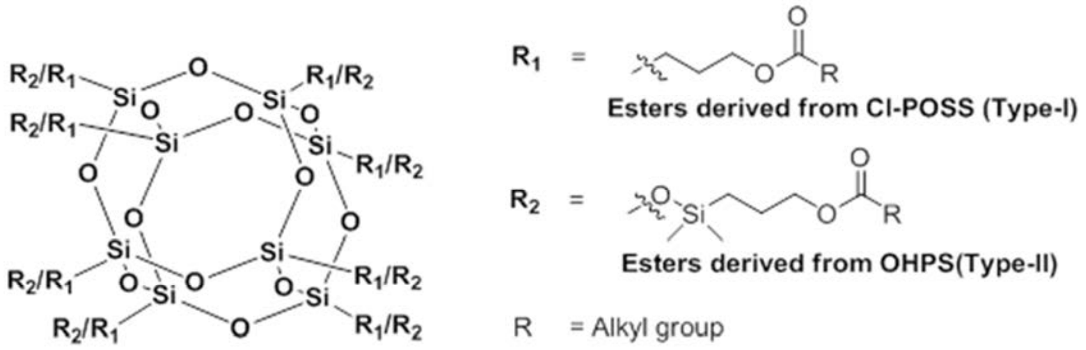
POSS derived hybrid ester type insulating oils

chirumarrysridhar Vijay kumar 신동수*

창원대학교 화학과

A new family of polyhedral oligomeric silsesquioxanes (POSS) based esters have been synthesized that consists eight ester functional groups. These are classified into Type-I and Type-II esters based on the starting materials, octakis(3-chloropropyl)silsesquioxane (Cl-POSS) and octakis(3-hydroxypropyldimethylsiloxy) octasilsesquioxane (OHPS) respectively (figure 1). These new POSS type ester moieties can be used as insulating oils and oil additives in the transformers and also considered to be alternatives to mineral and vegetable oils that are presently used in the insulation system.


R2/R1
Si
O
R1/R2
R1 =
O
O
R
Esters derived from CI-POSS (Type-I)
R2 =
O
Si
O
R
Esters derived from OHPS(Type-II)
R = Alkyl group

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발표코드: **ORGN.P-688**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Formal synthesis of PF-00951966: *(S)-3-(Methylamino)-3-((R)-pyrrolidin-3-yl)propanenitrile*

김승희 엄희성 하현준* 이원구[1,*]

한국외국어대학교 화학과 [1]서강대학교 화학과

(S)-3-(Methylamino)-3-((R)-pyrrolidin-3-yl)propanenitrile is a key intermediate in the preparation of PF-00951966, which is a fluoroquinolone antibiotic agent against pathogens causing community-acquired respiratory tract infections including *multidrug resistant*(MDR) organisms. This key intermediate was prepared from *azridine-2-yl acrylate* as a starting material via several key reactions including (a) stereoselective 1,4-addition, (b) methylative aziridine ring-opening reaction with cyanide nucleophile and (c) Chemoselective hydrogenation using *Polymethylhydrosiloxane* (PMHS).

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

Nucleophilic Aromatic Substitution Reaction (SNAr) of Cyanuric Chloride : NMR Study on the Products, (AnBm)triazine (A=dithiocarbamate, B=amine, n+m=3)

도희진 김영준*

충남대학교 화학과

Dibenzylcarbamodithioate group was introduced in 1,3,5-triazines by the reaction of potassium dibenzylcarbamodithioate and cyanuric chloride. Mono-, di- substituted 1,3,5-triazines were synthesized by the reaction of potassium dibenzylcarbamodithioate in THF with water at 0℃. In contrast, the anhydrous THF with base conditions is superior to produce tri-substituted with potassium dibenzylcarbamodithioate compound, at room temperature. The activation parameters of C-N bond rotation of the dithiocarbamates in DMSO-d_6 and Toluene-d_8 were measured by using variable-temperature ^{1}H NMR spectroscopy. Their Gibbs free energies (ΔG‡) were calculated as 16 ~ 18 kcal/mol from the coalescence temperatures and line shape analysis and will provide useful information about the electronic effects.

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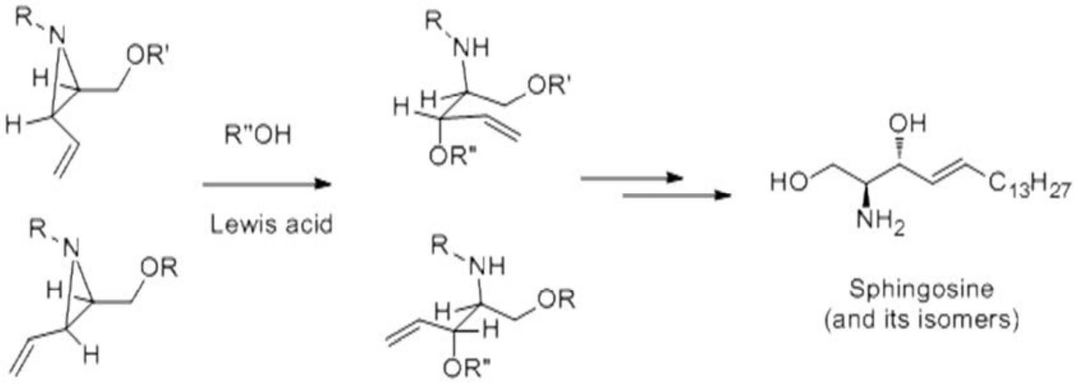
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of sphingosine and its isomers by ring-opening of 3-substituted-2-vinylaziridines

강한영* 신미리 강온유

충북대학교 화학과

During the investigation on the nucleophilic opening of cis-3-substituted-2-vinylaziridines we have learned that the openings, particularly in the presence of a Lewis acid (BF3.OEt2) occur in stereo- and regioselective fashion to give the 1,2-functionalized compounds efficiently. We, now, wish to extend this nucleophilic opening to trans-3-substituted-2-vinylaziridines in order to confirm the usefulness of the ring opening reactions through applying to the synthesis of possible stereoisomers of 1,2-functionalized compounds. Success of the selective ring opening would lead to the synthetic application to the compounds that contain 1,2-functionalized moiety. Sphingolipids belong to a large class of natural products which exhibit interesting biological activities in many physiological processes, including immune response, cell recognition, and so on. The application of the ring opening reactions to the synthesis of sphingosine, one of the most important and representative sphingolipids, as well as its isomers will be presented.



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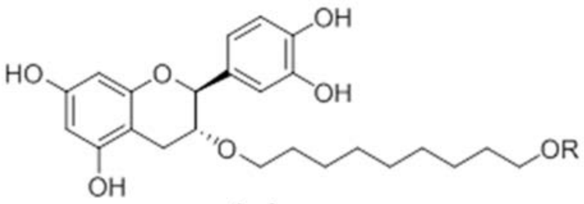
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis antioxidant and antimicrobial studies of (-)-catechin derivatives

kumar deepak VAIDYARAGHAVENDERRAO 신동수*

창원대학교 화학과

Catechins, which have been reported to have antimutagenic, antioxidant, anti-bacterial, antitumor and other biological acivities. Looking at the biological significance of (-)-catechin nucleus, some novel (-)-catechin derivatives (1a-1k) were synthesized and screened for their antioxidant, antibacterial and antifungal activities. Most of the compounds showed good antioxidant activity, whereas compounds 1a, 1b, 1c exhibited potent antimicrobial activities against both bacteria and fungi. In conclusion, novel (-)-catechin derivatives have been designed, synthesized and fully assigned by analytical and spectral data. Most of the synthesized compounds exhibited significant activities. This indicates that (-)-catechin derivatives can be considered as potential antioxidant and antimicrobial agents. Finally, it’s conceivable that further derivatization of such compounds can serve as novel templates for antimicrobial agents, which might lead to more active molecules in the field of antimicrobial treatment.



1a-k

R = alkyl, acyl, aryl, heterocyclic

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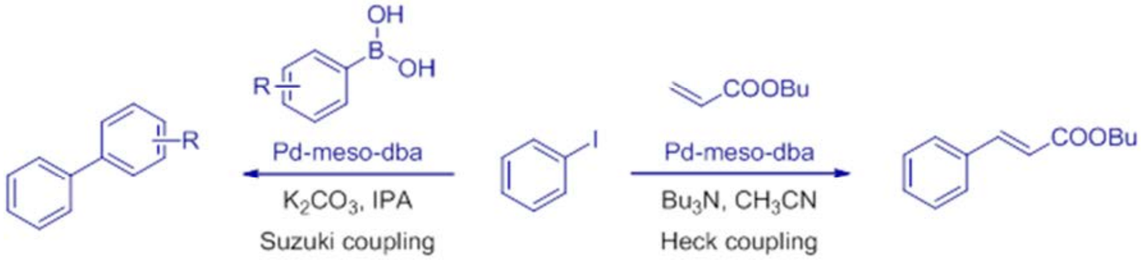
발표코드: **ORGN.P-692**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel recyclable mesoporous silica supported catalyst Pd-Meso-DBA for Suzuki and Heck reactions

Vijay kumar PATILKALPESHTUMADU 신동수*

창원대학교 화학과

Mesoporous silica with different textural and structural properties have been synthesized and studied extensively recently. This substance meet the key factors for improved catalytic activity with distinguished properties such as high surface area, narrowly and highly ordered pore system, high hydrothermal stability and surface functionalities that present inside and outside of pores. These heterogeneous mesoporous silica supported catalysts achieve the catalyst-free product with better yield when compared with the conventional catalysts. We herein, present a new mesoporous silica based palladium(0) complex ‘Pd-Meso-DBA’, along with its applications towards Suzuki and Heck coupling reactions.


OH
B
OH
R
COOBu
Pd-meso-dba
K_2CO_3, IPA
Suzuki coupling
I
Pd-meso-dba
Bu_3N, CH_3CN
Heck coupling
R
COOBu

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and electroluminescent properties of 10-(naphthalen-7-yl)anthracene derivatives with quinoline groups for OLEDs

김찬우 박수나 이슬비 윤승수*

성균관대학교 화학과

this work, we have designed and synthesized three blue host materials based on naphthyl-anthracene moieties with quinoline groups. These materials showed blue electroluminescences and the structural features of these materials have effects on their electroluminescent properties. Particularly, a material exhibited highly efficient blue electroluminescence with a luminous and power efficiencies of 1.64 cd/A and 0.93 lm/W at 20 mA/cm^2.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

[Pd(η^3-allyl)Cl]$_2$-Catalyzed Decarboxylative Trifluoroethylation of Aryl Akynyl Carboxylic Acids

황진일 노지은 김한성 이선우*

전남대학교 화학과

Trifluoroethylation of alkyne was developed through the palladium-catalyzed decarboxylative coupling reaction. When akynyl carboxylic acids and ICH_2CF_3 were allowed to react with [Pd(η^3-allyl)Cl]$_2$/XantPhos and Cs_2CO_3 in N,N-dimethyl formamide (DMF) at 80 °C for 1 h, the desired products were formed in good yields. This catalytic system showed high functional group tolerance.

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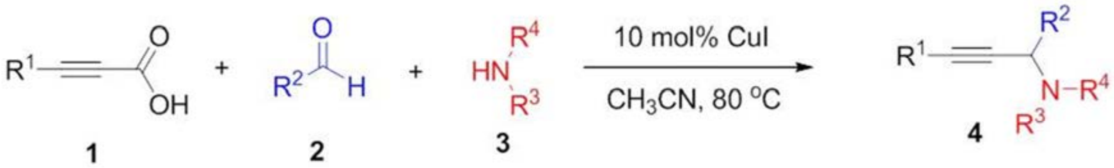
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed one-pot of Multicomponent Reactions for the Synthesis of Propargyl Amines

임정아 박경호 이선우*

전남대학교 화학과

When aryl alkynyl carboxylic acids were allowed to react with amines and aldehydes in CH_3CN at 80 °C in the presence of 10 mol% CuI, the desired propargyl amines were formed in good yields. This coupling reaction demonstrated to work across a broad range of reagents including functionalized aryl alkynyl carboxylic acids, aliphatic and aromatic aldehydes and cyclic and acyclic amines.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct Synthesis of Diaryl 1,2-Diketones from Aryl Iodides and Propiolic acid using by Copper-catalyst

최진섭 민홍근 이선우*

전남대학교 화학과

Benzil derivatives such as diaryl 1,2-diketones are synthesized via the direct decarboxylative coupling reaction of aryl propiolic acids and their oxidation. The optimized condition is that the reaction of aryl propiolic acids and aryl iodides is conducted at 140 oC for 6 h in the presence of 10 mol% CuI/Cu(OTf)2 and Cs2CO3, and then HI (aq) is added and further reacted. It showed good functional group tolerance toward ester, aldehyde, cyano and nitro groups. In addition, symmetrical diaryl 1,2-diketones are obtained from aryl iodide and propiolic acid in the presence of palladium and copper catalyst.

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발표코드: **ORGN.P-697**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Selective Synthesis of Isoindolin-1-ones and Isoquinolin-1-ones from the Three-Component Coupling of 2-Halobenzoic Acid, Alkynylcarboxylic Acid and Ammonium Acetate

<u>IRUDAYANATHANFRANCISMARIARAJ</u> GABRIELCHARLESEDWINRAJA 이선우*

전남대학교 화학과

Among the heterocyclic ring compounds, isoindolin-1-one and isoquinolinone ring systems are regarded as one of the key scaffolds in the field of medicinal and material chemistry applications. Isoindolin-1-ones and isoquinolin-1-ones were selectively synthesized from the reaction of 2-halobenzoic acid, arylalkynylcarboxylic acid and ammonium acetate (NH_4OAc) in the presence of cesium carbonate (Cs_2CO_3) and a copper catalyst. Changing the addition sequence of ammonium acetate after all reagents had reacted at 120 °C for 6 h selectively produced isoquinolin-1-ones. A variety of arylalkynylcarboxylic acids produced the corresponding isoindolin-1-ones and isoquinolin-1-ones in good yields. This method afforded the direct synthesis of the 5-exo-dig product with high regioselectivity, using arylalkynylcarboxylic acids, which are easily prepared from the coupling of propiolic acid and aryl halides. In addition, isoquinolin-1-one was selectively obtained via the formation of isocoumarin. A plausible mechanism was also suggested and proposed that isoindolin-1-one was formed through amide bond formation first or concerted coupling pathway.

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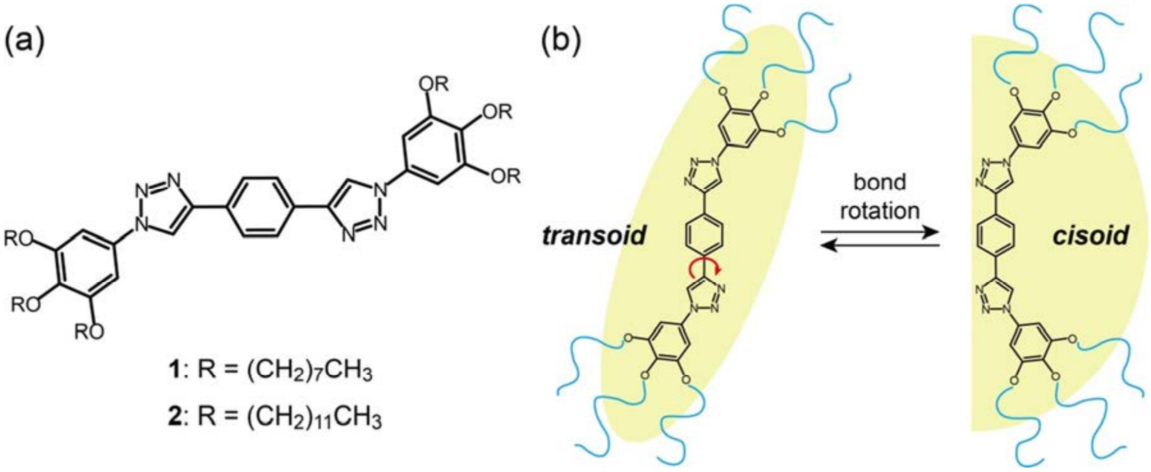
발표종류: 포스터, 발표일시: 수 16:00~19:00

Monoclinic to Two-dimensional Hexagonal Transformation in thermochromic Hexacatenar Molecules with a 1,2,3-Triazole-Based Conjugated Rod

한규원 조병기*

단국대학교 화학과

The polycatenar system consisting of an aromatic rod and multiple flexible chains would be a facile aromatic molecular candidate to create nanosegregated aromatic domains, because their assembling behavior shares the characteristics of calamitic and discotic liquid crystals. Indeed, various morphologies such as nematic, smectic, cubic, and columnar phases have been found depending on the number of terminal chains. Also, by incorporating extended π-conjugated aromatics, some polycatenar examples showed PL nanostructures in bulk states. In several cases, their fluorescence properties could be tuned in response to morphology variation. In this study, we prepared novel hexacatenar molecules based on a 1,2,3-triazole-extended aromatic rod, and examined their self-assembling and fluorescence properties. Interestingly, in their crystalline states, they formed 3D monoclinic lattices, which were transformed into hexagonal columnar LC phases upon melting. The phase transition may involve a conformational change from an anisotropic transoid to half-disk cisoid conformer. In a hexacatenar molecule with sixfold octyl chains, the crystal-to-LC transition accompanies a photoluminescence color change from sky blue to dark blue, which is attributed to the formation of higher-order aggregates in the crystalline state.



1: R = $(CH_2)_7CH_3$

2: R = $(CH_2)_{11}CH_3$

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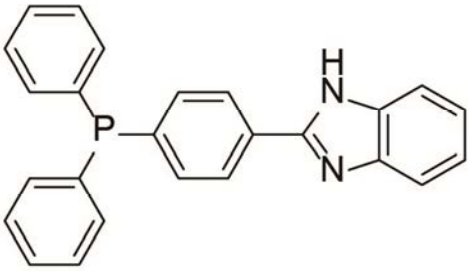
Synthesis of 2-(4-diphenylphosphino)phenyl)-1H-benzo[d]imidazole (4-DPI) and 2-(4-diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (4-DPPI) as OLED materials

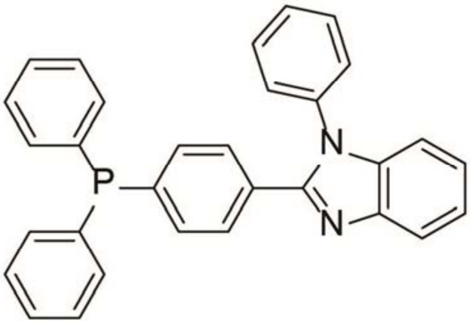
김경현 강은국 이범종[1,*] 조현희

인제대학교 화학과 [1]인제대학교 의생명화학과

In the process of investigation for finding novel organic light-emitting materials (OLEDs) based on phosphino-benzimidazole structure, 2-(4-diphenylphosphino)phenyl)-1H-benzo[d]imidazole (4-DPI) and 2-(4-diphenylphosphino)phenyl)-1-phenyl-1H-benzo[d]imidazole (4-DPPI) were synthesized. The cyclization reactions from o-phenylenediamine and 4-diphenylbenzoic acid (4-DPB), or 2-aminodiphenylamine and 4-DPB, which give phosphino-benzimidazoles have been carried out under mild conditions using tetrabutylammonium bromide (TBAB) as the reaction medium and triphenyl phosphite (TPP) as the catalyst. The chemical structures of 4-DPI and 4-DPPI were determined by 1H-NMR, 13C-NMR, FT-IR and UV-vis. Both 4-DPI and 4-DPPI showed a strong greenish-blue emission under excitation by UV-lamp of 365 nm. The electroluminescence (EL) properties of 4-DPI and 4-DPPI will be discussed.



4-DPI



4-DPPI

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발표코드: **ORGN.P-700**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-catalyzed oxidation of alcohols to their corresponding aldehydes and ketones in a microreactor

송주하 임효진 박찬필*

충남대학교 분석과학기술대학원

The oxidation of alcohols to their corresponding aldehydes and ketones has significant importance in organic chemistry. Palladium catalyst system was reported that is one of the most convinient and versatile catalyst systems for selective aerobic oxidation of alcohols. But, the traditional oxidation reaction of alcohols in a batch system was require long reaction time. In this research, we used an efficient continuous flow system which shows shorten reaction time than batch systems. Also, continuous flow system has some attractive merits, possible to reduce the waste of the expensive palladium catalyst by using microreactor, and has large reaction area that is efficient using oxygen gas as an oxidant.

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발표코드: **ORGN.P-701**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on the Chemical Shifts of Benzoic and Cinnamic Acids: Effect of a C-C Double Bond on the Transmission of Substituent Effect

한인숙* 정은정

강원대학교 과학교육학부

Series of aryl esters and anilides of benzoic and cinnamic acids were prepared by condensation of the acyl chlorides with m- and p-substituted phenols and anilines. 1H and 13C NMR spectra of the esters and anilides were obtained in 0.1 M DMSO-d6 solution. 13C chemical shift values were plotted against the substitutent constants (σ) to show good to excellent correlations (r = 0.953~0.990) except the 3-C of the esters (r = 0.826~0.878). The slopes of the correlations indicate that the electronic effect of the substitutent is transmitted in the amide series than in the ester series. Presence of a C-C double bond decreases the transmission of the substituent effect more significantly in the ester series than in the amide series. The inversed correlation of the chemical shifts of 13C=O in the ester series and the normal correlation in the anilides series may indicate the different polarization between the two series.

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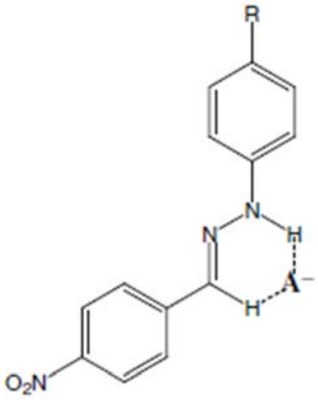
A chromogenic sensor for the recognition of anions based on phenylhydrazone

최유선 강종민*

세종대학교 화학과

Chromogenic anion receptors based on 4-nitrophenylhydrazone and phenylhydrazone have been designed and synthesized. UV?Vis and 1H NMR titration showed that receptor 1 responded to anions according to their basicity. Although the nature of hydrogen bonds in hydrazone N?H and vinylic C?H is weak, receptor 1 bound weakly basic anions such as chloride, bromide, iodide and hydrogen sulfate utilizing only hydrogen bond in CH3CN. No color change was observed with these anions. However, for more basic anions such as acetate dihydrogen phosphate and fluoride, color change due to deprotonation observed. Furthermore, the solution color of 1 changed to deep blue with fluoride. Fluoride could be distinguished from acetate and dihydrogen phosphate with naked eye. However, phenylhydrazone based receptor 2 showed only hydrogen bonding association with all anions investigated except fluoride. Due to low deprotonation tendency and its structure, color change of solution 2 was not observed.



R = NO_2 **1**
= H **2**

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Substituent Chemical Shifts of Benzylated Phenols

한선호 한인숙[1,*]

강원대학교 과학교육학부 화학교육전공 [1]강원대학교 과학교육학부

m- and p-substituted phenols were treated with benzyl alcohol in toluene in the presence of p-toluenesulfonic acid or methanesulfonic acid to give mono- and dibenzylated phenols. The procedure is more efficient than a typical Friedel-Crafts benzylation using benzyl chloride and aluminum chloride for the preparation of the benzylphenols. The mono- and dibenzylated phenols were separated and purified by column chromatography. 1H and 13C NMR spectra of the monobenzylated phenols were examined to find out the operation of substituent chemical shifts in the presence of the hydroxy group ortho to the benzyl group.

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유사세라마이드 구조를 가지는 신규화합물의 합성

김유미 김한영[1,*]

애경산업(주) 기반기술연구팀 [1]애경산업(주) 중앙연구소

피부 각질층은 피부 고유의 보습기능을 발휘하는데 매우 중요하며, 특히 각질세포간 지질은 각화된 세포사이에서 라멜라 구조를 형성하여 단단한 시멘트와 같은 역할을 함으로서 피부장벽기능의 근원이 된다. 이중 세라마이드는 지질 전체의 약 50% 이상이 될 정도로 매우 중요한 성분이며, 피부장벽기능의 필수적인 성분이라고 할 수 있다. 이러한 지질 성분은 어려운 제조방법으로 인한 단가 문제로 범용적인 사용이 어려운 단점이 있다. 이에 제조가 용이하여 범용적인 사용이 가능한 신규 유사세라마이드 소재를 합성하였다. 이는 서로 다른 두 화합물의 개환 반응으로 보다 편리하고 경제적으로 합성하였으며, 소재 평가를 위해서 보습력 실험을 실시하였다. 보습력 평가는 tape stripping 으로 피부 각질층을 손상 시킨 뒤 corneometer 를 사용하여 측정하였으며 손상 전, 후, 3 시간, 6 시간, 24 시간, 48 시간, 72 시간 측정하여 보습력 향상률을 계산하였다. 또한 소재의 안전성 데이터 확보 및 신규 소재의 독성 수준을 파악하기 위해 세포독성 실험을 하였다. 그리고 여드름균에 대한 항균활성을 알아보기 위해 MIC 측정 시험을 진행하였다.

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Synthesis of New Electron Transfer Material Based on Phenothiazine and Quinoline

정세양 박동규 권태우*

경성대학교 화학과

Phenothiazine is a well known electron donor component due to their low reversible oxidation potentials by virtue of the sulfur atom, which can facilitate the hole transport of the carrier. Phenyl quinoline moiety showed good electron transport properties as the acceptor in quinoline dendrimers, oligoquinolines and polyquinolines for OLEDs. Herein, we report an approach to a new electron donor-acceptor molecule based on phenothiazine and quinoline. The synthesis of 2-(6-bromo-3-alkyl-4-phenylquinolin-2-yl)-10-alkyl-10H-phenothiazine was accomplished via Grignard reaction and Friedlander condensation using 10-alkyl phenothiazine-2-carbonitrile as a starting material. The obtained compound was confirmed by ^{1}H, ^{13}C NMR, FT-IR, GC/MS. Detailed synthetic routes and characterization of novel donor-acceptor molecules will be discussed.

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Microchemical deoxygenation of benzylic alcohols in a biphasic medium

서승우 박찬필[1,*]

충남대학교 분석과학기술학과 [1]충남대학교 분석과학기술대학원

Deoxygenation of benzylic alcohols has been studied for a long time and used for broad industry area such as synthesis of drugs, the procedure to get biofuel from carbohydrate. An aqueous hydriodic acid (HI) is a catalyst to deoxygenation. Hypophosphorous acid (H_3PO_2) prevents consumption of HI by recycling I_2 as reducing agent. So HI is very economical catalyst with aqueous solution of H_3PO_2. However, this radical reaction was biphasic reaction and very harsh reaction. We introduce droplet based micro-tube reactor to improve these problems. Droplet system is able to increase surface to volume ratio. That occurred easy to transfer HI between organic phase with aqueous phase. In micro-tube reactor, organic phase and aqueous phase is separately injected to T-junction. Tiny droplets are formed by passing through T-junction and then the droplets are heated at 120 ℃, not need reflux condenser, to deoxygenate.In this study, we investigate the condition of suitable droplet length, reaction temperature and concentration of HI. And deoxygenation of benzylic alcohols (such as 2-methylbenzhydrol, 4-chlorobenzhydrol, bis(4-fluorophenyl)methanol, 2-phenyl 2-propanol, 1-phenyl ethanol, and triphenylmethanol) has high yield (99 %) for short reaction times (10 min) in micro-tube reactor. The results are anlysed by NMR and GC/MSD.Key words: deoxygenation/ micro-tube reactor/ biphasic reaction

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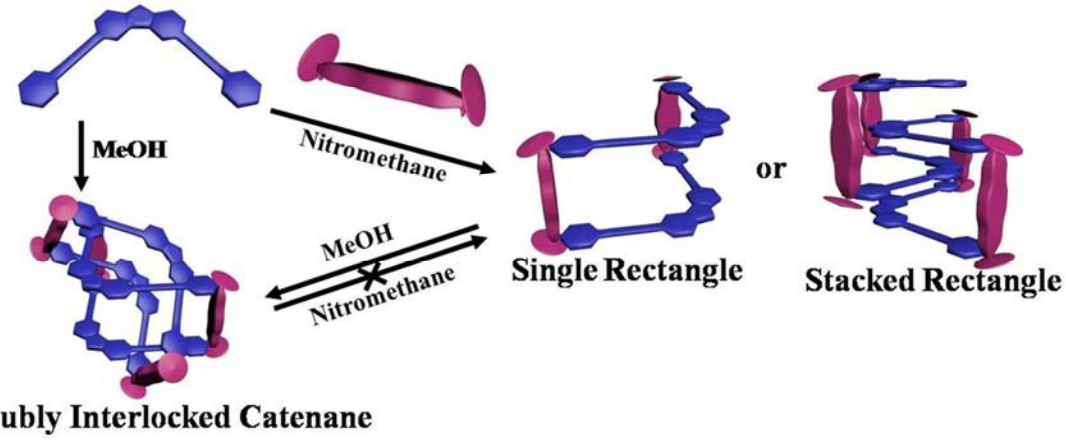
Coordination-Driven Self-Assembly of Self-Stacked Metallarectangle and Doubly Interlocked Catenane

송영호 지기환*

울산대학교 화학과

New interesting formation of supramolecular complexes were obtained from the self-assembly of carbazole based dipyridile ligand with some kind of arene-ruthenium acceptors. All these supramolecular complexes were characterized by ^{1}H and ^{13}C NMR spectroscopy, high-resolution electrospray mass spectrometry, and single-crystal X-ray diffraction.Self stacking of expected [2+2] macrocycle has been confirmed from X-ray crystal structure at specific case of self-assembly reaction.Especially, unique formation of doubly interlocked catenane (DIC) by combination of 90 degree carbazole based ligand with tetracene Ru acceptor was observed at specific reaction condition.



Scheme. Self-assembly of various formation of macrocycles using carbazole based dipyridile ligand with similar series of accepters.

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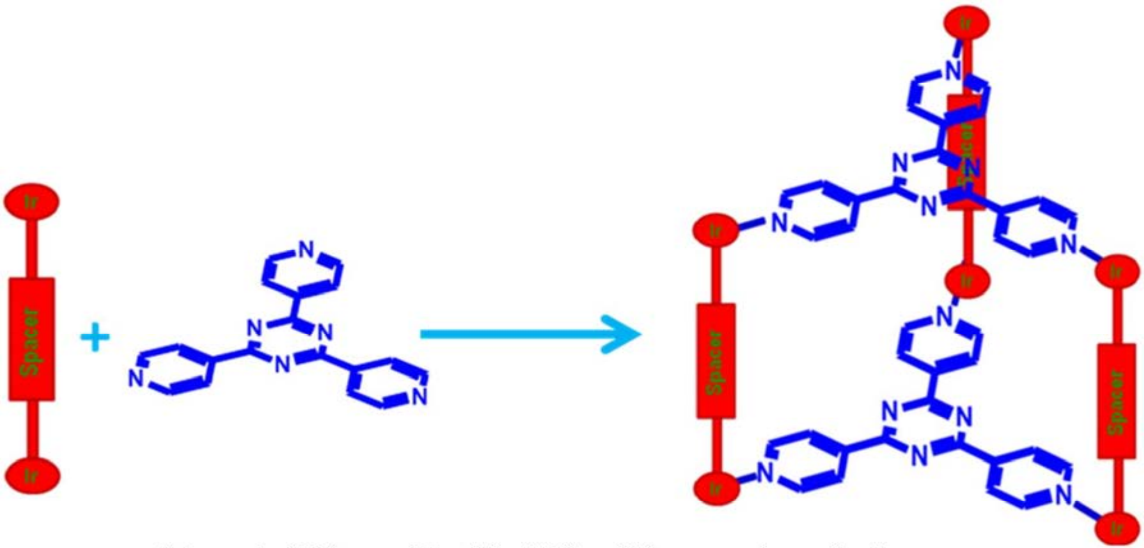
Self-assembly of a nanosized iridium coordination cage and encapsulation studies

SINGH NEM 조재호 송영호 지기환*

울산대학교 화학과

Since last decade self-assembled coordination cages are being successfully used in various challenging applications such as encapsulation and exploration of insoluble and reactive molecules, recognition of reactive intermediates by encapsulation, photo- and electrochemical studies by encapsulation, constructing pillars of aromatics, catalysis and so on. Most of the coordination cages capable of demonstrating these applications are self-assembled by square planer 90° Pd and Pt acceptor. The present work demonstrates the self assembly of coordination cage by octahedral iridium acceptor which is capable of incapsulating three planer aromatic guests (scheme 1). All the new complexes have been characterized by various spectroscopic analysis and single crystal X-ray diffraction. The X-ray crystallographic analysis revealed the expected cage structure. The poster will address a detail comprehensive account of the mentioned work.



Scheme 1: Self-assembly of the iridium(III) cornered coordination cage.

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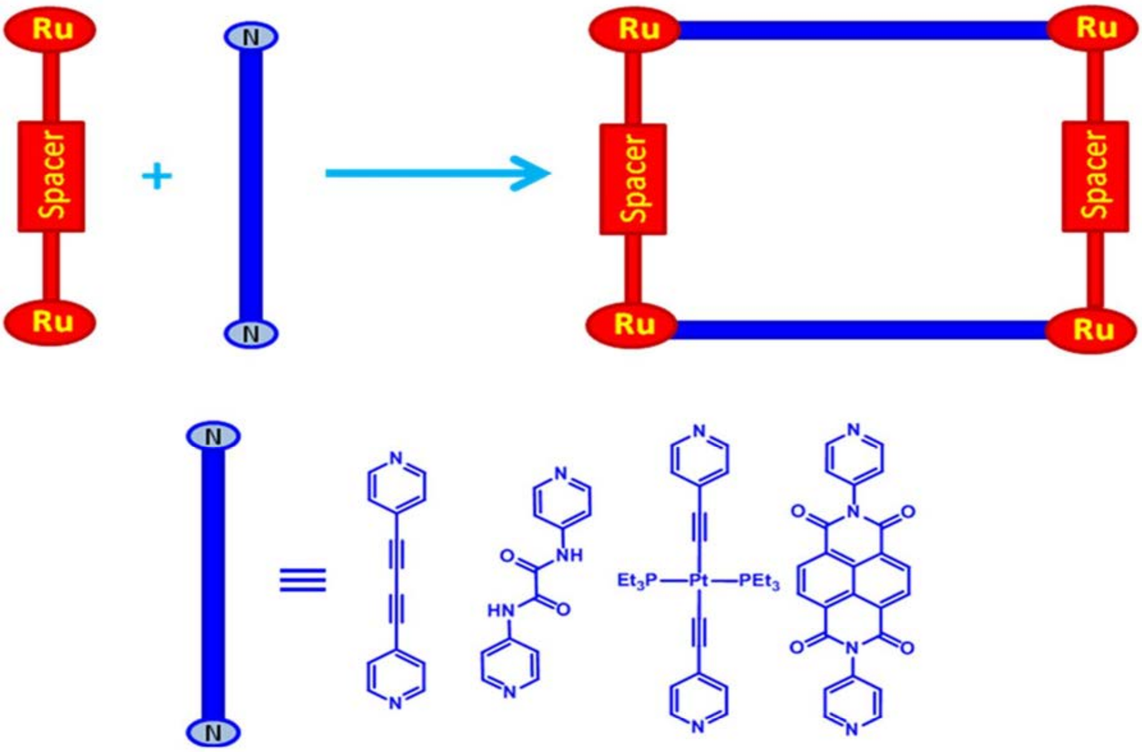
Coordination-driven self-assembled molecular rectangles incorporating pyridyl donors and arene ruthenium acceptor

SINGH NEM 조재호 지기환*

울산대학교 화학과

In the past two decades, coordination-driven self-assembly has emerged as an effective tool for constructing functionalized metalla-supramolecules with promising applications such as molecular recognition, separation, catalysis and encapsulation of various guests. In the search for new building blocks for the synthesis of supramolecular rectangles with comparable but modified properties, there has been an increasing interest in using transition metal complexes with octahedral geometry. The present work demonstrates the spontaneous formation of molecular rectangles by coordinating various lineour 4-pyridyl donors and acceptors based on octhedralmetal centers (scheme 1). The resulting supramolecular rectangles have well-defined internal cavities to stack large guest molecules. All the new complexes have been characterized by various spectroscopic and single crystal X-ray diffraction. The poster will address a detail comprehensive account of the mentioned work.



Scheme 1: Synthetic route to the self assembled metall-rectangles

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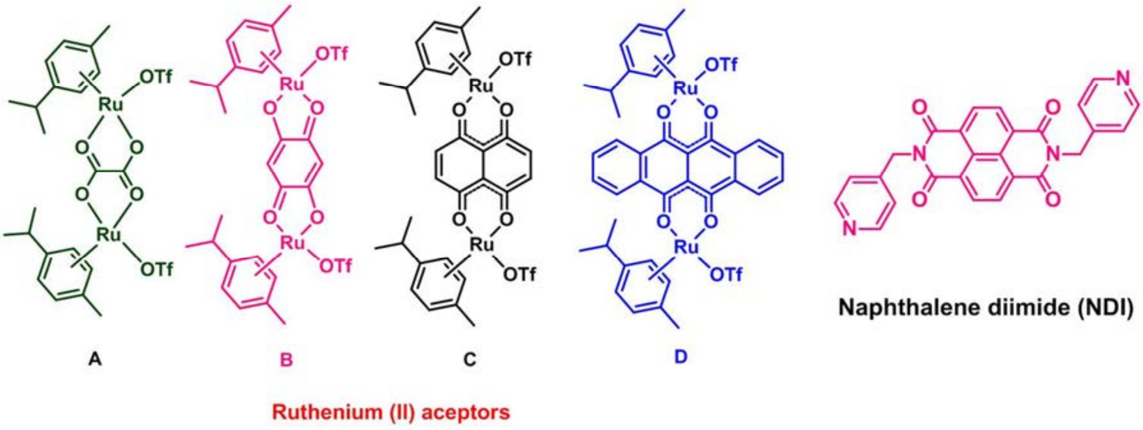
Rational Design and Synthesis of Organometallic Ruthenium(II) Supramolecular Self-assemblies of Flexible Naphthalene Diimide

PALANIELUMALAI 지기환*

울산대학교 화학과

The design and synthesis of supramolecular coordination driven, self-asseblies (SCDSs) via the rational combination of bridging multidentate ligands with various transition metal ions is of intense interest in the current field of supramolecular chemistry, and many complexes have been constructed in this aspect to exhibit either appealing architectures or encouraging the chemical properties such as catalysis, photoluminescence, sensors and nano material devices. Particularly, the platinum group metals coordinated SCDSs offer biological and chemical diversity that is distinct from that of organic drugs. Herein, we report the four supramolecular self-assembled metallacycles of arene-ruthenium acceptor with flexible naphthaline diimide ligand. The organometallic arene-ruthenium based metalla cycles architectures were achieved from an arene ruthenium acceptor (A-D) and electron rich, flexible ditopic napthaline diimide NN donor (NDI).



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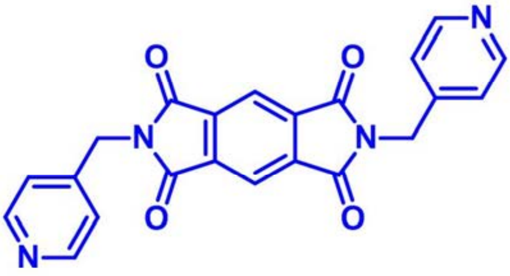
Flexible Pyromellitic Diimide Scaffold Organometallic arene-Ruthenium(II) Supramolecular Self-Assemblies

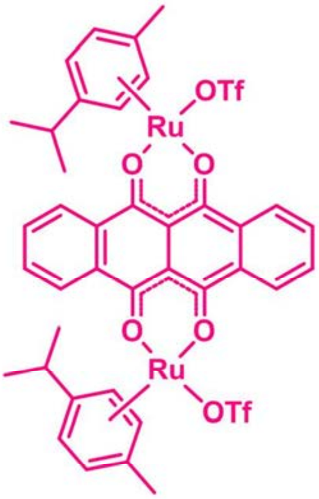
PALANIELUMALAI <u>김동환</u> 지기환*

울산대학교 화학과

Over the past few decades the significant progress has been made towards building new classes of supramolecular coordination-driven self-assemblies (SCDSs). Due to their simplicity, the interest on SCDS is significantly growing not only their intriguing structures and topological importance, but also their vital role in various fields, including catalysis, host-guest and biomedical applications. The SCDSs constructs by a multible of metal acceptors and suitable organic donors ligands and have extended beyond a simple two-component paradigm to encompass selective self-assembly, in which multiple assemblies form from a mixture of subunits, to multicomponent assemblies. Herein, we report the flexible pyrolmellitic diimide with arene ruthenium based supramolecular self-assemblies. The arene-ruthenium supramolecular architectures were achieved from a electron rich flexible N,N'-bis(4-pyridylmethly)pyromellitic diimide (PDI) and organometallic arene ruthenium acceptors (Ru-A).



Pyromellic Diimide (PDI)



Ruthenium (II) aceptor (Ru-A)

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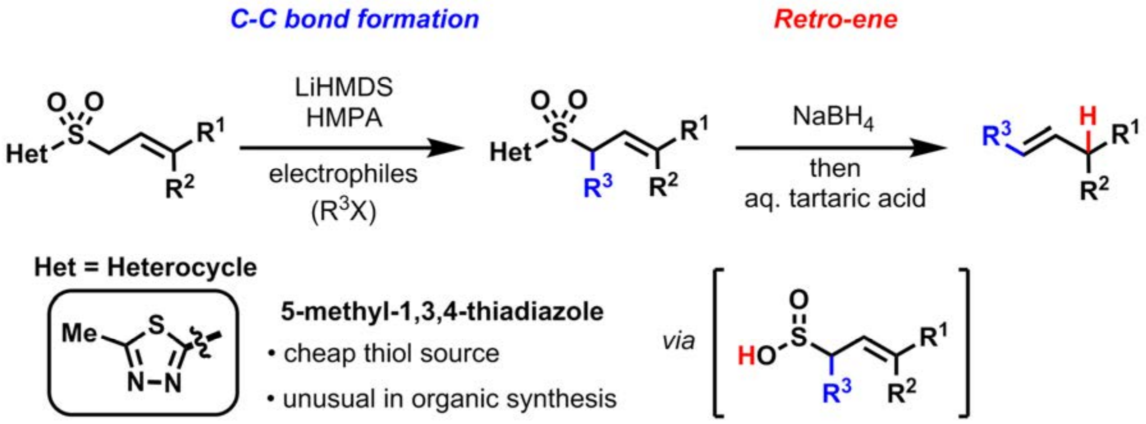
Traceless C-C bond Formation via Tandem Alkylation and Retro-ene Reactions Using Heterocyclic Sulfones

채영현 최진 이철범*

서울대학교 화학부

Our laboratory has been interested in the retro-ene reactions of allylic sulfinic acid that can be performed in tandem with the Diels-Alder reaction.1 As a follow-up study, we developed tandem alkylation and retro-ene reactions using unusual heterocyclic sulfones. This tandem protocol was aimed to form C-C bonds in a traceless fashion that was distinct from classical C-C bond forming reactions. Diverse allylsulfones as the precursor of the allylic sulfinic acid could be prepared through various C-C bond forming reactions (alkylation, aldol, and Michael reaction etc.). Subsequently, the retro-ene reaction was performed in one-pot under mild conditions and to yield functionalized reductively rearranged alkenes. It was found that thiadiazole substituted sulfones were more suitable precursor of allylic sulfinic acid than previously known heterocyclic sulfones. We anticipate that the traceless tandem methodology will be useful to synthesize various functionalized alkenes via allylsulfone substrates that can be prepared through a range of C-C bond forming reactions. The details of our studies will be shown in this poster.



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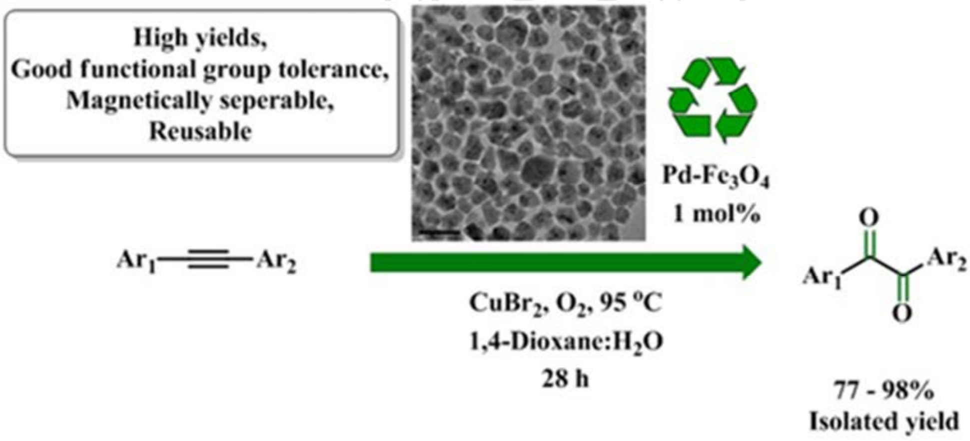
Efficient Synthesis of Benzil Derivatives via Oxidation of Alkynes Catalyzed by Pd-Fe3O4 Heterodimer Nanocatalyst

변상문 김병문*

서울대학교 화학부

An efficient, iterative, catalytic, Wacker-type oxidation of alkynes to 1,2-diketones using Pd?Fe3O4 heterodimeric nanocrystalline catalyst has been developed. This process has a wide substrate scope and affords 1,2-diketo compounds in excellent yields under atmospheric pressure. The operational procedure using the Pd-Fe3O4 nanocatalyst is extremely straightforward, and the catalyst can be recovered through the employment of simple magnetic separation, enabling the recycling of the catalyst for five times without loss of catalytic activity.



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Synthesis and Characterization of Novel Material for Organic Light Emitting Diodes (OLEDs)

노영리 윤순병 장용주 이다현 SHAIK BAJI 이상경* 천민경

경상대학교 화학과

Nitrogen-rich heterocyclic molecules have focusing for development of electron transporting materials (ETMs) because they have high electron mobility. The heterocycle compound which has nitrogen-rich was synthesized by Suzuki and Stille coupling. The obtained material was characterized by 1H-NMR, 13C-NMR and mass. Optical property of material was measured by UV absorption and photoluminescence (PL). It’s thermal and electrochemical properties were confirmed by thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC) and cyclic voltammetry (CV). Herein reported for the development of synthetic method, optical character, thermal and electrochemical properties of the synthesized novel material.

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Synthesis and Characterization of Asymmetric Anthracene Derivatives for OTFTs

윤순병 노영리 장용주 이다현 SHAIK BAJI 박민주 이상경[*]

경상대학교 화학과

Synthesis and physical properties of a novel p-type organic thin film transistors (OTFTs) materials containing thieno[3,2-b]thiophene and anthracene derivatives were studied. Suzuki, McMurry and Shonogashira coupling reaction were used for the synthesis of these materials at the final step. The obtained compound was confirmed by Mass, FT-IR, ^{1}H-NMR, ^{13}C-NMR spectroscopy and elemental analysis. The synthesized ACSTT, ACDTT and ACTTT have moderate solubility in common organic solvents such as chloroform, methylene chloride and THF. The thermal properties of thermal gravimetric analysis (TGA) differential scanning calorimetry(DSC). Optical and electrochemical properties of the compounds were confirmed by UV-vis and cyclic voltammetry.

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Synthesis and Physical Properties of New ETL Materials

이다현 노영리 윤순병 장용주 SHAIK BAJI 강훈민 이상경*

경상대학교 화학과

We synthesized new anthracene derivative, which contains nitrogen-rich heterocycle ring for electron transport layer (ETL) material in organic light-emitting diodes (OLEDs). Usually, ETL layer adopted electron rich molecules. So nitrogen-rich heterocycle compound was designed and synthesized. Anthracene derivatives have been widely used as emitting materials in OLEDs because anthracene derivatives have good photo-, electroluminescenet properties and electrochemical properties. The compound was synthesized by Suzuki coupling reaction. The obtained compound was confirmed by ^{1}H-NMR and ^{13}C-NMR. Thermal stability was characterized by TGA and DSC, physical properties was characterized by UV, PL and electronic stability was characterized by cyclovoltammetry.

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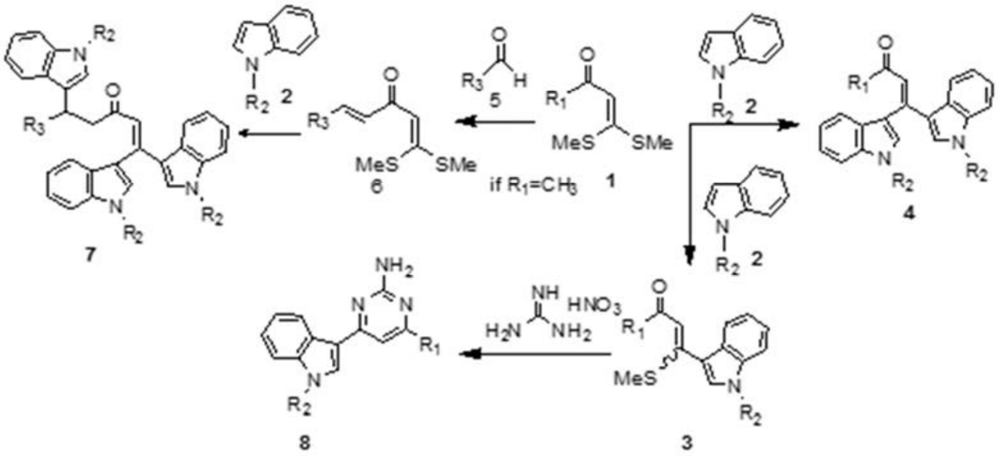
Indium(III) Chloride Mediated Michael Addition of Indoles to Ketene S,S-Acetals: Synthesis of Bis- and Tris-indolylketones

장용주 윤순병 노영리 **SHAIK BAJI** 이다현 이상경*

경상대학교 화학과

The indole nucleus is an important structural motif in medicinal chemistry. Bisindoles possess antitumor, genotoxicity, antihyper-lipidemic and antiobesity and radical scavenging activities and tris-indolyl scaffolds are known to show bacterial metabolic and cytotoxic agents. A series of bis and tris-indolyketones and meridianin alkaloids are prepared by one pot Michael reaction of indole and ketene S,S-acetals under solvent-free condition using mild Lewis acid InCl3. The ove-rall yields of the products are good and starting materials are cheaply available in compare to ethyl substituted dithioacetals.



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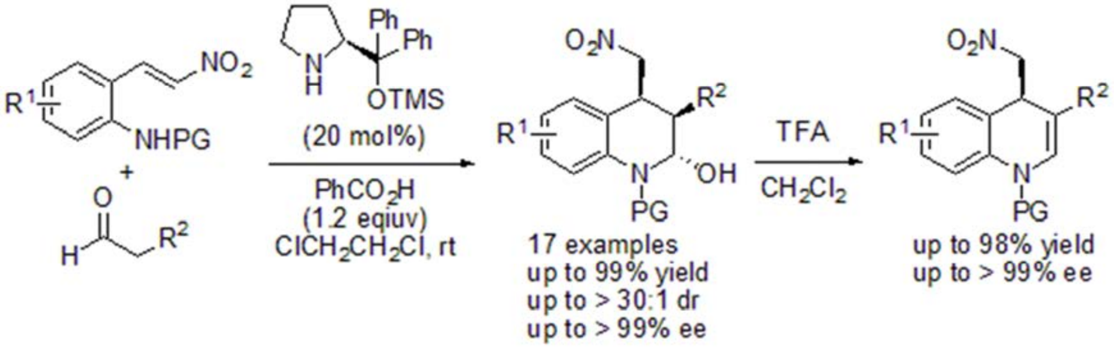
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Organocatalytic Michael addition?cyclization Cascade Reactions of Aldehydes to 2-Amino-β-nitrostyrenes

이요나 김성곤*

경기대학교 화학과

An organocatalytic enantioselective Michael addition/aza-cyclization cascade reaction of aldehydes with 2-amino-β-nitrostyrenes has been developed for the construction of fully substituted chiral tetrahydroquinolines. The reaction, promoted by diphenylprolinol TMS ether as an organocatalyst, generated the chiral tetrahydroquinolines in good to high yield with excellent diastereo- and enantioselectivities (up to >30:1 dr, >99% ee). The method also provided an alternative access to chiral 1,4-dihydroquinolines, which are difficult to synthesize by other methodologies.



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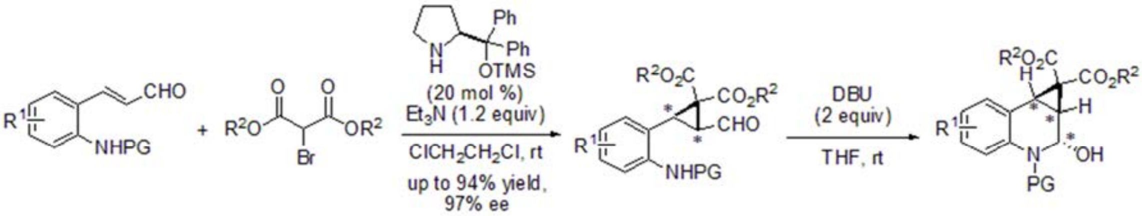
발표종류: 포스터, 발표일시: 수 16:00~19:00

Construction of chiral cyclopropane-fused tetrahydroquinolines: Enantioselective organocatalytic Michael/alkylation domino reaction and one-pot aza-cyclization

김철웅 김성곤[1,*]

경기대학교 화학 [1]경기대학교 화학과

An asymmetric two-step approach toward the synthesis of chiral cyclopropane-fused tetrahydroquinolines is described. In this synthesis, an asymmetric organocatalytic Michael/alkylation domino reaction of dialkyl bromomalonates with o-N-protected aminophenyl α,β-unsaturated aldehydes allows the process to proceed efficiently to afford corresponding 2-formylcyclopropane products in good yields with high enantioselectivities (up to 97% ee). In addition, a one-pot procedure for DBU-mediated aza-cyclization of the 2-formylcyclopropane adducts is applied for the formation of the chiral cyclopropane-fused tetrahydroquinolines.



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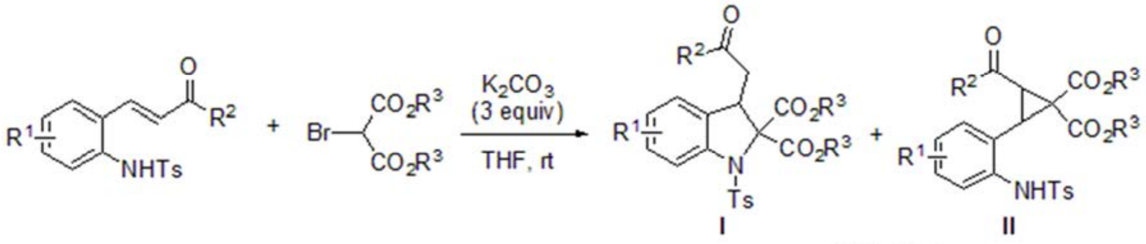
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Functionalized 2,3-Disubstituted Indolines via K_2CO_3-Promoted Cascade Michael/Aza-cyclization Reactions

김아름 김철웅[1] 김성곤[*]

경기대학교 화학과 [1]경기대학교 화학

The cascade Michael?cyclization reaction of o-N-tosylaminophenyl α,β-unsaturated ketones with dialkyl α-bromomalonates, which allows efficient construction of 2,3-disubstituted indolines, has been developed. The reaction, promoted by potassium carbonate, generated the functionalized indolines in good yields for a variety of o-N-tosylaminophenyl α,β-unsaturated ketones with high chemoselectivity.



up to 96% yield
ratio of I/II: up to 10/1

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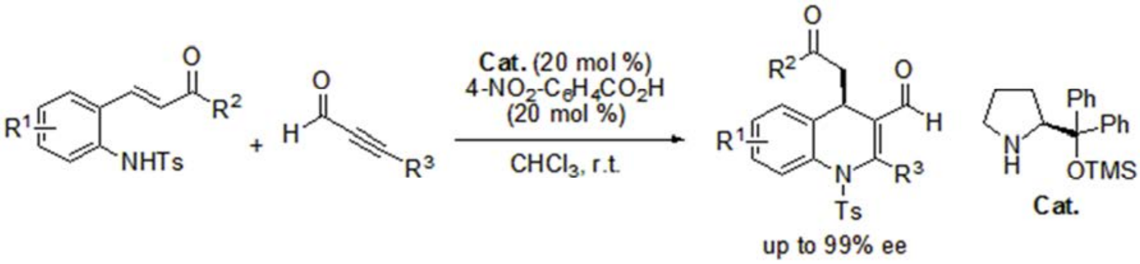
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Domino Aza-Michael-Michael Reaction of o-N-Protected Aminophenyl α,β-Unsaturated Ketones with Alkynes: Facile Synthesis of Chiral Highly Functionalized Dihydroquinolines

이요나 심종택 김성곤*

경기대학교 화학과

The enantioselective synthesis of dihydroquinolines has been developed through organocatalytic domino aza-Michael-Michael reaction of o-N-tosylaminophenyl α,β-unsaturated ketones with alkynes. This useful and simple domino process afforded diverse highly functionalized 1,4-dihydroquinolines, some of which are not easily accessible using other methodologies, in good yields and with good enantioselectivities (up to 99% ee).



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies of Rhodamine Cyclic Hydroxamate Derivatives as Fluorescent Probes

김재림 태진성*

연세대학교 화학과

We have prepared new rhodamine cyclic hydroxamate derivatives with various functional groups to establish a library of six-membered rhodamine probes. Several triazole derivatives are synthesized by copper(I)-catalyzed click chemistry with alkyne groups and rhodamines attached with a azide group. Metal ion selectivities and acid sensitivities of these derivatives are studied.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies of Rhodamine Cyclic Hydrazide Derivatives as Fluorescent Probes

오지민 태진성*

연세대학교 화학과

We have synthesized new rhodamine cyclic hydrazide derivatives containing different functional groups. These six-membered hydrazide derivatives were compared with the corresponding five-membered derivatives in terms of metal ion selectivities and acid sensitivities.

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The novel Palladium catalyst of Creative structure and its use

김미진 김영준[1] 정명진[2] 박찬필[3,*]

충남대학교 분석과학기술대학원 분석과학기술학과 [1]충남대학교 분석과학기술대학원/유기합성분석실험실 [2]충남대학교 분석과학기술학과 [3]충남대학교 분석과학기술대학원

Development of new catalyst is one of the oldest problems. Especially, Pd catalyst work effectively and efficiently to coupling reaction which formed C-C bond. While catalyst developed, ligands also have been developed. Herein, novel catalyst that we synthesized is not phosphine ligand or NHC ligand but, novel ligand of structure Bis(bidentate). It has advantage nontoxic, air-, moisture- stable and that doesn’t form intermediate for ligands. Specially, the novel catalyst that we used was synthesized through very simple process. It is remarkable that development of catalyst which has reasonable price and has a wide range of application because preparation process of catalysts at a high cost which need complicated synthesis route is restricted to industrial use for problem of cost. Also, synthesized novel catalyst is too stable to possible column and reaction with that catalyst synthesized high yield product without byproduct at high temperature.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Suzuki-Miyaura reaction using novel catalyst in the microreactor

김영준 김미진[1] 박찬필[2,*]

충남대학교 분석과학기술대학원/유기합성분석실험실 [1]충남대학교 분석과학기술대학원 분석과학기술학과 [2]충남대학교 분석과학기술대학원

In the past few decades, there are many palladium catalyzed studies that were used for heck, Suzuki-miyaura, sonogashira coupling reactions. Specially, Suzuki-miyaura coupling reaction with Pd is a powerful, convenient tool to form C-C bonding.In general, the traditional batch synthesis system have many demerits such as long time retention time, low conversion, products loss, low surface area to volume ratio, economic concern and environmental problem against the microreactor. However we can have high reaction efficiency with continuous flow microreactor. The traditional batch system was stirred to diffuse the two liquids. But it has randomly diffusion and non control the reaction condition. On the other hands, the microreactor has high surface area to volume ratio. So, this reactor could make the easy, convenient, efficient reaction condition. Also it can control the pressure in the tube, slug length, and can maintain the reaction condition stably. So the synthesis in the microreactor is suitable for lab scale reaction. In this study, we got the high efficiency through Suzuki-miyaura coupling reactionin the microreactor against the traditional batch system. In further study, we will control the temperature to confirm the catalyst stability and expect the high yield without side products.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Continuous flow synthesis of epoxy alcohols in a microchemical system

임효진 송주하 박찬이 박찬필*

충남대학교 분석과학기술대학원

The enormous potential of epoxy alcohols as key building blocks in production of valuable materials has led to intensive research for their preparation, metal-catalyzed epoxidation of allylic alcohols with hydroperoxides was the most practical route. However, the photooxygenation in batch system resulted in tedious reaction time and low selectivity, which was bottleneck in efficient mass production of epoxy alcohol. Therefore, it is difficult to complete the reaction by conventional one-pot synthesis. Herein we report a facile and efficient continuous flow process consisted of microchemical photooxygenation and epoxidation. Microchemical systems for photooxygenation provide new strategies and new challenges; it can be connected into the mass production of epoxy alcohols without delayed synthesis of peroxide intermediate. In addition, photocatalyst is decomposed immediately in microreactor, epoxidation is further faciltated in step2. Finally, the combination of methylene blue as photosensitizer and Ti(O-i-Pr)4 as epoxidation catalyst was perfect, alkenes were directly converted into epoxy alcohols with excellent yield and good selectivity.

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발표코드: **ORGN.P-727**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Phosphaannulation of Aryl and Benzyl Phosphonic Acids with Unactivated Alkenes via Palladium-Catalyzed C-H Activation/Oxidative Cyclization Reaction

전우형 손정유 김선웅 서보람 이필호*

강원대학교 화학과

An efficient phosphaannulation via Pd(II)-catalyzed C-H activation/oxidative cyclization by 6-*endo* mode is reported for the synthesis of 3-substituted phosphaisocoumarins from the reaction of aryl phosphonic acids with unactivated alkenes under aerobic conditions. Also, α,α-disubstituted benzyl phosphonic acids were phosphaannulated with unactivated alkenes, producing phosphaisochromanones having (*Z*)-alkylidenyl groups via *anti*-phosphoryoxypalladation by 6-*exo* mode.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Method of Pyrroles Starting from Terminal Alkynes, Sulfonyl Azides, and Alkenyl Alkyl Ethers

김철의 박상준 엄다한 서보람 손정유 이필호*

강원대학교 화학과

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

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Reversed-Polarity Synthetic Method for a Diversity of Unsymmetric Aryl Aryl and Aryl Alkenyl Ketones via Palladium-Catalyzed Cross-Coupling Reaction of Acylindium Reagents

류태규 박영철 손정유 서보람 이필호*

강원대학교 화학과

Transition-metal-catalyzed cross-coupling reaction of a number of electrophilic coupling partners with organometallic reagents is one of the most straightforward methods for C-C bond formation. To date, Pd catalysis has been applied widely in the synthesis of a variety of ketones constituting aryl aryl, alkyl aryl, and alkyl alkyl groups. We have developed a reversed-polarity synthetic method for a diversity of unsymmetric aryl aryl and aryl alkenyl ketones via Pd-catalyzed cross-coupling reaction of acylindium reagents generated in situ from acid chlorides and indium. Because the direct synthetic method of unmasked acyl anion equivalents from easily available acid chlorides with indium has been developed for the first time under mild conditions, the present reaction is highly useful and promising. The tolerance of formyl, ketone, ester, and nitrile groups is especially practical, providing an opportunity for further functionalization.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Diastereoselective Synthesis of Tetrahydrofurano- and Hexahydropyrano-dihydropyrroles Containing *N*,*O*-Acetal Moieties via Rhodium-Catalyzed Transannulation of *N*-Sulfonyl-1,2,3-triazoles with Oxacycloalkenes

김철의 박영철 박상준 <u>손정유</u> 이필호*

강원대학교 화학과

Rh-catalyzed [3 + 2] cycloaddition using iminocarbene intermediates derived from *N*-sulfonyl triazoles is well established. In this regard, we have developed a method for synthesis of pyrroles from the transannulation of *N*-sulfonyl triazoles with alkenyl alkyl ethers/elimination reaction. Tetrahydrofuranodihydropyrroles (THF-DPs) and tetrahydropyranodihydropyrroles (THP-DPs), which combine two unique heterocycles of dihydropyrroles and oxacycloalkanes, are valuable privileged structural motifs found in natural products. Herein, we have reported a diastereoselective synthetic method of tetrahydrofuranodihydropyrroles and tetrahydropyranodihydropyrroles containing *N*,*O*-acetal moieties via Rh-catalyzed denitrogenative transannulation of *N*-sulfonyl-1,2,3-triazoles with oxacycloalkenes. A myriad of functionalized pyrroles bearing hydroxyalkyl moieties at C3-position could be prepared via Rh-catalyzed denitrogenative transannulation/acid-catalyzed ring-opening reaction.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed C(sp^2)-H Activation/C-O Formation : Synthesis of Ethoxy Dibenzooxaphosphorin Oxides

신서현 강동진 전우형 백용현 이필호*

강원대학교 화학과

Unreactive C(sp^2)-H and C(sp^3)-H bonds are ubiquitous in organic compounds, so that the development of methods for the transition metal-catalyzed C-H activation is one of the challenging goals in organic synthesis. Recently, a variety of C-H activations by using new phosphoryl-related directing groups have been reported by our and other groups. We have developed an efficient synthetic method for a wide range of ethoxy dibenzooxaphosphorin oxides starting from 2-(aryl)arylphosphonic acid monoethyl esters and employing Pd-catalyzed C(sp^2)-H activation/C-O formation under aerobic condition.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Carbonylation of C-H Bonds of Phosphonic and Phosphinic Acids for the Synthesis of Oxaphosphorinanone Oxides

신서현 전우형 이은숙 서보람 이필호*

강원대학교 화학과

Because inhibition of β-lactamases remains a practical method to maintaining the efficacy of β-lactam antibiotics, the investigation for inhibitors of these enzymes has continued during the past 80 years. Since the cyclic phosphonates have been known to be reversible covalent inhibitors of the P99 β-lactamase, a new synthetic approach to these compounds was required. So, we have developed an efficient phosphaanuulation by Pd-catalyzed carbonylation of C-H bonds of phosphonic and phosphinic acids, leading to the construction of oxaphosphorinanone oxides, which are novel phosphorus heteocyclic privileged structures. Thus, this transformation opens a new avenue to sequential C-C/C-O bond formation in one pot vecause carbon monoxide represents an economical and atom efficient C1 building block.

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Synthesis of Dihydroazepines and Dihydropyrroles from Alkynes, Sulfonyl Azides, and 1, 3-Dienes through Aza-[4+3] and Aza-[3+2] Annulations

김상혁 모준태 김재은 류태규 이필호*

강원대학교 화학과

Azaheterocycles are a highly important class of compounds due to their biological activities and pharmaceutical usabilities. In particular, dihydroazepines, dihydropyrroles, and pyrroles are constituents of a valuable privileged structure in organic chemistry. For this reason, the development of efficient synthetic methods of multi-substituted azaheterocyclic compounds from simple and easily accessible starting materials has been continuously required. Now, we report an efficient aza-[4 + 3] annulation and aza-[3 + 2] annulation starting from terminal alkynes, sulfonyl azides, and 1,3-dienes in a one-pot.Recently, 1-sulfonyl-1,2,3-triazoles easily prepared from copper-catalyzed 1,3-dipolar cycloaddition of terminal alkynes with sulfonyl azides have been extensively investigated as precursors of α-imino metal carbenes. High reactivity of α-imino metal carbenes toward nucleophiles is caused by intrinsically electrophilic properties of the metal carbene species. In addition, it can react with electrophiles because the α-imino group having nitrogen atom is inherently nucleophilic. Accordingly, these amphiphilic α-imino metal carbenes smoothly react with nitriles, alkynes, allenes, isocyanates and isothiocyanates, furans, aldehydes and imines, α,β-unsaturated aldehydes, indoles, arenes, alkenes, amides, and furans to afford a multitude of heterocycles. More recently, we have reported that the reaction of triazoles with alkenyl alkyl ethers give rise to pyrroles through the corresponding dihydropyrroles. Next, we were interested in whether 1,3-diene can act as the dipolarophile to construct a dihydroazepine and dihydropyrrole scaffold.

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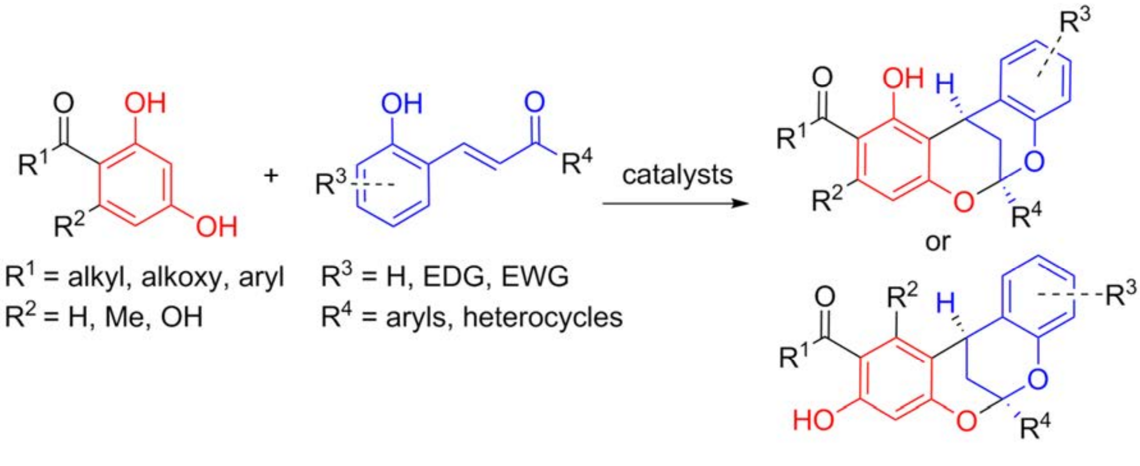
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regio- and Stereoselective Synthesis of Novel and Diverse 12*H*-6,12-Methanodibenzo[*d,g*][1,3]dioxocines

CAIHONGYUN 하립개 이용록*

영남대학교 화학공학부

The structural complexities of natural products have stimulated organic chemists to design novel and efficient strategies for the their syntheses. In particular, the synthesis of complex molecules from simple starting materials represents one of the most challenging goals in organic synthesis. Molecules bearing a 12*H*-6,12-methanodibenzo[*d,g*][1,3]dioxocine moiety are widely found in nature and have been shown to possess a number of important and potent biological activities. Given the importances of these biological and pharmacological activities, several synthetic methods have been devised for 12*H*-6,12-methanodibenzo[*d,g*][1,3]dioxocines, including 2,8-dioxabicyclo[3.3.1]nonanes.We present a facile one-pot regio- and stereoselective synthesis of diverse 1-hydroxymethanodibenzo[*d,g*][1,3]dioxocines and 3-hydroxymethanodibenzo[*d,g*][1,3]dioxocines using ethylenediamine diacetate (EDDA) or p-toluenesulfonic acid (PTSA) catalyzed reactions of various resorcinols and a number of 2-hydroxychalcones.



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발표코드: **ORGN.P-735**
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Diastereoselective *N*-Sulfonyl Aminoalkenylation of Azulenes from Terminal Alkynes and Azides via *N*-Sulfonyl-1,2,3-triazoles

박상준 용우순 김상혁 옥진표 이필호*

강원대학교 화학과

Azulenes, which are known to be a class of nonbenzenoid aromatic hydrocarbons, have attracted notable attention because of their significance as natural products, biologically active compounds, and molecular materials. Thus, development of efficient synthetic methods of these compounds from readily available starting materials has been in continuous demand. Although Hafner and co-workers reported a novel synthetic approach of azulene in one pot, introduction of valuable substituents onto azulene have limitations due to its unusual reactivity caused by the polarized π-electron system. For this reason, synthetic strategies of azulene through an introduction of a new functional group and its transformation are extremely desirable for the preparation of azulene derivatives. Herein, we report diastereoselective introduction of an enamine functionality on the azulenes from terminal alkynes and azides via *N*-sulfonyl-1,2,3-triazoles.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Metal-Free Azaphosphaannulation of Phosphonamides via Intramolecular Oxidative C-N Bond Formation

김예린 조승윤 김선웅 김성화 이필호*

강원대학교 화학과

Organophosphorus compounds have been broadly used in agricultural and pharmaceutical chemistry and material science, development of an efficient synthetic method for these compounds has been continuously required. In this regard, we were interested in transition-metal-catalyzed C-H activation/C-N bond formation and developed a Rh-catalyzed C(sp^2)-H activation/annulation and oxidative alkenylation/aza-Michael reaction directed by phosphonamide and phophinamide groups. We report an efficient metal-free azaphosphaannulation of myrid of phosphonamides through intramolecular oxidative C-N bond formation using $PhI(OAc)_2$ and iodine in acetonitrile under air, thus leading to the formation of benzazaphosphol-3-one 1-oxides, which are novel phosphorus heterocyclic privileged structures.

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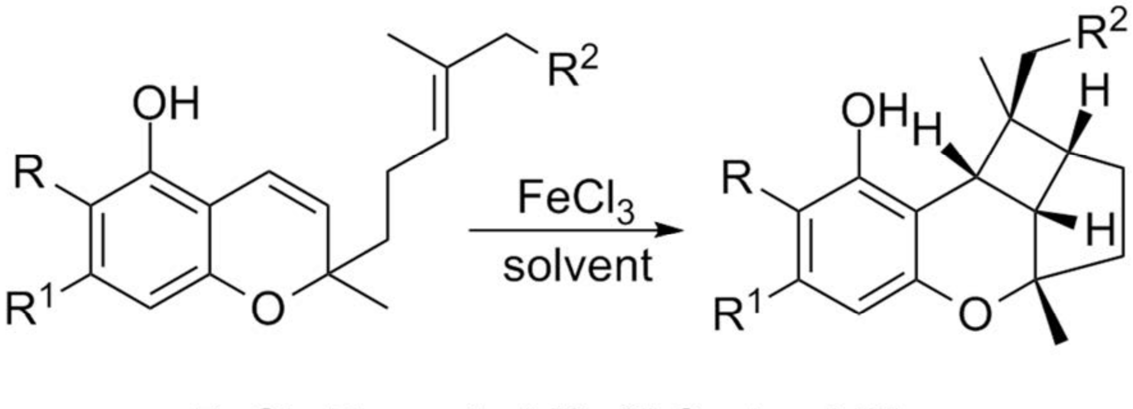
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Polycycles by FeCl3-Mediated [2+2] Cycloaddition

POUDELTEJNARAYAN 이용록*

영남대학교 화학공학부

Polycycles bearing a dihydropyran, a cyclopentane, and a cyclobutane ring are widely distributed in nature. They have a wide range of biological and pharmacological activities. Given the importance of these biological and pharmacological properties, several synthetic approaches have been devised for the synthesis of cyclol moieties that utilize intramolecular [2+2] cycloaddition.. Although several synthetic methods for polycycles bearing a cyclol moiety have been described using Brønsted acid or base catalyzed-reactions, efficient and facile synthetic methods are still demand. We present a facile FeCl3-promoted synthesis of biologically interesting polycycles bearing a cyclol moiety starting from readily available benzopyrans.



FeCl$_3$-Promoted [2+2] Cycloaddition

일시: 2014년 10월 15~17일(수~금) 3일간
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Mild Copper-TBAF-Catalyzed *N*-Arylation of Sulfoximines with Aryl Siloxanes

김재은 옥진표 김상혁 최원석 김선웅 이필호*

강원대학교 화학과

An efficient copper-TBAF-catalyzed C-N bond formation of sulfoximines with arylsiloxanes in dichloromethane at room temperature, affording the desired *N*-aryl sulfoximines in good to excellent yields under an oxygen atmosphere, is reported. The present method complements the previously reported synthetic approaches due to some advantageous properties of aryl siloxanes such as availability, low toxicity, ease of handling, high stability, and environmentally benignity under mild conditions, thus opening a new approach to practical C-N bond formation.

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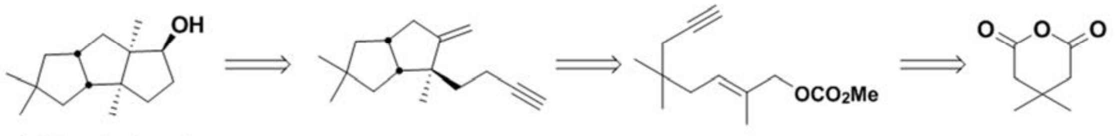
New radical reaction mechanism via Ruthenium catalyst : the case of (±)-Ceratopicanol synthesis

김리라 이희윤*

한국과학기술원(KAIST) 화학과

Ceratopicanol, which was first isolated by Hanssen and Abraham[1] from the fungus Ceratosystis Piceae Ha 4/82, is ceratopicane sesquiterpene natural product. Its highly congested structural feature with the cis/anti/cis-linearly fused triquinane structure that has five contiguous chiral carbon atoms, with two consecutive quaternary carbon centers, has challenged the synthetic chemistry community. Furthermore, recent reports have indicated that terpenes including ceratopicanol could be useful as prophylaxis or the treatment of pain while the pharmacological and clinical aspects of ceratopicanol were not fully explored as sesquiterpene hydrocarbons had not shown typical biological activities. We tried to solve the problematic step in Clive's synthesis[2] with other radical system but the reaction was achieved by palladium (0) catalyst with silyl hydride. The key intermediate was prepared by palladium-mediated ene reaction with cascade carbonylation that was reported on total synthesis of Hirsutene by Oppolzer[3]. In summary, (±)-Ceratopicanol was synthesized via two different palladium catalyzed reactions. References1. P. Hanssen; W.-R. Abraham, Tetrahedron. 1988, 44, 2175-2180.2. D. J. L.Clive; S. R. Magnuson; H.W. Manning, H.W; D. L. Mayhew, J. Org. Chem. 1996, 61, 2095-21083. W. Oppolzer.; C. Robyr, Tetrahedron, 1994, 50, 415-424



(+)-Ceratopicanol

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Synthesis of 2-Aryl-2*H*-benzotriazoles from Azobenzenes and *N*-Sulfonyl Azides via Sequential Rhodium-Catalyzed Amidation and Oxidation

류태규 민지애 최원석 전우형 이필호*

강원대학교 화학과

Development of synthetic methods of 2-aryl-2*H*-benzotriazole derivatives from easily accessible reactants is highly significant because it is an essential component of pharmaceuticals, UV stabilizers, and organic electronic materials. Because benzotirazoles exist as N^1-, N^2-, and N^3-substituted isomers, the selective preparation of benzotriazole represents an important synthetic challenge. Although a variety of synthetic methods for N^1-arylation of benzotriazole have been reported, a selective N^2-arylation of benzotriazole is still needed. For this reason, the selective synthesis of 2-aryl-2*H*-benzotriazoles has been continuously in demand. In our continuing efforts to develop efficient C-H activations, we report herein an efficient synthetic method for 2-aryl-2*H*-benzotriazoles from azobenzenes and *N*-sulfonyl azides through sequential Rh-catalyzed amidation (C-N bond formation) and oxidation (N-N bond formation) with $PhI(OAc)_2$ in one pot.

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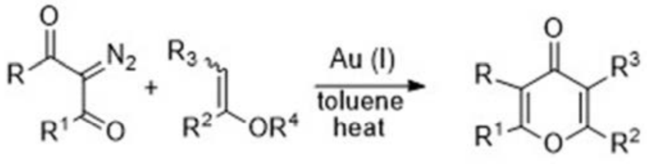
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold-Catalyzed Cascade Reactions for Substituted 4-Pyrones

KHANALHARIDATTA 하립개 이용록*

영남대학교 화학공학부

4-Pyrones are important heterocyclic compounds that are widely distributed in nature. They are frequently encountered as the skeletons of a variety of natural products and biologically active synthetic materials. They have been also used as versatile building blocks and valuable intermediates for the syntheses of complex natural products and bioactive molecules. Due to their remarkable biological activities, a number of synthetic approaches have been devised for the preparation of 4-pyrones. We present herein the simple and efficient one-pot synthesis of a variety of substituted 4-pyrones by sequential gold-catalyzed Wolff rearrangement of diazodicarbonyl compounds followed by [4+2] cycloaddition and elimination.



Gold-catalyzed reactions for the synthesis of 4-pyrones

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Bronsted Acid-Catalyzed Intermolecular Carboalkoxylation of Alkynes

엄지원 신승훈*

한양대학교 화학과

Our group reported gold-catalyzed intermolecular couplings of sulfonylacetylenes with allyl ethers via a [3,3]-sigmatropic rearrangement(Eq. 1)1. When the reaction partners were changed from allyl ethers into the more nucleophilic allyl amines, the reaction could be best catalyzed by Brosted acids. The resulting product will find its use as potential precursors of β-amino acids and therefore, various efforts toward asymmetric transformation have been made. References1.(a) Jun, J.; Yeom, H. ?S.; An, J. ?H.; Shin, S. “Gold-Catalyzed Intermolecular Coupling of Sulfonylacetylene with Allyl Ether: [3,3]- and [1,3]-Rearrangement” Beilstein J. Org. Chem. 2013, 9, 1724 (b) Park, S. R.; Kim, D. ?G.; Thrimurtulu, N.; Yeom, H. ?S.; Jun, J.; Shin, S.; Rhee, Y. H. “Entry to β-Alkoxyacrylates via Gold-Catalyzed Intermolecular Coupling of Alkynoates and Allylic Ethers”, Org. Lett. 2013, 15, 1166

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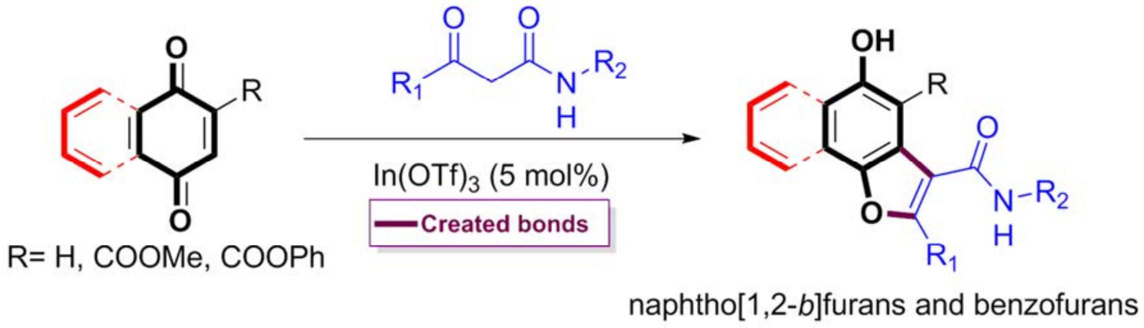
발표코드: **ORGN.P-743**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

In(OTf)$_3$-Catalyzed Formal [3+2] Cycloaddition of Benzo-/1,4-Naphthoquinones with β-Ketoamides: Regioselective Synthesis of Diverse Benzo-/Naphtho[1,2-*b*]furan-3-carboxamides

윤상현 하립개 이용록*

영남대학교 화학공학부

We describe a novel and efficient synthesis of naphtho[1,2-*b*]furan-3-carboxamides and benzofuran-3-carboxamides via the In(OTf)$_3$-catalyzed cascade formal [3 + 2] cycloaddition of 1,4-naphthoquinones or benzoquinones with β-ketoamides. This methodology has broad substrate scope that can afford novel and diverse naphtho[1,2-*b*]furan-3-carboxamides and benzofuran-3-carboxamides with high regioselectivity in good to excellent yields. Furthermore, this methodology is expected to be applicable to the synthesis of biologically-active complex molecules bearing naphtho[1,2-*b*]furan-3-carboxamides and benzofuran-3-carboxbenzamides.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Radical scavenging properties of novel 3,4,5-trisubstituted piperidine derivatives

김진호 장혜영[1] 이정태[*]

한림대학교 화학과 [1]아주대학교 화학과

Reactive oxygen species are present in the body of all animals and plants and can protect our body from bacteria and virus. However, overproduction of reactive oxygen species can cause aging and cancer due to their attack to normal cells. Antioxidants scavenge the reactive oxygen species protecting normal cells. Therefore, they have been the center of attention. A series of novel 3,4,5-trisubstituted piperidine derivatives were tested for their antioxidant activity. The effect from the presence of tempo was studied.

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Syntheses and anion binding studies of a series of meso *p*-substituted aryl calix[4]pyrroles

김주연 이창희[1] 이정태[2,*]

한림대학교 화학 [1]강원대학교 화학과 [2]한림대학교 화학과

The human body is composed of more than 60 trillion cells and has a large number of anions. These anions are recognized as an integral part on the organism to survive. Because calixpyrroles have widely been known as receptors for these anions and used as chemical sensors, intensive research on calixpyrroles has been conducted. In this study, the anion binding ability of various calix[4]pyrroles bearing different meso aryl groups has been compared by NMR titration. We synthesized a series of meso *p*-substituted aryl calix[4]pyrroles and studied the effect of these *p*-substituted aryl groups on the equilibrium constants using the Hammett equation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Diversity oriented synthesis of 2-arylbenzo[*b*]furan

윤소라 전종갑*

한림대학교 화학과

The 2-arylbenzo[*b*]furan structure is a heterocyclic compound consisting of fused benzene and furan rings and is an important scaffold for drug development. Several 2-arylbenzo[*b*]furans have shown antioxidant, anti-HIV, antifungal, antiplasmodial, anticancer, anti-inflammatory and estrogenic activities. Diverse synthetic routes can be applied to the synthesis of benzofurans. We have attempted Pd-catalyzed Sonogashira cross coupling reation, intramolecular Wittig reaction, Suzuki cross coupling reation, Al_2O_3 mediated cyclization reation and Horner-Emmons type condensation by utilizing umpolung property of α-aminophosphonates to construct 2-arylbenzo[*b*]furan.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of anti-inflammatory active piperlongumine and its derivatives

서영화 전종갑*

한림대학교 화학과

Piperlongumine (PL) and its derivatives were synthesized by the direct reaction between acid chloride of 3,4,5-trimethoxycinnamic acid and various amides/lactams. Later their anti-inflammatory effects were evaluated in lipopolysaccharide (LPS)-induced RAW-264.7 macrophages. Of the piperlogs prepared in this study, the maximum (91.3%) inhibitory activity was observed with PL (IC_{50} = 2.68 μM) but showed cytotoxicity whereas compound 3 (IC_{50} = 6.01 μM) which possess α,β-unsaturated γ-butyrolactam moiety offered good level (64.8%) of activity with no cytotoxicity. This study revealed that amide/lactam moiety connected to cinnamoyl group with minimum 3 carbon chain length and α,β-unsaturation is fruitful to show potent anti-inflammatory activity.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of puerariafuran which was extracted from *pueraria* root and its derivatives

김철기 윤현호 전종갑*

한림대학교 화학과

We wish to describe an effective synthesis of benzo[*b*]furan natural compound puerariafuran. This compound has been extracted from *Pueraria lobata Ohwil*. This is also known as nontoxic, and good for treating and preventing diabetic complications. It has been synthesized from the Al_2O_3 mediated coupling reaction between phenol and α-brominated ketone compounds.The total synthesis of puerariafuran was applied by using Al_2O_3 mediated cyclizationreaction between α-bromoketone compound and substituted aryl benzaldehydes instead of Sonogashira coupling reaction. This method will provide shorter total reaction procedures and better yield. However, the yield of this key step is still very low and should be improved through adjusting various reaction conditions including catalysts, solvents and temperatures.

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Synthesis of natural stillbene compound

문인수 전종갑*

한림대학교 화학과

Stilbenes are a class of naturally occuring polyphenolic compounds, exist as *cis* or *trans* isomers and have exceptional antioxidant, anti-inflammatory, anti-tumor, anti-fungal, antibacterial and antiplatelet aggregation properties. These effects are well known as natural products resveratrol, piceatannol and combretastatins having stillbene structure. They have also been applied to photo-responsive OLEDs or NLO materials and photo-chemical or photo-physical cis-trans isomerization in different technological fields. The anti-inflammatory activity of stilbene derivatives differs from the type of position and substituents. Herein we wish to describe the synthesis of new natural stilbene derivatives using the Wittig-Horner reaction method.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An Expeditious Synthesis of Natural Benzofuran, Eupomatenoid-6 by Umpolung of α-Aminophosphonates

KONGARADAMODAR 전종갑[1,*]

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Simple and practical synthesis of natural benzofuran derivative eupomatenoid-6 *via* Horner-Emmons type condensation as the key step is described. The umpolung property of aldehyde derivative, α-aminophosphonate was efficiently employed in this reaction. α-Aminophosphonate of anisaldehyde subjected to Horner-Emmons type condensation with 5-bromo-2-methoxybenzaldehyde to yield the deoxybenzoin, which was further methylated and then underwent tandem demethylation-cyclodehydration to afford the benzofuran scaffold in excellent yield. Finally Suzuki coupling with propenyl boronic acid afforded eupomatenoid-6 with an overall yield of 56.8%.

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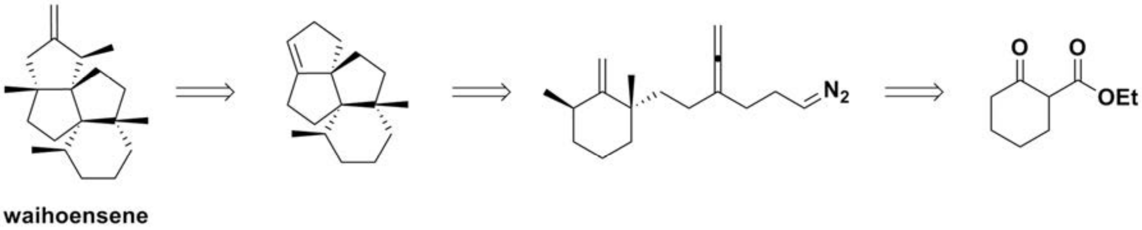
Tetracyclic Compounds through Single Operation Using TMM Diyl Intermediate; Application to the Total Synthesis of Waihoensene

이홍수 이희윤*

한국과학기술원(KAIST) 화학과

Recently, we developed the tandem cycloaddition route to triquinanes from linear substrates via an intramolecular [2+3] cycloaddition reaction of TMM diyls.1 The scope of the tandem cycloadditon reaction of TMM diyl can be extended to the synthesis of tetraquinanes framework.We envisioned that the total synthesis of Waihoensene2, the metabolite to be discovered whose structure is related to laurenene and has a unique skeleton among the known diterpenes can be achieved through the TMM-mediated tandem reaction to tetraquinanes strategy. We prepared the diazoallenyl precursor of the tetracyclic compound from cyclohexanone carboxylate and the tandem cycloaddition reaction produced the desired tetracyclic product as the major product. We will present the detailed synthesis of the tetracyclic intermediate and the completion of the total synthesis of waihoensene in stereo- and regio-selective manner.References1.Kang, T.; Kim, W.-Y; Yoon, Y; Kim, B. G.; Lee, H.-Y. J. Am. Chem. Soc. 2011, 133, 18050.2.Clarke, D. B.; Hinkley, S. F. R.; Weavers, R. T. Tetrahedron Lett. 1997, 38, 4297.



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Functional supramolecular electron donor-acceptor materials based on a TTF-C4Ps and PDI derivatives

김덕은 박정수*

숙명여자대학교 화학과

Considerable effort has been focused on the preparation of supramolecular systems with the capability of recognizing specific chemical species. Among a variety of artificial supramolecular host frameworks, calix[n]pyrroles are multi-pyrrolic macrocycles that consist of the same number of pyrroles and *sp*^{3}-alkyl substituted bridging *meso*-carbon atoms. Recently, in the context of the effort to combine calix[n]pyrrole and tetrathiafulvalene (TTF) chemistry, a series of tetrathiafulvalene (TTF) functionalized calix[n]pyrroles (TTF-C[n]Ps) were synthesized and studied as functional receptors for various guest species such as anions, electron deficient guest species, and fullerenes. Here, the recent discovery in supramolecular chemistry of TTF-calix[n]pyrroles as electron donors and perylene-3,4,9,10-tetracarboxylic diimide derivatives (PDIs) as electron accepting chromophores will be discussed in details.

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Oxidative compling reaction of alkylamine with various heteroaromatic diamines

김건우 정대일* 이언진 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Benzimidazole moiety plays an important role in chemistry and is also present in a variety of biologically active and therapeutically useful compounds. A simple and efficient transformation using readily available reagents under solvent-free and metal-free conditions is considered as a key solution for pollution problems generated by large-scale reaction. In contract to oxygen, which in a biradical in the ground state, sulfur in less reactive. Here in, we report a chemoselective method for an oxidative coupling reaction of alkylamine with heteroaromatic diamines for the formation of substituted 2-carbodiimides benzimidazoles.

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Cyclization reaction of isobenzofuran-1-(3H)-ones with o-phenylenediamine or heteroaromatic diamines

권연근 이도훈 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

In medicinal chemistry, aromatic heterocyclic compounds have remained a major source of chemotypes used in drug discovery. Specially, 1,4-and 1,5-benzodiazepine scaffolds structures have already proven their utility in medicinal chemistry. Recent trends in drug discovery show an attempt to move away from flattened aromatic structures to their saturated counterparts. Implementation of this idea to 1,4 and 1,5-benzodiazepine scaffolds, as well as to their fused analogues gives rise to three-dimentional molecular frameworks which potentially might preserve the 'privileged' status of their aromatic preunsorp. Herein, we report two-step reaction sequence for the preparation of isoindolo[2,1-a][1,5]benzodiazepin-1,2-ones. pthalaldehydic acid has been prepared by the alkaline oxidation of naphthalene. Cyclization reaction of isobenzofuran-1-(3H)-ones with o-phenylenediamine or heteroaromatic diamines led to the formation of isoidolo[2,1-a][1,5]benzodiazepin-1,2-ones.

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Synthesis and kinetic study of 7-azabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylates

김성태 이용균 정대일* 김인식[1] 한정태[2]

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Indole is a common component of fragnances and amino acid the precusor to many pharmaceuticals(tryptophan and serotonin) indoline is an aromatic heterocyclic organic compound and based on the indole structure.By oxidation/dehydrogenation it can be converted to indoles. The pupose of the research is to report that pyrrole also gave the 1:2 adduct(indole) when refluxed with DMAD in ether.Indoline was obtained by rearrangement (an ester group on the 3a position shift to a 3 position and the 1,3shift of the hydrogen atom) of indole.In this research, we with to propose a mechanism for the rearrangement nationalized by chemical kinetics.

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Highly efficient one-pot synthesis of novel phenylpyrimido[1,2-*c*]thienopyrimidinones

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목원대학교 화학과대학원 [1]목원대학교 화학과

New phenylpyrimido[1,2-*c*]thienopyrimidinones 4A/4B were easily prepared in good yields by the one-pot reaction of formamidine derivatives 2 of 4-aminothienopyrimidine with phenylacetyl chlorides. The application of this convenient and reliable method could be used for the synthesis of a variety of pyrimido[1,2-*c*]thienopyrimidinones derivatives of biological importance.

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N-glycosylaion vs Amadori reaction of glucose

권순정 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

sugar compound like glucose and fructose can be used as energy source which can be synthesized easily and concisely. biomass and biofuel are typical energy material which can be converted from sugar. It is a nonpolluting and clean object to efficiently synthesize the glucose containing nitrogen compounds. Amadori rearrangement and N-glycosylation reactions are efficient tools for the synthesis of the above compounds which can be proceeded from the same substrates. The study on the control of the reaction conditions leading either to N-glycosylation or to Amadori has been carried out. The concentration of the acid on the product yield is examined in order to determine the optimum conditions for Amadori rearrangement. The control of temperature is more important than the amount of acid in the optimization of the Amadori product.

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A study on the synthesis of various 2,7-substituted-oct-4-enedials as a key subunit for Unnatural Carotenoids

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Carotenoids present in nature as natural pigment of yellow and orange, can be classified as the xanthophylls and carotenes depending on the presence or absence of oxygen respectively. Most of the carotenoids are composed of 40 carbon atoms to form a conjugate polyene chain. Carotenoids may exhibit conductivity by the polyene chain present in it and can be used as molecular wire. We synthesized the titled dials by coupling 1,4-dibromo-2-butene and 2-substituted acetate, followed by LiAlH4 reduction and swern oxidation. And we studied the importance of crown ether functional group that is able to bind the metal ion. The unnatural carotenoids can be assembled by our sulfone-mediate coupling and double elimination strategy utilizing allylic sulfone and the above-mentioned dials. The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would offer an extra stability and excellent electronic characteristics compared with those of the natural carotenoids.

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A study of molecular wire synthesis with crown ether

김윤지 구상호[1,*]

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Carotenoids have a conjugated polyene chains, which could be utilized as materials for conductive molecular wire. We already know that unnatural carotenoids which have different substituent have different conductance from that natural carotenoids. And we think that these might be some different conductance if there are Crown ether that coordinate with metal ions in the molecular wires.These molecular wires can be obtained by coupling with allylic sulfones and crown ether-dialdehyde. Chloro sulfone unit is the key compound, contain aromatic substituents, which can be prepared form the acetophenone derivatives. Allylic sulfone was prepared by Indium mediated addition of chloro sulfone unit to aldehyde followed by Oxonia-cope rearrangement.

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Research on synthetic method of Unnatural carotenoid

임보람 구상호[1,*]

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We plan to synthesize the conjugated polyene chain containing phenyl substituents.It is postulated that two phenyl substituents in 1,6-position are orthogonal to conjugated polyene chain which can coordinate with specific metal ions.And then subsequent double elimination, carotenoids, it is necessary to design efficient building blocks.;Allylic sulfone unit containing phenyl substituents can be readily prepared from acetophenone derivatives via indium mediated addition and oxonia-cope rearrangement. Allylic aldehyde unit can be easily obtained. Based on our design, it is feasible to synthesize the conjugated polyene chain with di phenyl substituents.

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Single-Step Synthesis of Pyrralines from Readily Available Sugars: Scope, Limitation, Mechanistic Investigation and Applications

DASADHIKARYNIRMAL 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Single-step Synthesis of various N-substituted 5-(hydroxy)methylpyrrole-2-carbaldehydes (pyrralines) was performed using oxalic acid in dry DMSO at 90 °C for 30 min. Initially the reaction goes through Amadori intermediate which upon several steps of rearrangement followed by dehydration lead the formation of the desired pyrallines in 21-53% yield. Use of α-amino esters produced the expected intramolecular lactonization products which were reported to be biologically active pyrrolo-lactone natural products, synthesized in multistep process earlier. Further cyclization of the highly functionalized pyrralines afforded the pyrrole-fused poly heterocyclic compounds as potential intermediates for drug and functional materials.

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Carotenoid Derivatives: Synthesis and Incorporate Effect of Various Substituents on Electrical Conductance of these as Molecular Nanowires

ALAMMOHAMMADSHARIFUL 구상호[1,*]

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An efficient synthetic method for the different carotenoid compounds consisting different substituents and aliphatic macro cyclic ring(or aromatic fused ring) at middle position and incorporate consequence of electrical conductance in these carotenoid molecular nanowires. These carotenoid derivatives can be synthesized by coupling with dihelomethyl toluene through successively producing metacyclophane and corresponding sulphonium compounds. Finally carotenoid derivatives obtained by coupling with allylic sulfone after further halogenations. Specially can be done a systematic study on the combined effect of the different substituents of synthesized carotenoid derivatives as a molecular nanowires.

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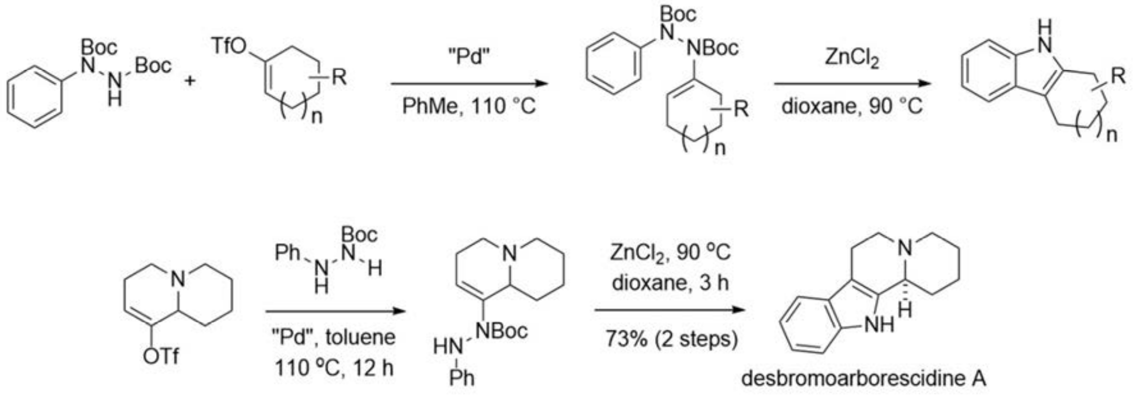
Ene-hydrazide from Enol Triflate for the Regioselective Fischer Indole Synthesis

임병윤 정보은 조천규*

한양대학교 화학과

Indole alkaloids are important class of natural products possessing intriguing molecular structures and biological activities. Over the years, many synthetic elaborations have been directed toward the indole-based natural products. The advance of the transition metal catalyzed C-N coupling reaction has particularly enriched the repertoire in indole synthesis. Despite the recent developments, the historic Fischer indole synthesis, reported in 1883, is still and often practiced because of its simplicity and reliability. However, it also suffers from two major drawbacks: the poor availability of the starting aryl hydrazine and the lack of regioselectivity.

Ene-hydrazide prepared from enol triflate undergoes Fischer indolization reaction to give the indole with complete regioselectivity. The starting enol triflate is readily accessed in regiochemically defined form from the corresponding ketone via well-established thermodynamic/kinetic control in the enolate formation. This new protocol was successfully applied to the synthesis of desbromoarborescidine A, a natural β-carboline alkaloid, difficult to prepare with conventional Fischer indole synthesis.



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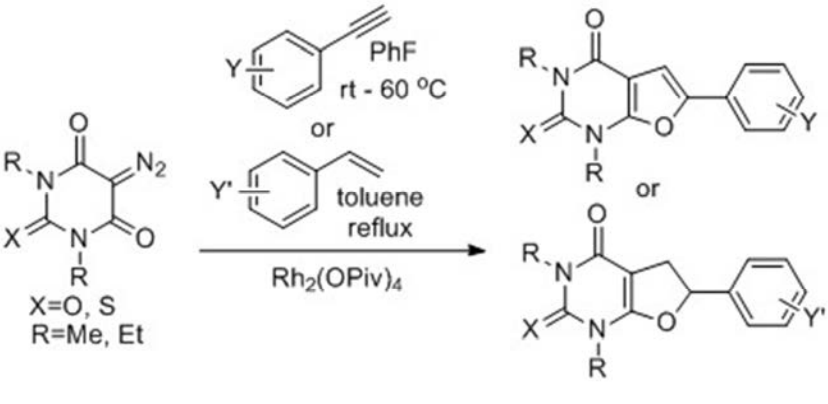
Rhodium (II) Catalyzed Synthesis of Various Furo[2,3-d]pyrimidinediones and Thioxofuro[2,3-d]pyrimidineones

MAEZONO SHIZUKA MEI BAUTISTA 소마이마가크리쉬나 이용록*

영남대학교 화학공학부

Furopyrimidine derivatives have shown a variety of biological activities such as antimalarial, antifolate, antitumor, antiviral, antibacterial, antifungal, and antihypertensive properties. Because of their importances, several methods have been devised to synthesize furopyrimidines. There is a need for more convenient and efficient synthetic methods for the preparation of furo[2,3-d]pyrimidinedione derivatives, and in particular, the synthesis of thioxofuro[2,3-d]pyrimidinedione derivatives. We present the rhodium (II)-catalyzed reactions of cyclic diazo compounds with arylacetylenes and styrenes.



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A Study on the reaction of Anthraniloyl hydrazine and Aldehydes with diphenyl phosphate

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The pyridine analog is quinoline or isoquinoline. especially quinazolinone compounds are class of fused heterocycles compounds well known for a long time and still continue the object of considerable interest. quinazolinones have been reported to be biologically versatile compounds posses variety of activity including anticancer, antifungal, antibacterial activities. The quinazolinones have immense interest because of their broad spectrum of in-vitro activity and their in-vivo chemotherapeutic activity. Recently, the synthesis of 2,3-dihydro-4-(1H)-quinazolinones by using Lewis acids and heteropoly acids has been described and their catalyst free synthesis in ionic liquids or 2,2,2-trifluoroethanol has also been reported. We now report reactions of anthraniloyl hydrazine(or salicylamide) and aldehydes with diphenyl phosphate(DPP), cyanuric chloride and tungstosilicic acid as catalysts. And we will try synthesis of N-substitued- quinazolinones from 2-amino-quinazolinones.

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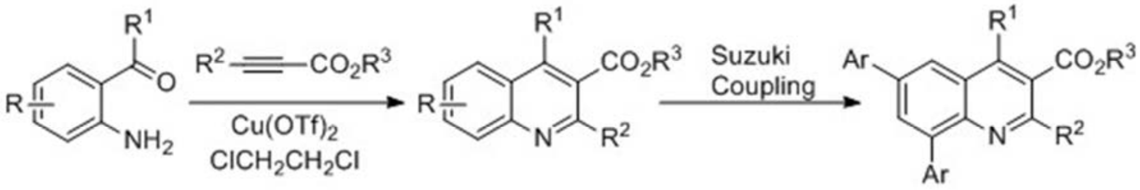
Copper-Catalyzed Cascade Process for the Synthesis of Diverse Quinoline Carboxylates

KALIAPPANKALIRAJ PANDIT RAMESHWAR PRA 이용록*

영남대학교 화학공학부

We describe an efficient cascade process for the synthesis of quinoline caroboxylates employing 2-aminoarylcarbonyls and acetylene carboxylates. Use of catalytic copper(II) triflate in the domino process has yielded diverse quinoline carboxylates. Initial Michael addition of nitrogen nucleophile to the acetylene carboxylates (Michael acceptor) followed by cyclization and aromatization are the essential steps involved in the domino process. Furthermore synthetic extension of the developed method has been demonstrated via Suzuki coupling.



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A study on the synthesis of 2-Amino-4-arylthiazoles and 2-Substituted-4-arylthiazolesrt

김수완 송주현 정대일* 한정태[1]

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It's well known that thiazole devatives are important compounds in medicinal chemistry due to their broad range of biological activities. Thiazoles are found in a variety of specialized products, often fused with benzene derivatives, the so-called benzothiazoles. This type of heterocycles have shown wide variety of pharmaco active protecties as anti-inflammatory, anti-tubercular, antibacterial, fungicidal, local anesthetic, tranquilizers, insecticidal, anti-microbial, anti-tumor and diuretic. Considerable efforts have been devoted to the synthesis of this type of compounds. Taking in consideration the advantages of microwave heating on solvent-free reactions, we report the rapid solventless synthesis of a series of 2-amino-4-aryl-1,3-thiazoles under microwave irradiation, prepared from the cyclocondensation of heteroaromatic ketones with thiourea and iodine. And also we report the reactions of 2-amino-4-arylthiazole with 2,5-dimethoxytetrahydrofuran, 1,3-acetonedicarboxylic acid and the reactions of 2-amino-4-arylthiazole with acyl chloride.

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Bridging of photochromic dye for application in lens

이상희* 이유석 김동희

군산대학교 화학과

Photochromic dyes are light-responsive molecules, which undergo a reversible change in color when exposed to UV radiation. This color change is accompanied by intramolecular rotational transformation which is sensitive to viscocity of their environment. Therefore, in rigid polymeric matrices, a dramatic slowing of coloration and kinetics is seen when compared with solution speeds. Fast decoloration is required for the application of photochromic dyes to lens. In this research, dyes were bridged using appropriate linker to modify rotational freedom in lens matrices. The synthesis of bridged dye and bridging effect on decoloration rate will be discussed.

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발표분야: 유기화학
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Structural modification of Naphtopyrane photochromic dye to control fade rate in lens matrices

이상희* <u>이정구</u> 유수창

군산대학교 화학과

Under near-UV light irradiation, naphthopyrans undergo an electrocyclic pyran-ring-opening to give colored photoisomers with a strong absorption in the visible. Ring formation rate, fading rates, of these phtochromic dye depend on rigidity of lens matrix. In this study, we would like show that simple structural modification of naphtopyran can increase the fading rate of photocromic dye in rigid lens matrix. Longer alkyl groups (DB6 and DB4) make free space for coformational change of photoisomer in lens matrix, therefore, fading rate is faster comparing to that of DB1.

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발표코드: **ORGN.P-770**
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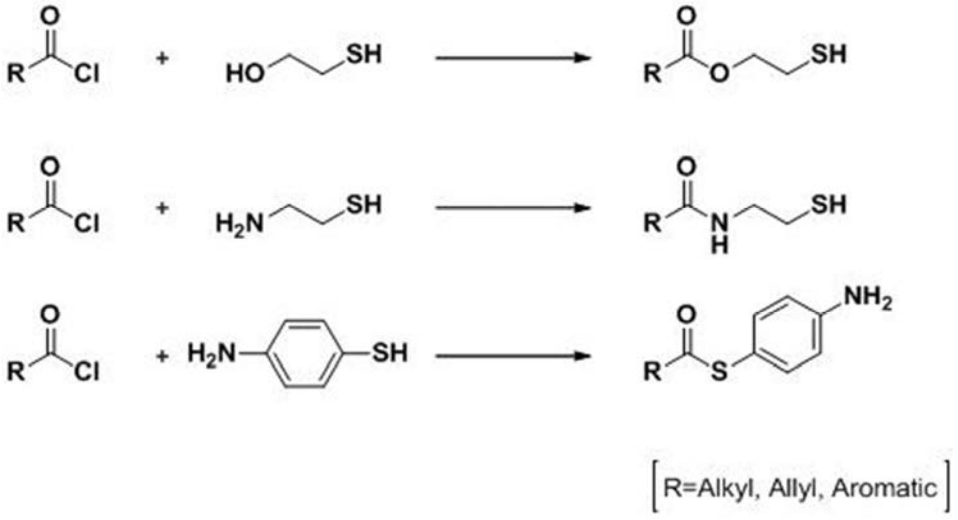
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Investigation and mechanistic study of Chemoselective O-Acylation of β-mercapto alcohol and N-Acylation of β-mercaptoamine with Acid Chloride Derivatives

김예진 안철진*

창원대학교 화학과

The chemoselectivity in O-acylation of β-mercaptoalcohol and N-acylation of β-mercaptoamine are synthetically important to prepare the organic compounds with free-SH. In this paper, the investigation to the chemoselective O-acylation of β-mercaptoalcohol and N-acylation of β-mercaptoamine with acid chloride derivatives and mechanistic study are reported. Also, we try to figure out the chemoselectivity in N-acylation or S-acylation with acid chloride and 4-aminothiophenol.



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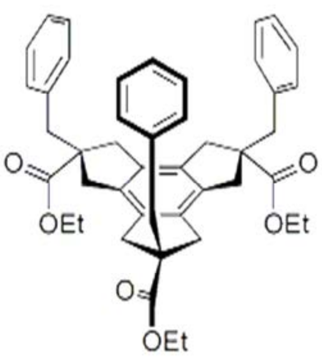
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-771**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photophysical Properties of Trindane-based Anion Molecular Sensors with Guanidine Recognition Motif

김원 김기동 최홍진*

경북대학교 응용화학과

Novel C_{3v}-symmetric tripodal anion receptors having guanidine recognition motif with 2-aminobenzimidazole were synthesized from *cis,cis,cis*-2,5,8-tribenzyltrindane-2,5,8-tricarboxylate (1). The C_{3v}-symmetric scaffold 1 has non-polar benzyl moieties on one side and polar ester moieties on the other side. These moieties were selectively functionalized to afford the C_{3v}-symmetric anion molecular sensors to recognize selectively and effectively towards anions with C_{3v}-symmetry guests such as F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, HSO_4^-, NO_3^-, HCO_3^- ions, expecting shape-selectivity.Interestingly the tripodal receptor which has 2-aminobenzimidazole recognition motif showed a superior recognition towards $H_2PO_4^-$ by NMR titration, but selectively recognized with HSO_4^- emitting blue fluorescence under UV irradiation, which can be further developed to fluorescent anion sensors. New compounds 2 with electron-donating and electron-withdrawing groups 5,6-disubstituted on benzimidazole moieties are expected for more red-shifted fluorescence light emission than the unsubstituted one.



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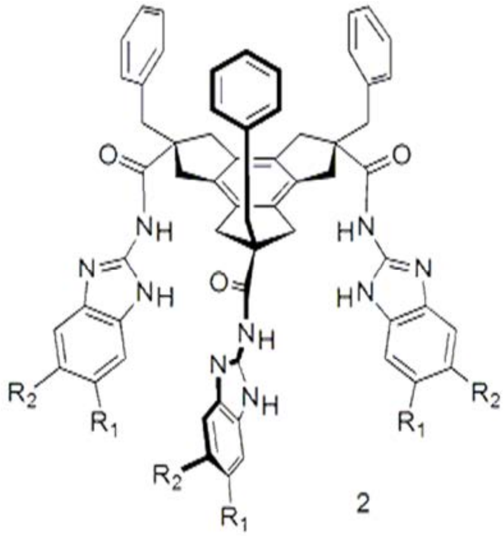

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일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-772**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence “turn-on” peptide sensor for metal ions

박유진 이건형[1,*]

인하대학교 화학화공융합학과 [1]인하대학교 화학과

Tetraphenylethene(TPE) labelled peptide is synthesized using a solid phase synthesis. This fluorescent sensors show turn-on response for heavy transition metal(HTM) ions. TPE fluorophore shows weak fluorescence in solution, but they become strong emission after aggregation. We herein designed a water-soluble chemosensor by incorporating TPE fragment with peptides.

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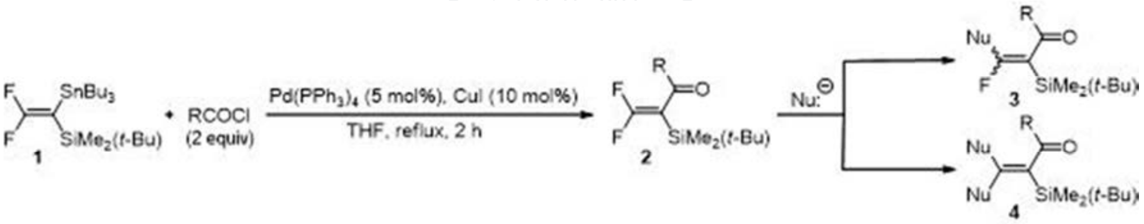
발표코드: **ORGN.P-773**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 1,1-difluoro-2-(*tert*-butyldimethylsilyl)enone and it's reactions with nucleophiles

정예림 안혜진 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

The cross-coupling acylation reaction of 2,2-difluoro-1-(*tert*-butyldimethylsilyl)ethenyltributylstannane (1) with acid chlorides in the presence of catalytic amount of Pd(PPh$_3$)$_4$ and CuI in THF at reflux temperature for 2 h provided 1,1-difluoro-2-(*tert*-butyldimethylsilyl)enone (2) in good yields. Reaction of 2 with Grignard reagents in THF at -78 ℃, followed by warming to room temperature gave the mono-substituted products 3 stereoselectively in good yields. The use of excess Grignard reagents in this reaction afforded the di-substituted enones 4 in good yields. Sulfur or oxygen nucleophiles under the similar reaction condition also provide the mono- and di-substituted products.



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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-774**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient and simple colorimetric fluoride ion sensors

조은진 이영주[1] 이기복[2] 배현종[3,*]

전남대학교 바이오에너지 연구소 [1]한국기초과학지원연구원 광주센터 [2]전남대학교 화학과 [3]전남대학교 바이오에너지공학과

Among the anions, fluoride ion is one of the most important anions because of its role in prevention of dental caries and the treatment of osteoporosis. However excess intake fluoride can cause many serious disease such as gastric and kidney disorders, skeletal fluorosis. Thus the development chemosensor for fluoride anion is of great importance for enviroment and human health care. An azo naphtalene based colorimetric chemosensor has been developed and demonstrated for the highly selective detection of fluoride ion in DMSO solution. To examine their application as anion receptors by UN-vis and ^{1}H NMR spectroscopy results revealed their higher selectivity for fluoride ion than other anions.

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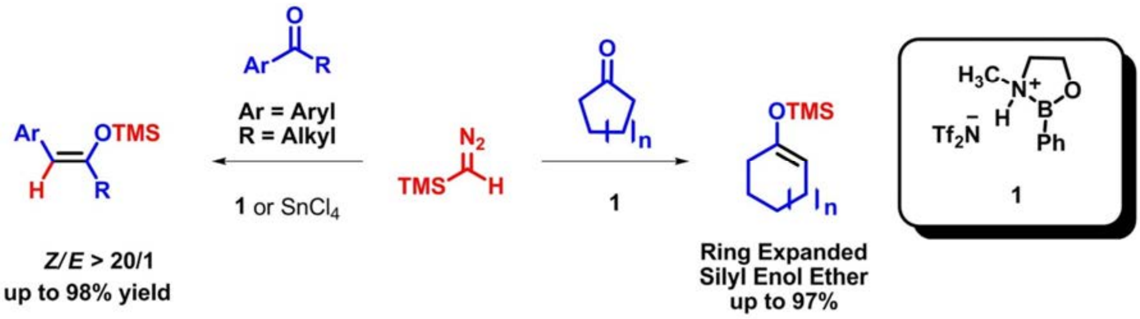
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly stereoselective synthesis of (Z)-silyl enol ethers from (trimethylsilyl)diazomethane(TMSD) catalyzed by SnCl4 or oxazaborolidinium ion

심수용 강병철 김태형 정현실 백은희 류도현*

성균관대학교 화학과

Silyl enol ethers are very useful intermediates in organic synthesis including aldol reactions, Michael reactions, and cycloaddition reactions. Because the configuration of silyl enol ether can affect the stereochemistry of subsequent events, many regio- and stereo-defined synthetic methods have been developed. However more efficient and milder methods are required, especially for acyclic ketone substrates.In this research, highly (Z)-selective silyl enol ethers were prepared from alkyl aryl ketones or cyclic ketones and (trimethylsilyl)diazomethane(TMSD) by using oxazaborolidinium ion or SnCl4 as Lewis acid catalyst.Also, the synthetic utility of the present reactions was demonstrated by applying it to the one-pot tandem Mukaiyama aldol reaction and [2+2] cycloaddition.



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발표코드: **ORGN.P-776**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of a New Synthetic Method to the Synthesis of Axially Chiral Diol Compounds Bearing Different Dihedral Angles

윤정민 천철홍*

고려대학교 화학과

Axially chiral diol compounds, such as BINOL and VAPOL, have been widely used as chiral ligands and catalysts in asymmetric synthesis. Since the reactivity and selectivity with these chiral diols show a strong dependence on substituents on the main framework of the chiral diols, many chiral diol derivatives bearing different substituents along the chiral axis have been developed and extensively studied. Although the dihedral angle in the axially chiral ligands and catalysts is known to have a profound influence on the reactivity and selectivity in asymmetric catalysis, in particular those with axially chiral diphosphine ligands, however there has been little study on the influence of the dihedral angle of chiral diol ligands in asymmetric catalysis. This lack of the research on the dihedral angle in asymmetric synthesis with chiral diols might be due to the fact that there are not efficient synthetic routes to access these important compounds. In order to address this issue, we have initiated a program for the development of an efficient method to access several axially chiral compounds bearing different dihedral angles via the diastereomeric resolution of rac-boronic acids with a chiral boron ligand. The boronic acid moiety in the resulting diastereromers was further transformed to other functional groups, which allowed us to synthesize several axially chiral compounds with various dihedral angles.

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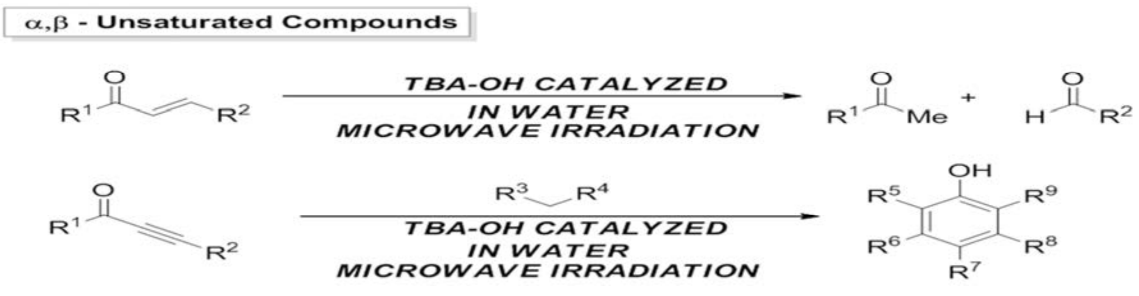
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Modification of Polybutadiene with Sodium Formate and Alcohols by Ruthenium-Catalyzed One-Pot Hydroesterification

이창희 박우진 김동수 이혜정 전철호*

연세대학교 화학과

Transition-metal catalyzed hydroesterification reaction is a useful synthetic method to prepare valuable carboxylic ester. Recently we developed a new three component hydroesterification reaction of alkenes with alcohols and sodium formate under the cooperative catalytic system comprised of Ru3(CO)12 and 2-pyridinemethanol. In this reaction, sodium formate is decomposed to carbon monoxide and sodium hydroxide. The former supplys carbonyl group in the ester and the latter catalyzes transesterification. This reaction overcomes some limitations of previously developed hydroesterification such as use of toxic CO gas and multistep synthesis. However, this reaction does not require toxic carbon monoxide gas and can be performed as one-pot reaction. In this poster, we present polymer modification using this protocol. In the modification of polybutadiene, vinyl group can be readily transformed to ester group bearing various functional group. A mixture of alcohols can be also applied for the modification of polybutadiene in one pot synthesis.



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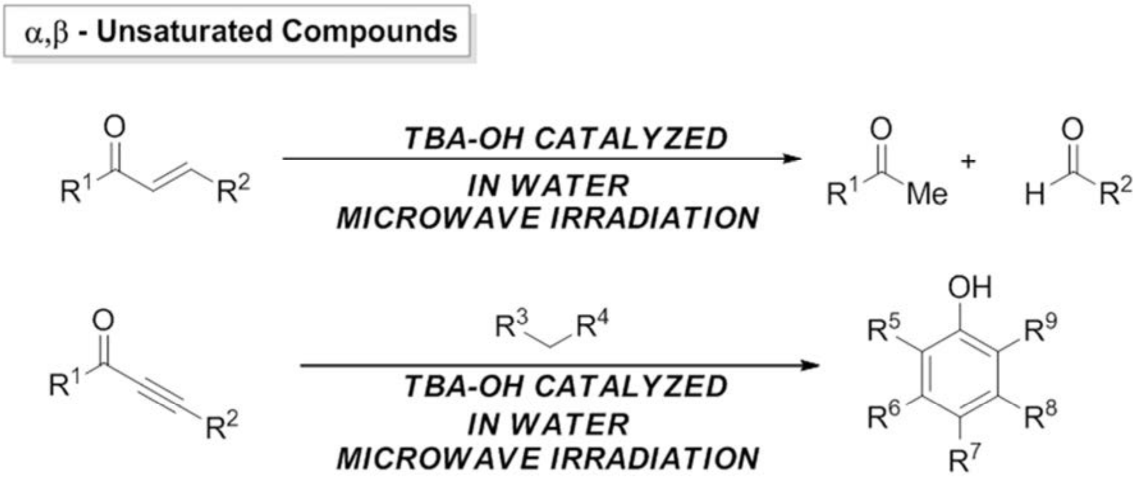
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

TBA-OH Catalyzed 1,4-Addition of H2O into α,β-Unsaturated Ketone by Microwave Irradiation

이혜정 전철호*

연세대학교 화학과

Green chemistry becomes one of interesting subjects in organic synthesis since it gives multi-benefits in industrial process, such as reduction of chemistry waste, use of benign solvents and atom-economy. Since water is inexpensive, non-toxic, non- corrosive and easy to handle, water is a good candidate for reagent and solvent compared with traditional organic solvent. With environmentally benign H2O solvent and MW heating, we found that water can be used as a nucleophile in the 1,4-addition reaction of α,β-unsaturated ketone. And further reaction of the resulting β-hydroxy ketone affords retro-aldol or tandem organic transformations. We found the cleavage reaction of C-C double bond of α,β-enone and enal through the base catalyzed retro-aldol type fragmentation. In addition, multi- substituted phenols were also obtained from α,β-ynones and diketones through base-triggered Michael reaction, followed by annulation reaction.



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

Synthesis of Anthracene Based Organic Light Emitting Diodes and Evaluation of their physical properties

이지은 권수한* 정용석*

충북대학교 화학과

청색발광은 풀칼라를 위한 전자발광 소자로의 응용에 매우 중요하다. 청색발광소자의 발광물질로서의 가능성을 확인하기 위하여 anthracene 을 기반으로 한 새로운 형광 물질을 합성하였다. 이 신규화합물은 anthracene 의 2 번 위치에 (trifluoromethyl)phenyl group 을, 9 번과 10 번 위치에는 phenyl, naphthyl, biphenyl group 을 도입하였다. 합성한 새로운 anthracene 유도체의 광학적, 전기적 특성을 평가하였다.

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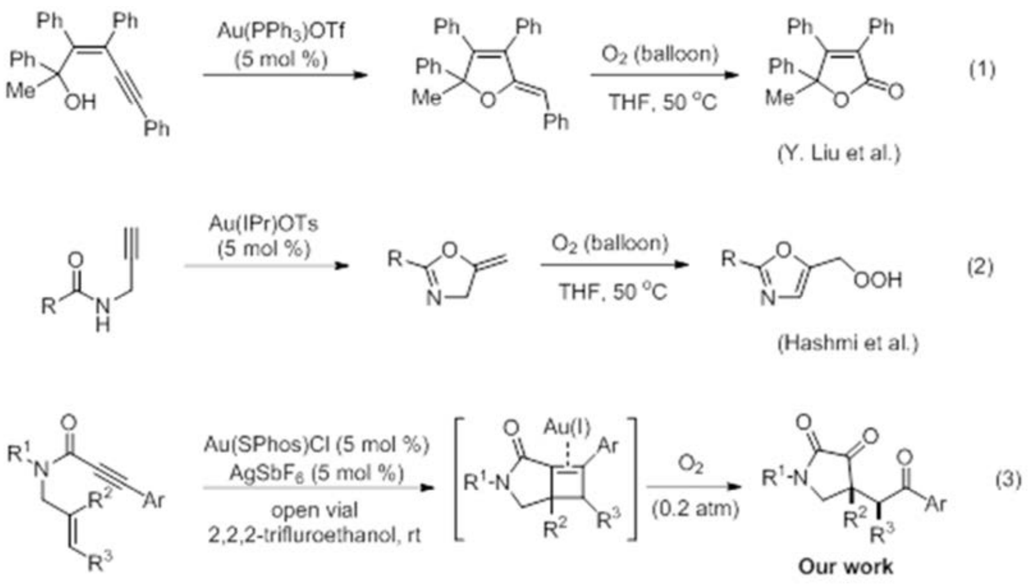
발표종류: 포스터, 발표일시: 수 16:00~19:00

Gold Catalyzed Aerobic Cleavage of Electron-Deficient Triple Bonds

PATILDILIPVITTHAL 신승훈*

한양대학교 화학과

Transition metal catalyzed cleavage of triple bonds have been reported with Rh, Ru and Pd complexes.1 In these, cleavage of triple bonds are initiated by hydroamination of alkynes, followed by retro Mannich-type fragmentation. In gold catalysis, electron-rich olefin intermediates, such as enol ethers, obtained by gold catalyzed cyclization have been reported to undergo oxidative cleavage in the presence of air.2 For the latter process (Eq. 1), the most likely mechanism involves autoxidation by hydroperoxides generated from ether solvents, such as THF2 that occurs independent of Au-catalyst (Eqs. 1 and 2).2b-c In this presentation, we have found a unique cleavage of electron-deficient triple bonds catalyzed by Au-complexes.3 The Au-catalyzed reaction of propiolamide-derived 1,6-enynes under air led to oxygenative cleavage of triple bonds into 1,4-dicarbonyl compounds. Interestingly, the optimal conditions were found to be 0.2 atm of O2 at RT (Eq. 3). Radical inhibition tests suggests that the oxygenative cleavage occurs via a gold-bound metallo-radical species. The resulting 1,4-dicarbonyl compounds can be precursors of fused pyrroles.References:1.(a) Jun, C. ?H.; Lee, C. ?H.; Moon, C. ?W., Hong, H. ?S. J. Am. Chem. Soc. 2001, 123, 8600; (b) Shimada, T.; Yamamoto, Y. J. Am. Chem. Soc. 2003, 125, 6646.2.(a) Liu, Y.; Song, F.; Guo, S. J. Am. Chem. Soc. 2006, 128, 11332; (b) Song, F.; Liu, Y. J. Organomet. Chem. 2009, 694, 502; (c) Hashmi, A. S. K.; Jaimes, M. C. B.; Shchuster, A. M.; Rominger, F. J. Org. Chem. 2012, 77, 63943.Patil, D. V.; Park, H. ?S., Koo, J.; Han, J. W.: Shin, S. Chem. Commun. 2014, DOI: 10.1039/c4cc04153d.


Au(PPh3)OTf
(5 mol %)
O2 (balloon)
THF, 50 °C
(1)
(Y. Liu et al.)
Au(IPr)OTs
(5 mol %)
O2 (balloon)
THF, 50 °C
(2)
(Hashmi et al.)
Au(SPhos)Cl (5 mol %)
AgSbF6 (5 mol %)
open vial
2,2,2-trifluroethanol, rt
O2
(0.2 atm)
(3)
Our work

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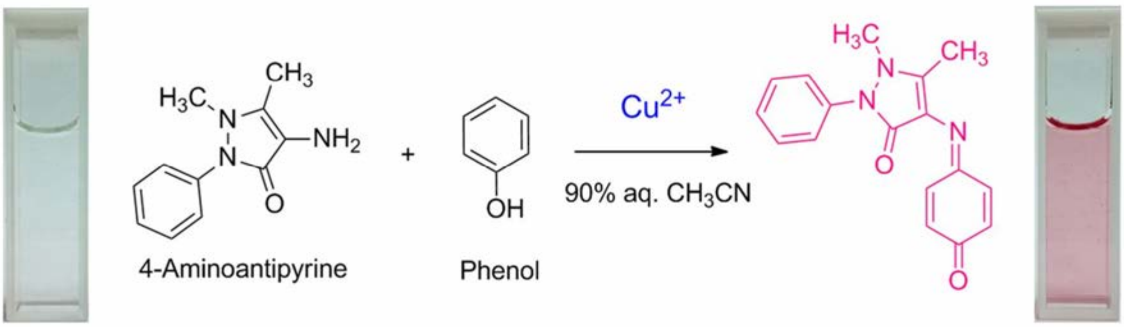
발표코드: **ORGN.P-781**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reaction-based colorimetric signaling of Cu^{2+} ions by oxidative coupling of phenols with 4-aminoantipyrine

김홍영 이효진 장석규*

중앙대학교 화학과

A new reaction-based colorimetric probe system utilizing Cu^{2+}-induced coupling of phenols with 4-aminoantipyrine was devised. A number of phenols having no or labile para-substituents could be used for the signaling of Cu^{2+} ions by oxidative coupling to form highly colored quinoneimine dyes. The Cu^{2+}-selective signaling was not affected by the presence of common metal ions as background. The phenol/4-aminoantipyrine probe system exhibited chromogenic Cu^{2+} signaling via prominent color change from colorless to pink with a detection limit of 8.5×10^{-7} M. The effects of pH, reaction time, 4-aminoantipyrine/phenol ratio, and signaling medium on the determination were elucidated.



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장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-782**

발표분야: 유기화학

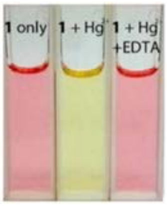
발표종류: 포스터, 발표일시: 수 16:00~19:00

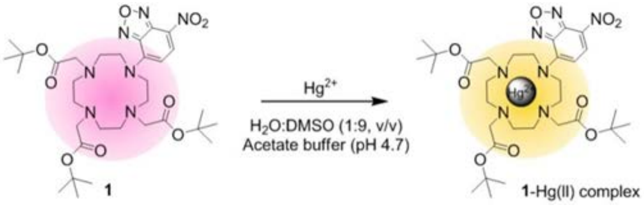
Colorimetric signaling of Hg^{2+} ions by a nitrobenzoxadiazole-appended cyclen-triester

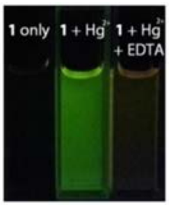
최지영 이슬기 장석규[*]

중앙대학교 화학과

A novel Hg^{2+}-selective colorimetric chemosensor based on a cyclen-nitrobenzoxadiazole (NBD) conjugate was investigated. Hg^{2+} ions are considered as one of the most toxic metal ions on human health and natural ecosystems. In this research, we report a new Hg^{2+}-selective sensor constructed using NBD chromophore as the reporting chromogenic subunit and a cyclen derivative with three ester ligands was used as the binding site. Upon treatment with Hg^{2+} ions, solution color dramatically changed from red to yellow. Fluorescence turn-on type signaling of Hg^{2+} ions was also possible. Selective signaling of Hg^{2+} over other common metal ions was possible with a detection limit of 1.5×10^{-6} M (0.3 ppm) in an aqueous DMSO solution.







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발표코드: **ORGN.P-783**

발표분야: 유기화학

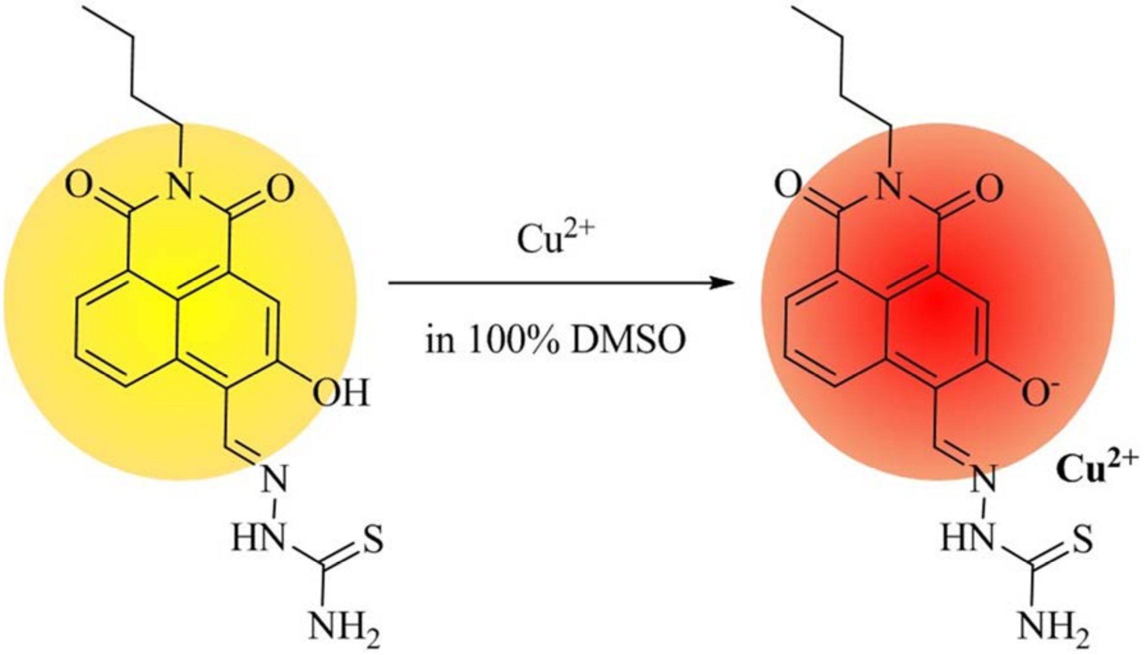
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colorimetric signaling of Cu^{2+} ions by a 3-hydroxynaphthalimide thiosemicarbazone derivative

박현지 김호원 장석규*

중앙대학교 화학과

A novel Cu^{2+}-selective colorimetric signaling behavior of a thiosemicarbazone derivative of 3-hydroxynaphthalimide was investigated. Chemosensor **1** showed pronounced selectivity for Cu^{2+} ions by revealing a significant color change from yellow to red. The signaling of Cu^{2+} ions by **1** was not affected by the presence of commonly encountered metal ions except Hg^{2+} ions. Interference from Hg^{2+} ions could be readily suppressed by using iodide ions as a masking agent. Cu^{2+}-selective colorimetric signaling was possible with a detection limit of 8.6×10^{-6} M in a DMSO solution. Application for the extractive signaling of aqueous Cu^{2+} ions in practical samples of semiconductor wastewater was tested.



1 **1**-Cu(II) complex

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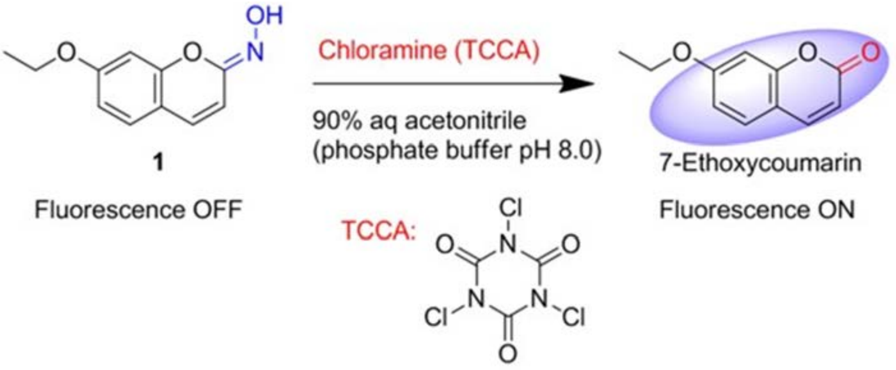
Signaling of chloramine: Trichloroisocyanuric acid-selective fluorescent probe based on deoximation of a coumarin oxime

이슬기 정용애 장석규*

중앙대학교 화학과

A new coumarin oxime based trichloroisocyanuric acid (TCCA)-selective probe was developed. The coumarin oxime 1 exhibited prominent TCCA-selective off-on type fluorescent signaling behavior in a phosphate buffered (pH 8.0) 90% aqueous acetonitrile solution. The signaling is due to the TCCA-promoted transformation of the oxime function to its carbonyl derivative. The TCCA signaling of the probe was not affected by other practical metal ions and anions as a background. Additionally, the TCCA-selective signaling was possible in the presence of other commonly used oxidants such as hydrogen peroxide, peracetic acid, superoxide, tert-butyl hydroperoxide, perborate, and percarbonate. The detection limit of coumarin oxime 1 for the TCCA signaling in 90% aqueous acetonitrile solution was estimated to be 7.58 X 10^{-7} M (176 ppb).



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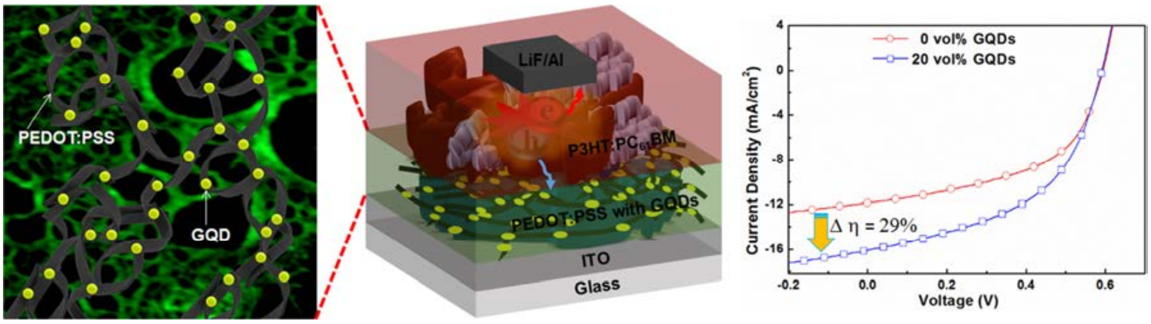
A Self-Assembled PEDOT:PSS/Graphene Quantum Dots Organogel with Reticulated Nanostructure for Efficient Charge Transport

임홍철 홍종인*

서울대학교 화학부

Organogels have received considerable attention in the field of material science because of their tunable characteristics. In particular, graphene allotropes have been employed for the construction of organogels with reinforcing their intrinsic properties. Among these materials, graphene and CNF were introduced into conjugated polymers to yield organogels with enhanced electrical properties. Although these organogels exhibit acceptable mechanical, thermal, and electrical properties, their growth morphologies and formation mechanism in electrical network structures has not yet been investigated. Herein, this study describes the development of reticulated charge-transporting networks with enhanced electrical properties of self-assembled PEDOT:PSS organogels containing GQDs. We propose a building model for the formation of the reticulated nanostructure in the organogels. This model is based on the time-dependent morphological characterizations during gelation. The effects of varying the polymer-to-gelator blend ratio on the nanostructural morphologies of the organogel solid films were investigated to gain insight into their fundamental charge transport processes. Reticulated nanostructures of the PEDOT:PSS solid films containing GQDs were applied as hole extraction layer (HEL) in OPVs using typical poly(3-hexylthiophene) (P3HT): [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) bulk heterojunction. The 29% improvement in the OPV performance is attributed to enhancements in the electrical percolation pathways of the PEDOT:PSS HEL.


PEDOT:PSS
GQD
LiF/Al
e
h
P3HT:PC61BM
PEDOT:PSS with GQDs
ITO
Glass
0 vol% GQDs
20 vol% GQDs
Δ η = 29%
Current Density (mA/cm2)
Voltage (V)
4
0
-4
-8
-12
-16
-0.2
0.0
0.2
0.4
0.6

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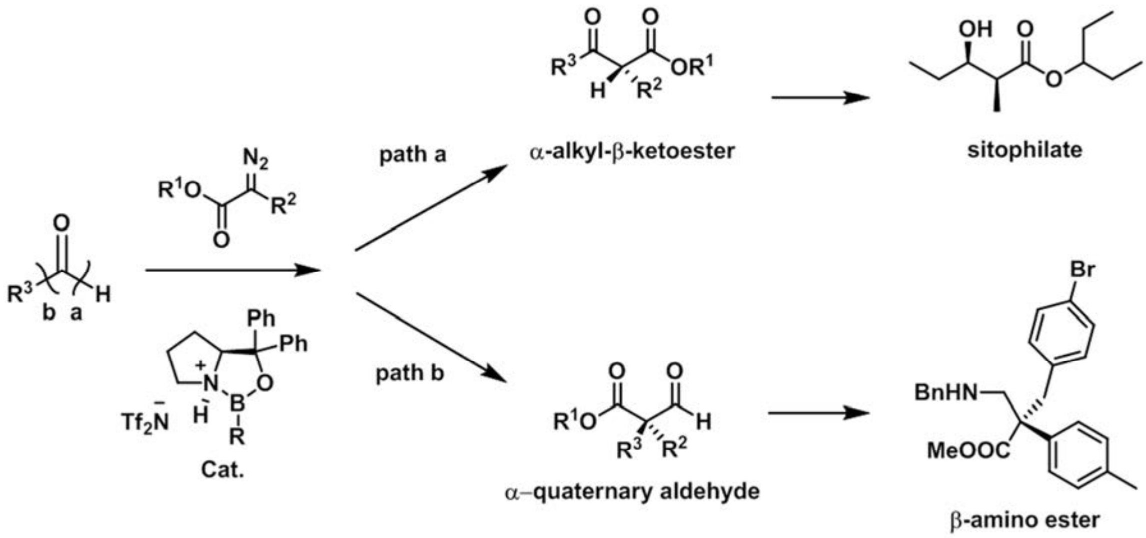
Oxazaborolidinium ion catalyzed stereoselective synthesis of α-alkyl-β-ketoesters or α-quaternary aldehydes with diazoacetate

강병철 강기태 신성호 심수용 정현실 백은희 류도현*

성균관대학교 화학과

Mild and selective C-H or C-C bond insertion reactions provide potential advantages for synthetic strategies to make useful molecules. Among developments in this area, the formal diazo carbon insertion into C-H or C-C bonds is a powerful tool for the homologation of aldehydes and ketones. In this type of reaction, the formal C-H bond insertion reaction of aldehydes via a 1,2-hydride shift, namely the Roskamp reaction, has been well established, and asymmetric methods providing chiral β-keto esters have recently been achieved (path a). Moreover, the corresponding formal C-C bond insertion was successfully achieved to provide one-carbon homologated aldehydes which is more challenging due to the difficulty of promoting the selective 1,2-shift of the R3 group in preference to the hydride (path b). This methodology is highly valuable since it leads to the enantioselective construction of all-carbon quaternary stereogenic centers in acyclic systems, which is one of the most challenging topics in current synthetic organic chemistry. Synthetic utilities of C-H and C-C bond insertions were demonstrated by the synthesis of aggregation pheromone sitophilate and α- and β-amino esters.

N2
R1O
R2
O
R3
H
b a
Ph
Ph
O
B
R
N
H
Tf2N
Cat.
path a
path b
R3
H
R2
OR1
α-alkyl-β-ketoester
OH
sitophilate
R1O
R3
R2
H
α–quaternary aldehyde
Br
BnHN
MeOOC
β-amino ester

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Spectroscopic investigation of Spiropyran-Fluorescein Conjugate

신은주* 김빛나

순천대학교 화학과

Artificial sensors for sensing and recognition of various metal ions have received considerable attention. Especially, the design and synthesis of sensors for colorimetric and fluorimetric detection of metal ions is a challenge to many chemists. Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, undergoing reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.Fluorescein(Fl) is highly fluorescent and widely used as a fluorescent tracer for many applications and a useful fluorescence probe for important biomolecules, and also known as a color additive. Incorporating Fl into SP is expected to lead to excellent light-controlled fluorometric ion sensing system. In this study, SP-Fl dyad with spiropyran and fluorescein units, was prepared. Their spectroscopic properties and photochromic reaction were investigated using absorption and fluorescence spectroscopy.

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

Photochromic Behavior of Spiropyran-Pyrene Conjugate

신은주* 정다영

순천대학교 화학과

Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, whose molecular structure can be altered after exposure to light, temperature, pH or electrochemistry. They would undergo reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.On the other hand, the pyrene(Py) moiety is one of the most useful fluorophores in the construction of fluorogenic chemosensors for a variety of important chemical species. Pyrene is widely employed as ratiometric fluorescent chemosensors, due to its wellknown photophysical properties in monomer/excimer emission switching.Incorporating SP into Py is expected to lead to interesting photoresponsive system with the properties of which can be manipulated by light. In this study, SP-Py conjugate consisting of spiropyran and pyrene units was prepared and its spectroscopic properties were investigated using absorption and fluorescence spectroscopy.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic approach toward tropane alkaloids : An Intramolecular Aza-Prins-type Cyclization via Oxidative C-H Activation

정승영 이재균[1] 최기항 민선준[2,*] 조용서[3,*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 케모인포매틱스연구단 [2]한국과학기술연구원(KIST) 뇌의약연구단 [3]한국과학기술연구원(KIST) 생체과학연구본부

Tropanes are known as an important class of alkaloids showing various pharmacological properties such as anticholinergics, stimulants and anesthesia. For example, hyoscyamine, a secondary metabolite found in certain plants of the Solanaceae family, acts as an antagonist of muscarinic acetylcholine receptors to block the action of acetylcholine in the central nervous system (CNS), which can modulate the symptoms of neurodegenerative diseases such as Parkinson’s disease and Alzheimers disease. On the other hand, cocaine, one of the Narcotic drugs, is a nonspecific voltage-gated sodium channel blocker, which causes it to anaesthesia at low doses. For a long time, the tropane alkaloids have been highly attractive targets for total synthesis because of these biological importance and their typical structures, azabicyclo[3.2.1] octane systems.In this study, we described an efficient synthesis of tropane alkaloids via aza-Prins-type cyclization of amino allylsliane. Unlike the conventional Prins-type reactions, we envisioned that direct C-H activation of cyclic amines by oxidants or photo-induced electron transfer could generate the corresponding iminium species in the kinetic way, which could undergo cyclization to afford the azabicyclo[3.2.1] ring systems.

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

Development of π-Extended Acedan Derivatives and Their Application for Two-Photon Microscopy Imaging of Amyloid-β Plaque

유혜근 김도경 안교한*

포항공과대학교(POSTECH) 화학과

The fluorometric analysis can provide an operationally simple and cost-effective detection method together with high sensitivity and selectivity. Therefore, many fluorescent probes have been developed for detection of various analytes; however, most of them are based on the one-photon dyes which need to use high energy one-photon excitation light. On the other hand, two-photon dyes can be excited by low energy two-photon light. Accordingly, the development of two-photon dyes and the corresponding two-photon probes have been received great attention owing to their advantages such as increased penetration depth, lower autofluorescence, and high special-resolution, in addition to the reduced photodamage and photobleaching.[1] Acedan, 1-(6-dimethylaminonaphthalen-2-yl)ethanone,[2] and its analogues are one of the widely used two-photon dyes but their maximum absorption wavelength (~370 nm) are rather short for two-photon excitation (~740 nm) which causes strong autofluorescence and restricted deep tissue penetration in two-photon microscopic imaging. Therefore, we developed π-extended acedan derivatives which exhibit longer maximum absorption wavelength (~400 nm) and the desired two-photon optical properties for deep tissue imaging. Moreover, one of these π-extended acedan derivatives display potential for application for TPM imaging of amyloid-β plaque in Alzheimer's disease model.

Reference

1. Zipfel, W. R.; Willians, R. M.; Webb, W. *Nat. Biotechnol.*2003, *21*, 1369.
2. Kim, H. M.; Cho, B. R. *Chem.-Asian. J.* 2011, *6*, 58.

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발표코드: **ORGN.P-791**
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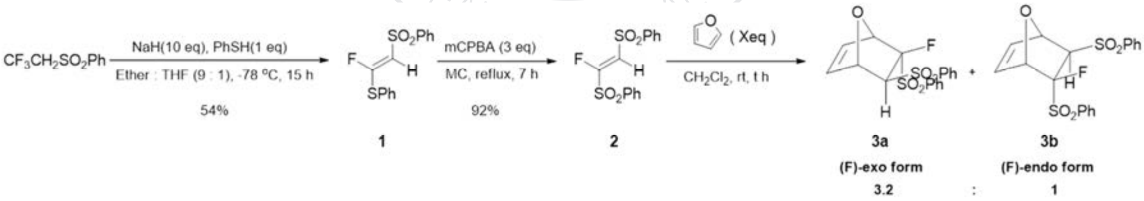
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of (*E*)-1,2-bis(phenylsulfonyl)fluoroethene and Diels-Alder reactions

김호영 김수진 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

(*E*)-1,2-Bis(phenylsulfonyl)fluoroethene 2 was prepared in 92% yield from the reaction of (*E*)-(1-fluoro-2-(phenylsulfonyl)vinyl)(phenyl)sulfane 1 with mCPBA in methylene chloride at reflux temperature for 7 h. The compound 1 was synthesized from the reaction of 2,2,2-trifluoroethylsulfone with NaH (10 eq) and PhSH (1 eq) in Ether : THF (9 : 1) at -78 ℃. The Diels-Alder reaction of 2 with several dienophiles affored cycloadduct 3 in good yields. The scope and limitation of the Diels-Alder reactions of 3 will be presented.



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발표코드: **ORGN.P-792**
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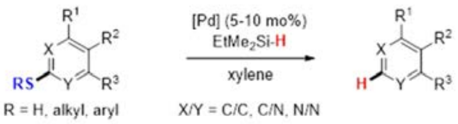
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-Catalyzed Reductive Cleavage of C-S Bonds

이현경 손정훈*

충남대학교 화학과

A novel palladium-catalyzed hydrogenolysis reaction method for the conversion of C-S bond to C-H bond in the presence of trialkylsilane is presented. The reaction method proceeded efficiently with a wide range of substrates possessing C(sp2)-SR(R = H, alkyl and aryl) groups. This chemistry allows a new synthetic strategy for target molecules, such as a general synthetic method for 4,5,6-trisubstituted pyrimidine derivatives.


R¹
R²
R³
X
Y
RS
R = H, alkyl, aryl
[Pd] (5-10 mo%)
EtMe₂Si-H
xylene
X/Y = C/C, C/N, N/N
H

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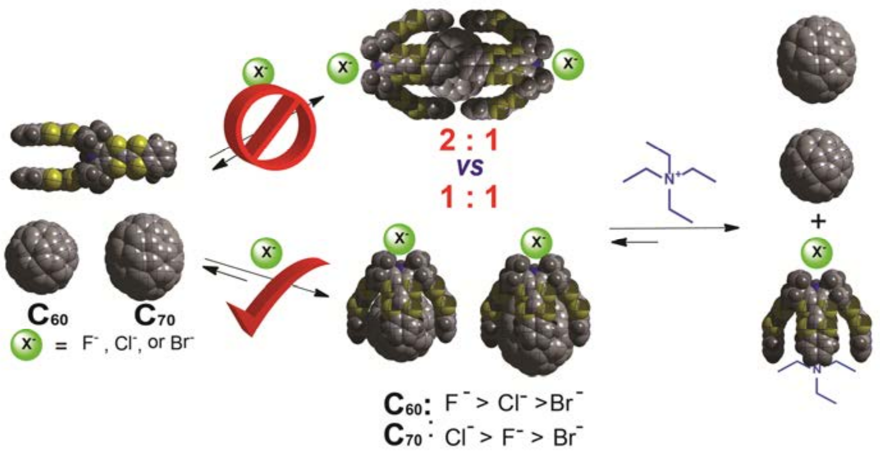
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ion Controlled Allosteric Binding of Fullerenes by Tetrathiafulvalene-Calix[4]pyrroles

박정수* 김덕은

숙명여자대학교 화학과

The significance of allosteric regulation in the realm of biological recognition processes has inspired many efforts to gain fundamental understanding of this process at molecular level and to imitate such elegant strategy in artificial supramolecular recognition systems. Herein, we investigated in-depth the effect of ionic species on allosteric binding pro-cesses between tetrathiafulvalene-functionalized calix[4]pyrroles (TTF-C4Ps) and fullerenes (C60 and C70). The binding properties of TTF-C4Ps to fullerenes were found to be highly influenced by both the nature of halide anions and its counter tetraalkylammonium cations. Particularly, we demonstrate that the appropriate choices of halides can be exploited to modulate the strength of the corresponding host-guest binding interactions and even alter the selectivity between TTF-C4Ps and fullerenes. Overall, the studied system is a clear example of how host-guest binding events and selectivity in the artificial system can be fine-tuned by addition of simple ionic species as allosteric modulators.


X⁻
X⁻
X⁻
2 : 1
vs
1 : 1
N⁺
+
X⁻
C60
C70
X⁻ = F⁻, Cl⁻, or Br⁻
X⁻
X⁻
X⁻
X⁻
C60: F⁻ > Cl⁻ >Br⁻
C70: Cl⁻ > F⁻ > Br⁻

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An FITC-BODIPY based FRET system for the highly selective detection of cysteine

배주량 안교한*

포항공과대학교(POSTECH) 화학과

Fluorescence resonance energy transfer (FRET) is widely used to elucidate biological processes. A donor fluorophore in a FRET couple may transfer its excited state energy to an acceptor fluorophore through nonradiative dipole-dipole coupling.[1]Fluorescein and its derivatives, along with the rhodamine family, constitute an important family of fluorescent tracers for many biological applications. Here, we disclose that an 8-amino-BODIPY dye is a promising FRET donor to fluorescein, as demonstrated though a new FRET probe that senses cysteine (Cys), an important biothiol, in the ratiometric manner. An amino-BODIPY dye was readily introduced to a commercially available fluorescein isocyanate to generate an efficient FRET couple. To demonstrate its potential in biological applications, a fluorescence sensing system for cysteine was prepared by introducing acryloyl groups to the fluorescein, according to a known reaction-based sensing strategy. This fluorescein-diacrylate probe was evaluated as a FRET probe for cysteine, including cellular imaging experiments. The probe exhibited promising ratiometric response to cysteine with high selectivity. The cellular imaging experiments also revealed that such aryl acrylate type probes are vulnerable to the ubiquitous esterase activity, warning that cellular imaging data obtained with the ester type probes, in general, may also contain the non-enzymatic hydrolysis portion. Also, the FRET probe was applied to determine the level of cysteine in human blood plasma. The results demonstrate that the FRET couple holds promise for the development of other molecular probes for biological analytes.[1] R. M. Clegg, Current opinion in biotechnology, 1995, 6, 103?110.

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Quantification of polyphosphates using aggregation-induced enhanced emission phenomena

김혜림 안교한*

포항공과대학교(POSTECH) 화학과

Inorganic polyphosphate (polyP) is a widely distributed biological polymer composed of phosphate residues linked by high-energy phosphoanhydride bonds, and found in every tested organism. polyPs are widespread in living organisms and are found in the cells of microorganisms, animals, and plants. Also, polyP accelerates blood clotting by activating the contact pathway including factor Ⅴ, and it delays clot lysis by enhancing a natural antifibrinolytic agent, thrombin-activatable fibrinolysis inhibitor. In spite of important role of polyP in our body, very few studies on the quantification of polyP have been reported. This is in part due to the lack of suitable methods for quantifying polyP, which are inaccurate due to polyP chain length heterogeneity, employ radioactivity and loss of inorganic components during sample preparation. Herein we report a fluorescence turn-on sensor for polyP detection by making use of the aggregation induced enhanced emission (AIE) feature of tetraphenylethene molecule. The Probe which has a positive charged group shows weak fluorescent in aqueous solution. But in the presence of polyP, the positive charged group in probe would interact with the negative charged phosphate residue of polyP through ionic interaction. After electrostatic interaction, aggregation is occurred and it shows highly blue fluorescent after aggregation. To the best of our knowledge, this is the first aggregation-induced enhanced emission (AIE) based probe for quantification of polyP.

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Synthetic Chloride Transporters Deactivated by an External Stimulus

박은빛 정규성*

연세대학교 화학과

Ion transport across cell membranes is crucial in biological systems. In recent years, much effort has been devoted to prepare small synthetic compounds that can facilitate ion transport across lipid membranes. Herein, we have designed and prepared synthetic chloride transporters which show the controlled transport activity in response to external stimuli. The transporters consist of two urea groups linked through an amide unit which can undergo conformational changes from cis to trans by chemical and enzymatic reactions. This isomerization leads to the changes in the chloride-binding affinity and lipophilicity, which in turn alter greatly the chloride transport activities across a POPC (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine) membrane. Details will be described in the presentation.

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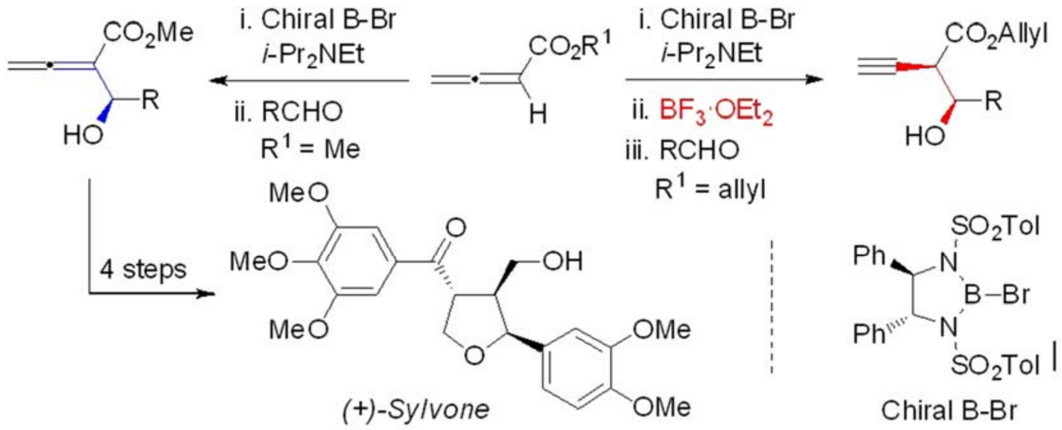
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regulation for the Formation of Isomeric Allenyl or Propargylic Aldol Adducts from Aldol Reaction of Allenoates: Concise Synthesis of (+)-Sylvone

방지윤 이은혜 유찬모*

성균관대학교 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity in the production of enantiomerically pure compounds is of considerable current interest in synthetic chemistry. A highly stereoselective synthesis of propargylic threo aldol adducts is achieved from the reaction of allyl allenoate with a chiral bromoborane in the presence of i-Pr2NEt, followed by addition of BF3?OEt2 as an additive to scavenge excess base and then aldehydes, whereas isomeric allenyl aldol adduct is formed in the absence of Lewis acid additive. The utility of this method has been demonstrated by the synthesis of (+)-sylvone in 5 steps



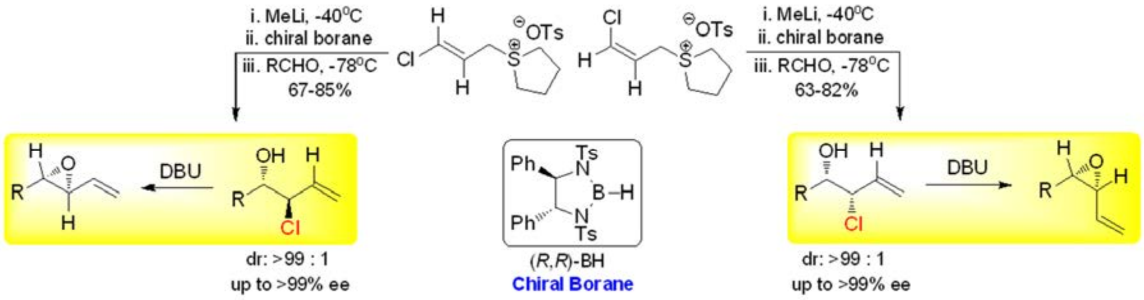
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-798**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cloroallylic Transfer Reactions for the Enantio- and Diastereoselective Synthesis of 3-Vinyloxiranes: Enantioselective Synthesis of Ponticaepoxide

이은혜 방지윤 유찬모*

성균관대학교 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity via catalysis is of considerable current interest in the field of synthetic chemistry. In this regard, allylic additions to carbonyl functionality in forming chiral homoallyl alcohols are considered as one of fundamental reactions in asymmetric synthesis. We would like to present herein several crucial points that have emerged from our recent investigations: new method for the preparation of functional allylic boranes from reaction of a sulfur ylide with chiral boranes: enantio- and diastereoselective synthesis of 3-vinyloxiranes in high levels of stereoselectivity: synthetic applications to high potent antifungal natural products, ponticaepoxide in short steps.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-799**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total Synthesis of Alternariol by BBr3-promoted Intramolecular Cyclization

원미희 권소현 김태현[1,*]

인천대학교 화학과 [1]인천대학교 자연과학대학 화학과

Alternariol, main metabolite of toxin-producing Alternaria fungi, leads to crop losses by fouling of some fruits such as tomatoes, apples despite of low toxicity as compared with others. Therefore, the isolation of that material is important for studying of a minimization of crop losses and toxicological residual risks. However, only sub-milligram amounts can be obtained from infected fruits, so artificial synthesis of alternariol should be studied. Total synthesis of alternariol is already proposed in other study, but the final procedure showed low yield and side-product. For this reason, we tried to search new high-yielded procedures and conditions using BBr3-promted intramolecular cyclization, and the new synthesis will be discussed in detail.

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발표코드: **ORGN.P-800**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Syntheses of 6-epi-Ieodomycin B and Its Analogs

설재희 이종석[1,*] 박솔[2] 이희승[3] 이연주[4] 신희재[5]

한양대학교 응용화학과 [1]한국해양과학기술원 해외생물자원 연구센터 [2]과학기술연합대학원대학교(UST) 해양생명공학과 [3]한국해양연구원 해양천연물연구실 [4]한국해양연구원 해양바이오센터 [5]한국해양연구원 천연물연구실

In our research program aiming to understand the chemical diversity of marine biological resources, four new antimicrobial fatty acids, ieodomycins A-D were discovered from bioassay-guided isolation of the culture extract of a marine Bacillus sp. 09ID194 from sediment in Ieodo, Rupublic of Korea’s southern reef. Due to the structural uniqueness and the biological activities (antimicrobial activities), we initiated the synthetic study of ieodomycins. In this presentation, the efficient synthesis of 6-epi-ieodomycin and its analogs will be described.The efficient syntheses of 6-epi-ieodomycin B and its analogs are described in this presentation. Our synthesis features (1) Ti-catalyzed asymmetric allylation of an aldehyde. (2) Stereoselective iodolactonization. (3) The Lewis Acid catalyzed Allylation of ketone with potassium allyltrifluoroborate. (4) Dehydration of allylic alcohol with Burgess reagent.

일시: 2014년 10월 15~17일(수~금) 3일간
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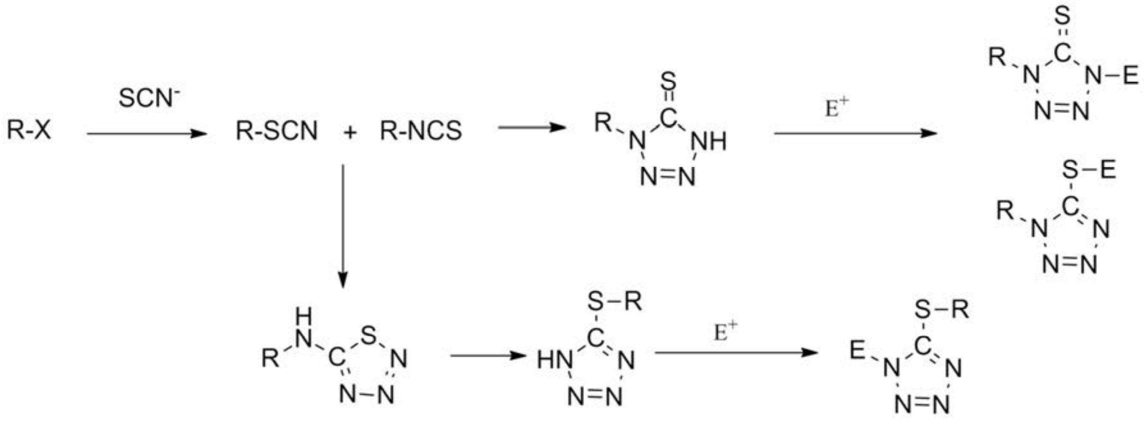
발표코드: **ORGN.P-801**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective synthesis of 1-substituted-tetrazole-5-thione derivatives from halides

경영수* 김은정 임홍규 박효원

강릉원주대학교 화학신소재학과

Tetrazole-5-thion derivatives were synthesized through constitutional isomers of isothiocyanate and thiocyanate from compatible halides. Using the nucleophilic character of tetrazole, various electrophiles were added to the N, and S atoms of tetrazole ring. We compared reactivity and regioselectivity of the tetrazoles.



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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-802**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Some Green Dopants for OLEDs Based onArylamine 2,3-disubstituted Bithiophene Derivatives

백오현 채규윤* 양두리[1] 배사랑[2]

원광대학교 화학과 [1]원광대학교 바이오나노화학과 [2]원광대학교 자연과학대학/바이오나노화학부

Abstract: A series of green dopants based on 2,2-diphenylvinyl end-capped bithiopheneand three different arylamine moieties (9-phenylcarbazole, triphenylamine, and N,N’-di-(ptolyl)benzeneamine) were successfully synthesized by the Suzuki and Wittig couplingreactions. The photophysical properties of these compounds are reported. The strongest PLemitting compound with the 9-phenylcarbazole moiety has been used for fabricating anOLED device with good overall performance.Keywords: green dopants; bithiophene; 2,2-diphenylvinyl; 9-phenylcarbazole;triphenylamine; N,N'-di-(p-tolyl)benzeneamine

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-803**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Electroluminescent Properties of OLED Green Dopants Basedon BODIPY Derivatives

김미진 채규윤[1,*] 양두리[2] 배사랑[3]

원광대학교 화학 [1]원광대학교 화학과 [2]원광대학교 바이오나노화학과 [3]원광대학교 자연과학대학/바이오나노화학부

The novel green dopants based on BODIPY and two different arylamine moieties, namely 9-phenylcarbazole and triphenylamine, have been successfully synthesized and characterized. Due to possessing the similar photophysical properties of these materials, the compound containing 9-phenylcarbazole moiety has been used as a standard for fabricating the OLED device with the structure of ITO/NPB/BODIPY (3 wt% in Alq3)/Alq3/LiF/Al. This device showed good performance with low turn on voltage (3.0 V), green emission (CIE = 0.40, 0.57), maximum brightness, current efficiency and power efficiency of 30,000 cd/m2, 4.32 cd/A, and 5.43 lm/W, respectively.Keywords: green dopant, BODIPY, 9-phenylcarbazole, triphenylamine, and OLED.

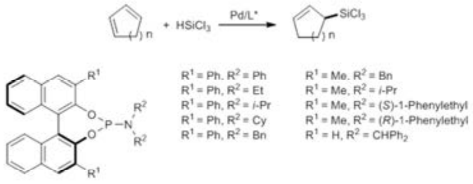
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-804**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric palladium-catalyzed hydrosilylation of cyclic 1,3-dienes with 3,3’-disubstituted chiral phosphoramidite ligands

박현섭 김민영 신수연 한진욱*

한양대학교 화학과

Catalytic asymmetric functionalization of olefins is an important goal in synthetic organic chemistry. The asymmetric hydrosilylation of olefins with trichlorosilane in the presence of palladium catalysts coordinated with chiral monodentate phosphorus ligands is a well-established methodology to obtain chiral organosilanes.1 The resulting organosilane is readily oxidized into alcohol with retention of configuration at the streogenic center.2Herein, we report that palladium-catalyzed asymmetric hydrosilylation of cyclic 1,3-dienes, including 1,3-cyclohexadiene and 1,3-cyclopentadiene, with trichlorosilane by use of chiral phosphoramidite ligands. Chiral phosphoramidite ligands prepared from 3,3’-disubstituted (S)-1,1’-binaphthols and secondary amines were examined in order to evaluate the influence of binaphthyl part of the phosphoramidite ligands in both catalytic activity and enantioselectivity.


+ HSiCl3
Pd/L*
SiCl3
n
R1
R2
R1
R1 = Ph, R2 = Ph
R1 = Ph, R2 = Et
R1 = Ph, R2 = i-Pr
R1 = Ph, R2 = Cy
R1 = Ph, R2 = Bn
R1 = Me, R2 = Bn
R1 = Me, R2 = i-Pr
R1 = Me, R2 = (S)-1-Phenylethyl
R1 = Me, R2 = (R)-1-Phenylethyl
R1 = H, R2 = CHPh2

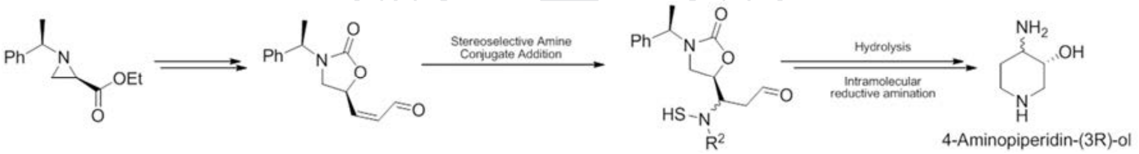
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-805**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of 4-amino-(3R)-hydroxypiperidine from Chiral Aziridine

이영석 이원구[1,*] 하현준[*]

한국외국어대학교 화학과 [1]서강대학교 화학과

4-Amino-(3R)-hydroxypiperidine known as a convenient precursor for the preparation natural and synthetic aminohydroxylated piperidine alkaloid analogs some of which has potent biological activities including BMS-690514 and Cisapride. This was prepared from stereoselective conjugate addition of amine or its equivalent to 3-(2-oxo-3-(1-phenylethyl)oxazolidin-5-yl)acrylaldehyde originated from aziridin-2-carboxylate.



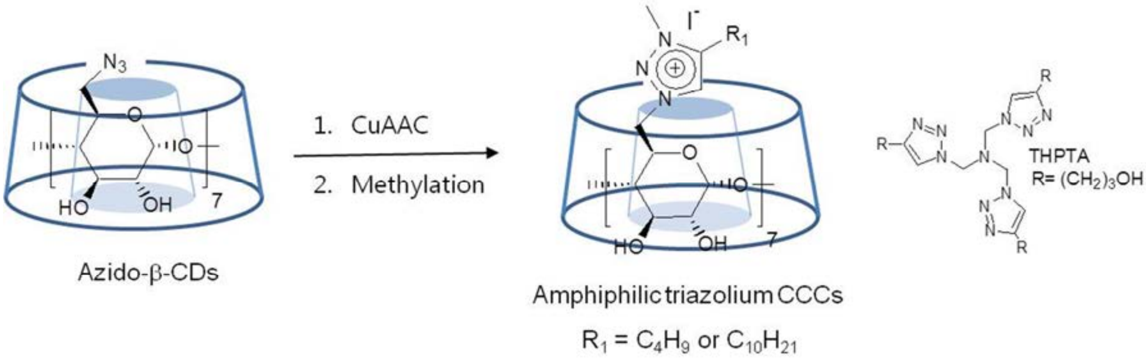
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-806**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of amphiphilic triazolium cyclodextrin click clusters

송영란 송정은 윤영민 임춘우[1,*] 김태우[*]

경희대학교 동서의학대학원 [1]한남대학교 화학과

Cyclodextrin click clusters (CCCs) are a kind of chemically-modified cyclodextrin (CD) derivatives, in which all the primary alcohols of CDs are transformed to triazole units by copper(I)-catalyzed azide-alkyne cycloaddition (CuAAc). The conventional amphiphilic CCCs are composed of three parts: CD as a scaffold, long alkyl chain at secondary OH as a hydropholic tail, and charged group at primary OH as a polar head. The amphiphilic CCCs have been used for gene delivery or supramolecular chemistry.In this study, we synthesized two amphiphilic triazolium CCCs by two straightforward reactions (CuAAC and methylation) from 6-azido-6-deoxy-?-CD and full characterize them using 1H, 13C NMR, HH COSY (homonuclear correlation spectroscopy) and HSQC (heteronuclear single quantum coherence). Their applications to liposome, gene delivery, and host-guest chemistry are under investigation.



1. 1-hexyne or 1-dodecyne, $CuSO_4$/**THPTA**, sodium ascorbate, THF/phosphate buffer, MW
2. CH_3I, DMF, MW

일시: 2014년 10월 15~17일(수~금) 3일간
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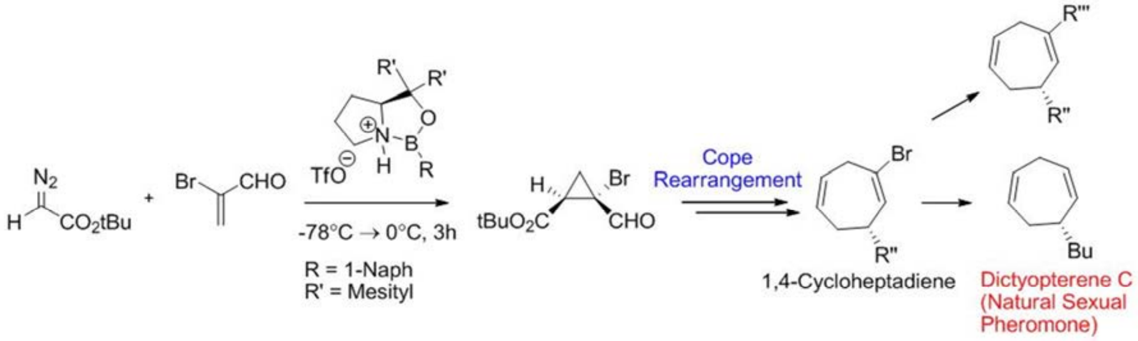
발표코드: **ORGN.P-807**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Chiral 1,4-Cycloheptadiene through Cope Rearrangement and its Applications

김태형 강기태 심수용 신성호 정현실 백은희 류도현*

성균관대학교 화학과

Seven-membered ring skeleton is frequently found among natural products; such as, occidenol, miscandenin, dictyoxepin, clavubicyclone, etc. These compounds can exhibit a wide range of bioactivities such as anti-tumor, anti-HIV, anti-bacterial, and anti-inflammatory.One of the powerful tools used for the construction of seven-membered carbocycle is sigmatropic rearrangement of cyclopropane moiety. In 2011, our research group reported the synthetic method for highly enantioselective cyclopropane.We were able to anticipate optically active cyclopropanes to be useful precursors for chiral cycloheptadienes through cope rearrangement. Additionally, we are expecting this synthetic methodology to be useful for synthesize medicines or natural products which contain seven-membered rings.In order to highlight the chemical utility, we applied this novel synthetic method for synthesis of Dictyopterene C, which contains unsaturated C-11 hydrocarbons bearing an enantiopure 1,4-cycloheptadiene. Dictyopterene series are a group of chemical compounds that are naturally present in freshwater environments. These compounds embrace a family of sexual pheromones for the marine brown algae (Phaeophyceae), exhibiting a remarkable activity including their sperm attracting physiological ability and which is responsible of the intense ocean smell.



N2
H
CO2tBu
+
Br
CHO
R'
R'
O
N
B
H
R
TfO
-78°C → 0°C, 3h
R = 1-Naph
R' = Mesityl
H
Br
tBuO2C
CHO
Cope
Rearrangement
Br
R''
1,4-Cycloheptadiene
R'''
R''
Bu
Dictyopterene C
(Natural Sexual
Pheromone)

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-808**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Conformational analysis of α/β-peptide oligomers containing (1R,2S)-2-aminocyclohexanecarboxylic acid (Cis-ACHC)

김유진 최수혁[1,*]

연세대학교 화학부 [1]연세대학교 화학과

Peptidic foldamare consisting of α- and β-amino acid residues adopt a variety of helical secondary structures. Oligopeptides containing D-Alanine and cis-ACHC have been reported to exhibit a high propensity to form 11/9 helical structures. 11/9 helix and 9/11 helix can be distinguished depending on whether an amide proton participates in an 11-membered H-bond or 9-membered H-bond. Oligopeptides having a-aminoacid residues at the both side of terminus prefer 11/9-helix. From this result, we supposed if the β-amino acid residues exist at the terminus, 9/11-hleix will prefer. Through the IR, CD, NMR studies, 3 kinds of peptides were studied to confirm N-H hydrogen bonding. Two-dimensional NMR experiments suggest that the αβ-oligopeptides form 9/11/9-mixed helix. NOESY and ROESY spectra for the oligomers are consistent with the characteristic NOEs for the 11/9-helix and 9/11helix. Long range NOEs such as NH6-α2 tell us other helix formations might exist.

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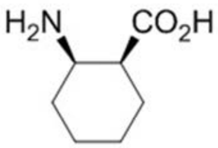
발표코드: **ORGN.P-809**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

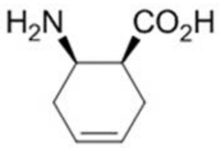
11/9-Helical folding propensity promoted by different β-residues

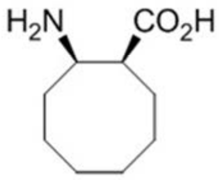
이재연 최수혁*

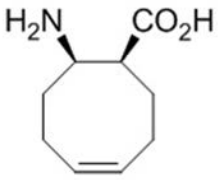
연세대학교 화학과

In the past decade, increasing work has been devoted to the study of foldamers that describe any polymer with a strong tendency to adopt specific compact conformation. Mixed helices are distinct and most unconventional helical structures, which arise from two types of hydrogen bonds with alternating directions. Here, We will discuss the residue requirements and the modification of building blocks to improve the mixed-helix stability. We synthesized several penta-peptide units that have different β-residue to test the helix stability









일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of D-glucosamine

김세진 조형진*

인하대학교 화학과

glucose 는 D-glucose 와 L-glucose 2 종이 존재한다. 이 둘은 서로 광학이성질체로 D-glucose 는 천연적으로 존재하며 L-glucose 는 인공적으로 합성하여 만들 수 있다.이 2 종 중 본 연구에서는 천연적으로 존재하는 D-glucose 를 사용하여 D-glucosamine 과 D-mannosamine 의 새로운 합성법을 발견하였다.본래 glucosamine 은 주로 갑각류의 껍질에서 키틴, 키토산을 추출하여 그 성분을 분해 추출하는 방법으로 얻어진다.

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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-811**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Benzocoumarin analogues: Synthesis and Characterization of Their Photophysical Properties

조서원 김도경 안교한*

포항공과대학교(POSTECH) 화학과

Benzocoumarins having a π-extended coumarins constitute a promising family of photonic materials. Disclosed here are synthesis and characterization of the photophysical properties of a series of Benzocoumarins that contain both an electron donor and an electron acceptor which are electronically conjugated through the benzocoumarin core.[1] The maximum absorption and emission wavelengths of benzo[g]coumarins are at longer wavelengths than the corresponding benzo[f]coumarins, as the former family has favourable intramolecular charge transfer from the donor to the acceptor moiety due to linear conjugation. The emission behaviour of the benzocoumarins is dependent on solvent due to their dipolar nature. The fluorescence of benzo[f]coumarins that have a dimethylamino donor at the C9 or C7 position is much weaker in polar media such as dimethyl sulfoxide (DMSO) and water compared with that of the corresponding benzo[g]coumarins. Comparison of a benzo[g]coumarin and a benzo[h]coumarin[2] that have the same donor and acceptor groups shows that the former shows a larger Stokes shift than the latter. Considering that some of the benzo[g]coumarins are already shown to be two-photon excitable around 900 nm, an optimum biological optical window, the benzo[g]coumrain series are highly promising for bioimaging applications.[3] The synthetic routes established here provide a basis to functional benzocoumarin derivatives.

References

1. D. Kim, Q. P. Xuam, H. Moon, Y. W. Jun, K. H. Ahn. Asian J. Org. Chem. 2014, DOI: 10.1002/ajoc.201402107 (VIP)

2. H. M. Kim, X. Z. Fang, P. R. Yang, J.-S. Yi, Y.-G. Ko, M. J. Piao, Y. D. Chung, Y. W. Park, S.-J. Jeon,

B. R. Cho. Tetrahedron Letters 2007, 48, 2791-2795

3. D. Kim, S. Sambasivan, H. Nam, K. H. Kim, J. Y. Kim, T. Joo, K.-H. Lee, K.-T. Kim, K. H. Ahn. Chem. Commun. 2012, 48, 6833-6835

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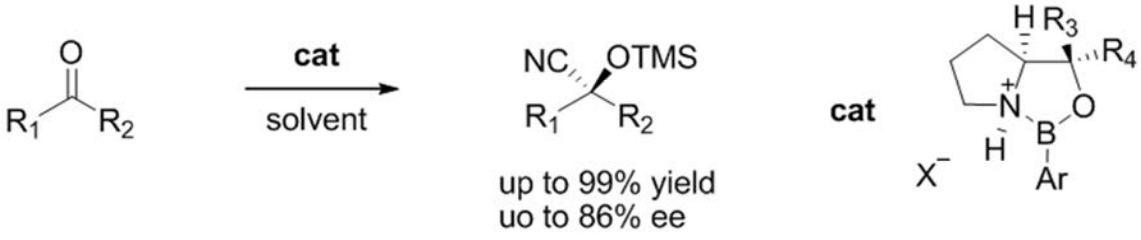
Enantioselective Cyanosilylation of Prochiral Ketones with Trimethylsilyl Cyanide Catalyzed by Oxazaborolidinium Ion

<u>JINMINGYU</u> 정현실 김태형 강기태 강병철 신성호 심수용 백은희 류도현*

성균관대학교 화학과

One of the most useful C-C bond-forming reaction is asymmetric synthesis of cyanohydrins by the addition of trimethylsilyl cyanide (TMSCN) to a wide range of ketones. The cyanohydrins compounds are useful avenue for the synthesis of important organic intermediates such as ?-hydroxy acids, ?-hydroxy amines, 2,3-substituted piperidines, ?-amino nitriles and ?-fluro nitriles.1 These intermediates are used in further stereoselective reactions. This paper describes an enantioselective cyanosilylation of prochiral ketones with TMSCN catalyzed by oxazaborolidinium ion,2 the reaction proceeded in excellent yield (up to 99%) with excellent enantioselectivity (up to 86% ee). The synthetic potential of this method was illustrated by conversion of the products to chiral atrolactic aicd.



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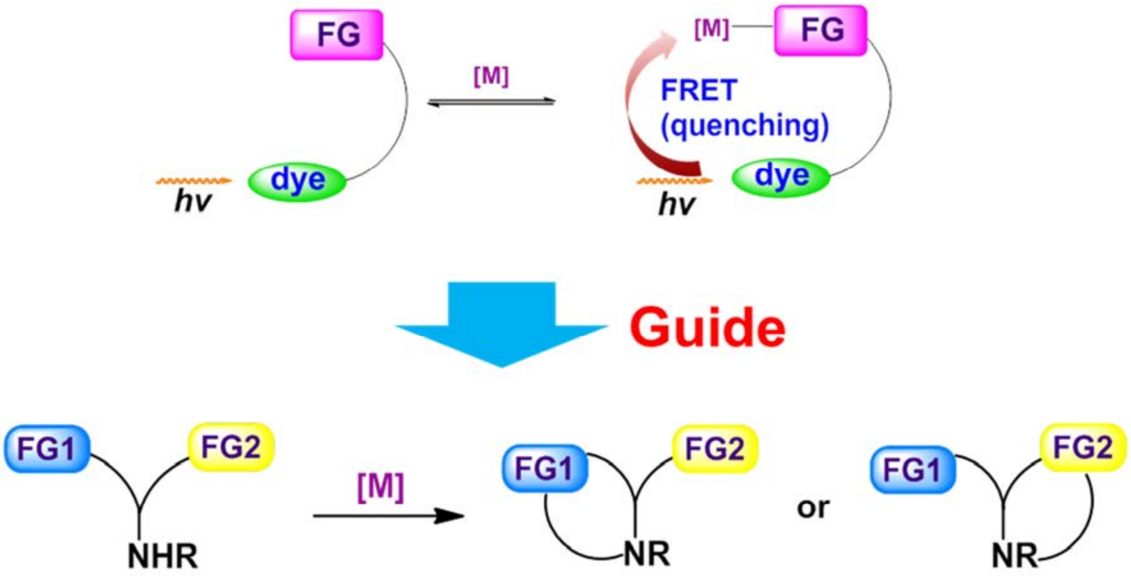
Studies on functionality preference of catalyst for site-selectivity guide

이옥숙 손정훈*

충남대학교 화학과

Metal-catalyzed tandem coupling reactions involving multiple functionalities are apodictically of importance to organic chemists for rapid synthesis of target compounds. In metal-catalyzed coupling reactions involving multiple functionalities, the functionality preference of catalyst, which determines the reactivity between the catalyst and functional group, might be critical to determine overall reaction pathway and final product with site-specificity. Therefore, the final products can be predicted and become an indicator for the development of new reactions if the functionality preference of metal catalysts were identified. Despite the importance of the functionality preference, there is no information of functionality preference of metal catalysts. In our research we established the preference of various metal catalysts toward alkene, alkyne and allene using FRET-based method1 and applied it to hydroamination reactions2 of the substrates containing the alkene/alkyne, alkene/allene, and alkyne/allene pairs to achieve site-specific cyclization



FG = alkene, alkyne and allene

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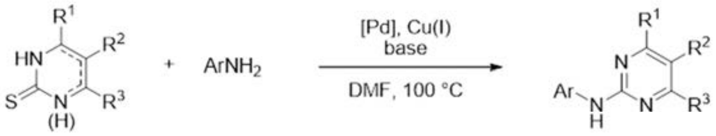
Palladium Catalyzed Desulfitative C-N Cross-Coupling Reaction of (Dihydro)Pyrimidinethiones with Arylamines

PHANNGUYENHUUTRONG 손정훈[1,*]

충남대학교 화학 생화학과 화학 [1]충남대학교 화학과

As a general method for the synthesis of 2-arylaminopyrimidine derivatives, we have developed a novel palladium-catalyzed desulfitative C-N cross-coupling of (dihydro)pyrimidinethiones with arylamines in the presence of Cu(I)-cofactor and base. The reaction was successful with a wide range of dihydropyrimidinethione/pyrimidinethione substrates and arylamines.


R1
R2
R3
HN
S
N
(H)
+
ArNH2
[Pd], Cu(I)
base
DMF, 100 °C
Ar
N
H

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Synthesis of Reactive Mesogens for reducing Optical Retardation

이승희 이명훈[1,*]

전북대학교 유연인쇄전자전문대학원 [1]전북대학교 고분자나노공학과

반응성 메소젠(reactive mesogen, RM)은 결정의 방향성과 액체의 유동성을 동시에 갖는 액정분자의 말단에 중합, 가교 또는 경화가 가능한 불포화기를 포함하고 있는 단량체 분자를 말한다. LCD 는 서로 수직하는 두 편광자 사이에 존재하는 액정들이 전압이 인가되면 한 방향으로 정렬되는 특성을 이용하고 있다. 빛의 편광특성으로 인해 본래 직교하는 두 편광자엔 빛이 투과할 수 없지만, 매우 큰 광학이방성을 가진 액정 분자들이 특정방향으로 위상지연을 발생시켜 편광자에서 빛을 빠져나오게 한다. 반면 이러한 특성은 시야각에 따라 빛 투과율 차이를 심하게 발생시켜 화면을 왜곡시키는 단점으로 작용 하기도 한다. 본 연구에서는 반응성 메소젠을 합성하고 이를 네마틱 액정과 혼합하여 uv 를 조사함에 따라 위상지연 값의 차이를 줄이고자 한다.

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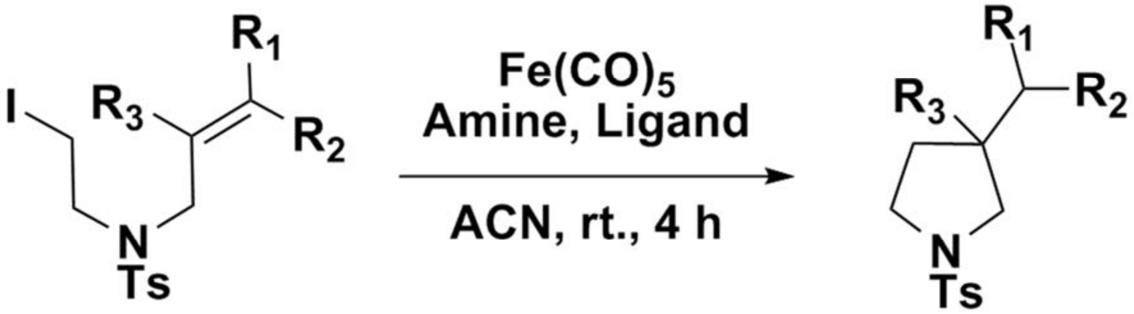
Iron(0) Pentacarbonyl-Mediated Cyclization Reaction of Alkyl Iodide Substrates

황준영 강은주[1,*]

경희대학교 응용과학대학 응용화학과 [1]경희대학교 응용화학과

Radical cyclization of alkyl iodides with a variety of common organic functionalities is reported. These substrates were subjected to the Fe(CO)5-mediated radical cyclization process in mild reaction conditions, leading to the formation of 1-tosyl pyrrolidines. This process appears to be a ligand-accelerated reaction, and iron(0) pentacarbonyl compound gives single-electron to alkyl iodides by SET mechanism. This Fe(CO)5-mediated cyclization process ensures an efficient access to a variety of reductive type-cyclizations.



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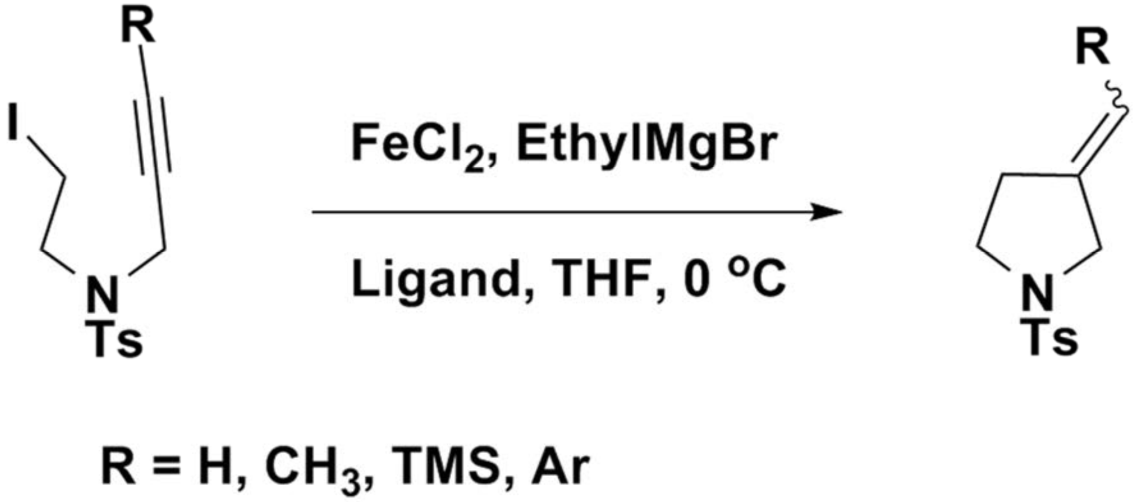
Iron(II)-Catalyzed Cyclization Reaction of 6-Halo-1-hexyne Derivatives with Grignard Reagent

김재곤 강은주[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

The metal-catalyzed Heck-type reaction of unactivated alkyl iodides has been well-known. However, it has been a major challenge of substrates. The sp3-hybridized alkyl halides resist oxidative addition, and the predisposition of assumed alkyl-metal complex to undergo β-hydride elimination. In addition, the cyclization reactions of 6-halo-1-hexyne derivatives have been reported with a few examples and needed the complicated condition. Herein, we report Iron(II)-catalyzed cyclization reaction of 6-halo-1-hexyne derivatives in the present of equimolar alkyl Grignard reagent.



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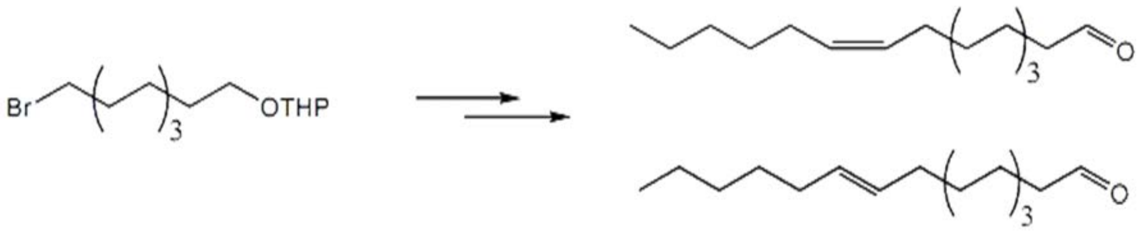
발표종류: 포스터, 발표일시: 수 16:00~19:00

Economical Synthesis for the Sex Pheromone of Peach Pyralid Moth

홍용표* 최종하 유건상 최선희[1]

안동대학교 응용화학과 [1](주)그린아그로텍 부설연구소

Peach Pyralid Moth, Dichocrocis punctiferalis Guenee attacking fruits, mainly apple, peach, chestnut is widely distributed in Asia and Australia. Sex pheromone of this moth may not only be an effective monitoring tool for timing insecticide application, but also a eco-friendly control agent. The sex pheromone components of peach pyralid moth, (Z)-10-hexadecen-1-al and (E)-10-hexadecen-1-al were economically synthesized 1,9-nonanediol and 1-heptyne. C9-Protected nonyl bromide and 1-heptyne were coupled and then, reduced to give (Z) and (E)-C16 compounds. They were easily deprotected and oxidized to produce peach pyralid moth sex pheromone.



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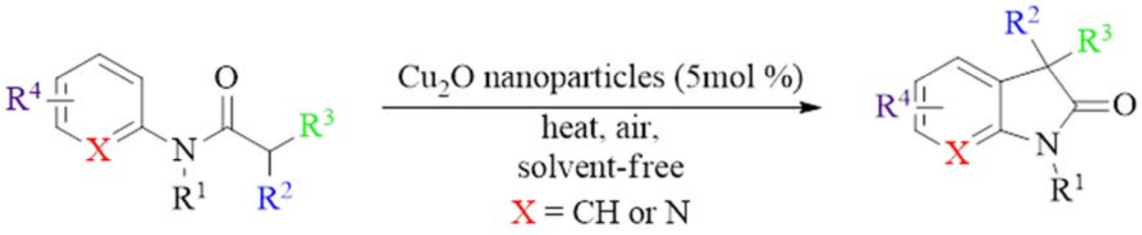
Atom-Economic and Environmentally Friendly Methodology For Oxindole Compounds

손세인 이재탁[1] 이재성[1] 송호림[1] 신현아[1] 이원구[1,*] 하현준[2,*]

서강대학교 화학 [1]서강대학교 화학과 [2]한국외국어대학교 화학과

Oxindole derivatives are used for a wide range of applications including traditional herbal medicine like Horsfiline1, anti-inflammatory agents2, molecular probes for pharmacological research3 and radical olefination reactions for the preparations of biologically interesting compounds4. Therefore, much effort has been made to develop efficient methodologies for preparing these molecules including famous named reactions such as Buchwald?Hartwig amination which require pre-functionalization by using halogen-substituted material 5-10. Previous experiments use halogen substituted materials because it is difficult to obtain oxindole derivatives without pre-functionalization by halogen which activates the ring at the initiation of the reaction. We recently developed methodology which does not need pre-functionalization with halogens, making this reaction environmentally friendly. While we studied CH activation, we realized that the organic solvent was not the important reagent for obtaining products. Therefore, we synthesized oxindole derivatives without organic solvent or extra additives. The required oxidant in this methodology is oxygen from air, and the reaction does not require an inert atmosphere. We used air to oxidize the intermediate and the method is appropriate for the preparation of pyridine derivatives which are rarely prepared through C-C bond formation.



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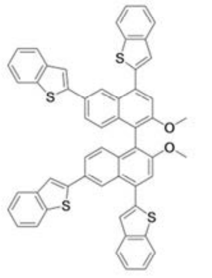
Blue organic-light emitting materials based on 4,4',6,6'-tetrabenzothiophenyl-2,2'-dimethoxy-1,1'-dinaphthyl

천지현 김태우* 임춘우[1,*] 신송이[2] 김영철[2,*]

경희대학교 동서의학대학원 [1]한남대학교 화학과 [2]경희대학교 화학공학과

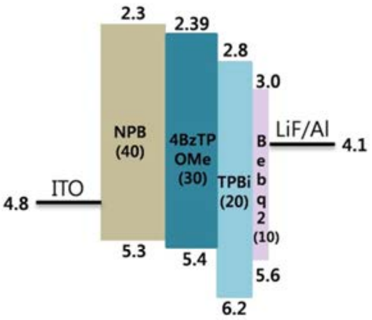
In this study, we synthesized a blue emitter, 4,4',6,6'-tetrabenzothiophenyl-2,2'-dimethoxy-1,1'-dinaphthyl (4BzTP-OMe), which was cross-coupled by Suzuki-Miyaura reaction between 4,4',6,6'-tetrabromo-2,2'-dimethoxy-1,1'-dinaphthyl and benzo[b]thiophene-2-boronic acid. Its photophysical, electrochemical, and thermal properties were investigated. Multilayered OLEDs were fabricated by using 4BzTP-OMe as an emitting material. A representative device structure was ITO / NPB (40 nm)/ 4BzTP-OMe (emitting materials, 30nm)/TPBi (20 nm)/Bebq$_2$ (10 nm)/LiF/Al. The device showed blue electroluminescent properties with luminance (1,100 cd/m² at 13 V), current density (160 mA/cm² at 13 V), and external quantum efficiency (0.91 % at 15 mA/cm²).

Molecular structure

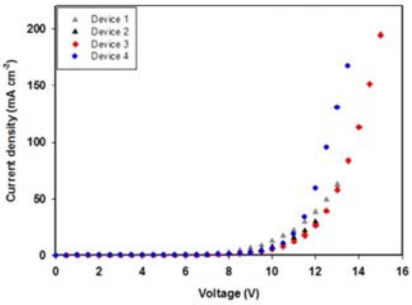


4BzTP-OMe

Device structure



Device performance



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Synthesis of Dendrimers by Homo-coupling of Alkyne-focal Aromatic PAMAM Dendrons

윤성희 한승철 이재욱*

동아대학교 화학과

Dendrimers are particularly attractive because they can have a high fluorescence quantum yield, and their modular monodisperse macromolecular structure enables tailoring of their properties to specific applications. Recently, dendrimers have attracted great attention as synthetic light-harvesting antennae, which means that some dendrimers can emit strong fluorescence from their core unit owing to energy transfer from dendron units to the core unit even when the core unit does not absorb light directly. In continuation with our research on the synthesis of symmetric dendrimers via homo-coupling using alkyne derivatives, we were fascinated to develop the fusion methods for the construction of the water-soluble dendrimers containing a fluorophore at core.The homo-coupling of terminal alkynes is a straightforward method for the synthesis of buta-1,3-diynes, which are important building blocks in the organic synthesis of natural products, pharmaceuticals, organic/inorganic composites, and polymers. Since Rossi's group used a palladium/CuI catalytic system to catalyze the homo-coupling of terminal alkynes, this method has attracted a great deal of interest due to its mildness and wide-ranging substituent tolerance. Taking advantage of these facts, herein we will present the efficient strategy for the convergent synthesis of emissive PAMAM dendrimers containing a chromophore by fusion method through homo-coupling of dendrons with a profluorophore at core.

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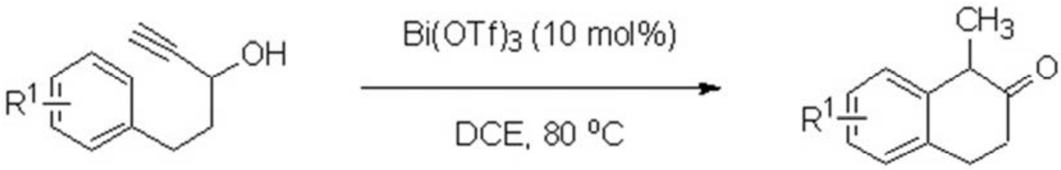
Bi(OTf)$_3$-Catalyzed Intramolecular Hydroarylation and Isomerization of Propargylic Alcohols for Synthesis of 2-Tetralone Derivatives

박정민 이구연*

강원대학교 생명건강공학과

2-Teralones are important scaffolds in biologically active natural products, pharmaceuticals, and other useful materials; however, they are difficult to synthesize. Therefore, a more efficient method needs to be developed for the synthesis of 2-tetralone considering their importance. Herein we have developed that bismuth catalyzed intramolecular cyclization of arylpropargylic alcohols to provide an efficient method for 2-tetralones. Bi catalysts, are inexpensive, non-toxic, and environmentally benign, and therefore, they are advantageous from the perspective of sustainable chemistry. 5-Phenylpent-1-yn-3-ol was treated with 10 mol% of Bi(OTf)$_3$ to give 1-methyl-2-tetralone in good yields. This highly efficient transformation involves tandem intramolecular hydroarylation, isomerization, and tautomerization in the same flask.



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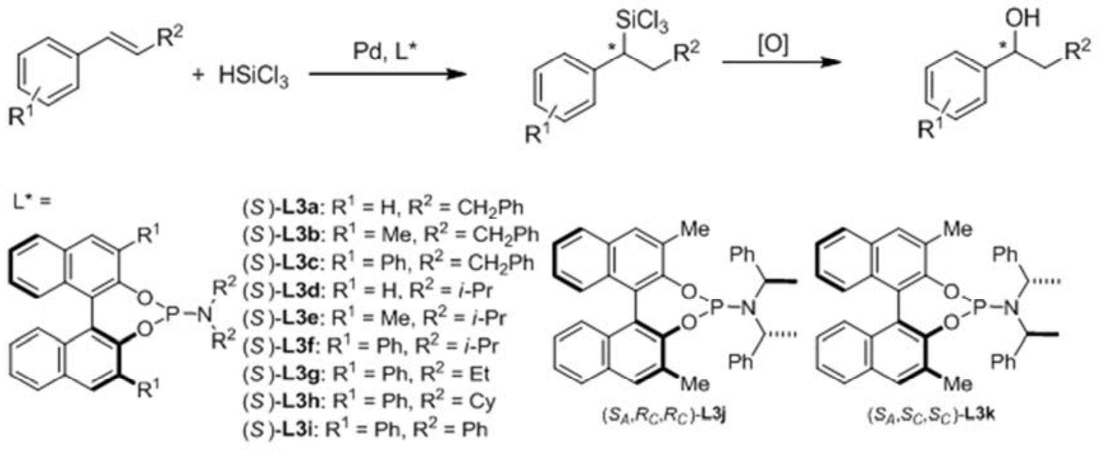
Asymmetric palladium-catalyzed hydrosilylation of styrene and its derivatives with 3,3'-disubstituted chiral phosphoramidite ligands

박희건 안효진 한진욱*

한양대학교 화학과

Palladium-catalyzed asymmetric hydrosilylation of styrene has become a potent methodology to show their efficiencies of newly-developed chiral monodentate phosphorous ligands.1 A significant improvement for catalytic activity and enantioselectivity in the hydrosilylation of styrenes was achieved by chiral monophosphine (MOP) ligands based on the 2-diphenylphosphino-1,1'-binaphthyl skeleton.2 Herein, we report a palladium-catalyzed asymmetric hydrosilylation of styrene with trichlorosilane using chiral phosphoramidites derived from (S)-3,3'-disubstituted 1,1'-binaphthols and secondary amines. In addition, asymmetric hydrosilylations of styrene derivatives with a substituents on the phenyl ring or at the β-position have been examined with the chiral phosphoramidite ligands. Optically active organosilanes were transformed to alcohol by a stereospecific oxidative cleavage of the C-Si bond with retention of configuration.



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Stereoselective Synthesis of 4-Substituted-Cyclic Sulfamidate-5-Carboxylates By Asymmetric Transfer Hydrogenation Accompanied By Dynamic Kinetic Resolution

서연지 김진아[1] 이현규[1,*]

과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]한국화학연구원 한국화합물은행

Dynamic kinetic resolution driven, asymmetric transfer hydrogenation reaction of cyclic sulfamidate imine-5-carboxylate esters proceed efficiently to give the corresponding chiral cyclic sulfamidate-5-carboxylate esters with excellent level of selectivity. This process is employed to prepare (-)-epi-Cytoxazone (1) and Taxotere side-chain (2).

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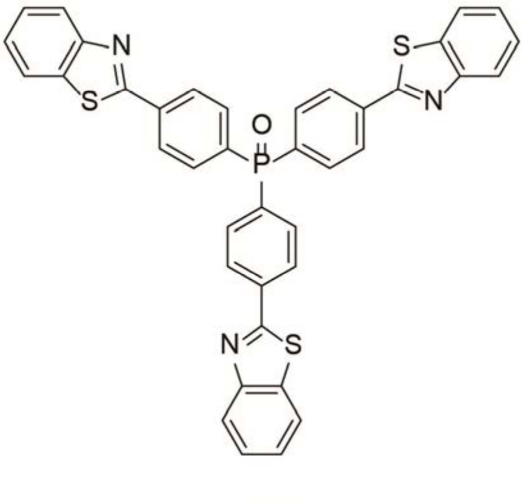
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-825**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Tris(4-(benzo[d]thiazol-2-yl)phenyl)phosphine oxide (4-TBTPO) and Tris(4-(benzo[d]oxazol-2-yl)phenyl)phosphine oxide (4-TBOPO) for Organic Light-Emitting Diodes

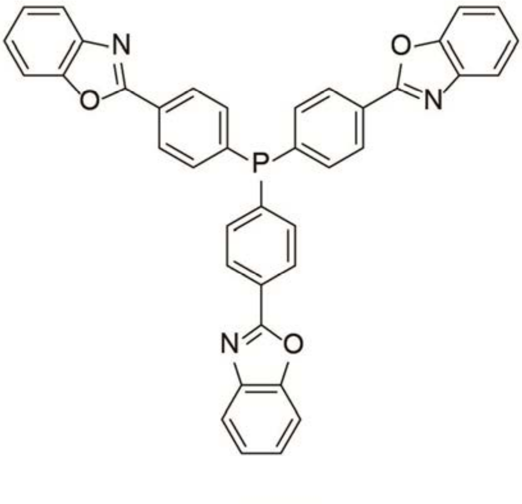
조현희 반은희 김경현 이범종[1,*]

인제대학교 화학과 [1]인제대학교 의생명화학과

The organic light-emitting diodes (OLEDs) have a variety of characters such as fast response, wide viewing angle, natural color, and low power. In the course of finding new OLED materials, we have synthesized novel compounds based on tris(benzothiazolyl or benzooxazolyl)phosphine oxide structure. The robust one-pot synthesis of tris(4-(benzo[d]thiazol-2-yl)phenyl)phosphine oxide (4-TBTPO) and tris(4-(benzo[d]oxazol-2-yl)phenyl)phosphine oxide (4-TBOPO) have been carried out in polyphosphoric acid (PPA) with P2O5 as solvent and catalyst. The chemical structures are characterized by 1H-NMR, 13C-NMR, FT-IR, UV-VIS, and elemental analysis (EA). The EL properties of the materials will be discussed.



4-TBTPO



4-TBOPO

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-826**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design and Synthesis of Boron Based Organic Semiconductors

류가연 김경곤[1,*] 김원석[2,*]

이화여자대학교 화학/나노과학과 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학 나노과학과

A new A-π-A type small molecules based on pyridine-borane complex (π-spacer) and 2,5-bis(alkyl)-3,6-di(thiophen-2-yl) pyrrolo [3,4-c]pyrrole-1,4(2H,5H)-dione (DPP) were designed and synthesized via Pd-catalyzed Suzuki cross-coupling reaction. The synthesized boron based complex exhibited high electron affinity, which indicates such π-materials have low LUMO level and high thermal and chemical stability. Herein, we report new types of boron based organic semiconductors for solar cells.

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발표코드: **ORGN.P-827**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A fluorescent chemical sensor for detecting water contents in organic solvents

이유진 김희문 김형진[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부

Water in organic solvents is considered as impurity. Measurement of water in organic solvents is therefore an important technology in various scientific and industrial fields. In this study, a water-soluble fluorescent 1,8-naphthalimde derivative attached with a guanidine moiety was synthesized and its ability to be used for the quantitative determination of water was investigated in various water-miscible organic solvents, such as ethanol, methanol, acetonitrile, dioxane, tetrahydrofuran, and dimethylformamide. This dye displayed the fluorescence "on-off" detection for water over a wider operating sensing range. The synthesis and water-sensing properties of the designed molecule will be presented.

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발표코드: **ORGN.P-828**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

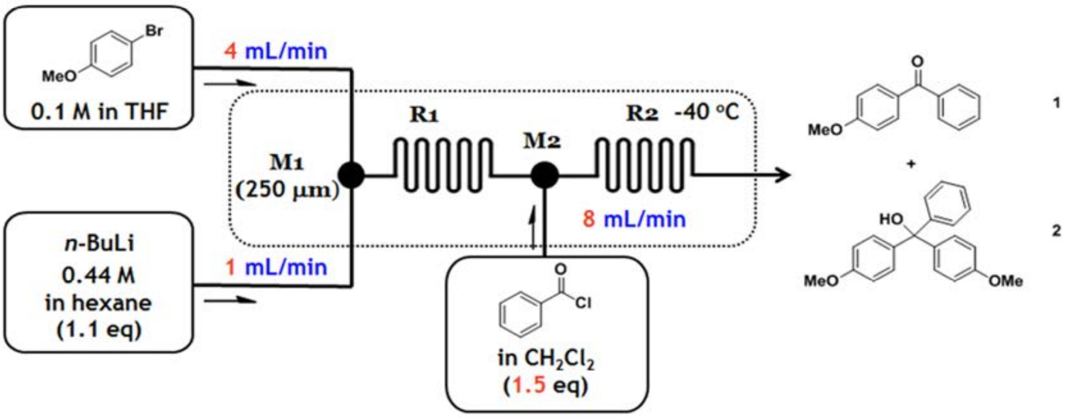
Synthesis of Unsymmetrical Biary Ketones Using Continuous Flow Microreactor

문수연 김원석*

이화여자대학교 화학 나노과학과

In recent years, continuous flow microreactor have been recognized as powerful tools for chemical synthesis from the viewpoint of both academia and industry due to the advantages, such as (1) controlled heat transfer, (2) controlled mixing (both fast and slow) (3) increased solution-solid phase interactions (4) controlled use of high reactive materials, and (5) tailor-made reactor to run serial reactions. Unsymmetrical Ketones are useful compounds present in many area, including materials, fragrances, and natural product synthesis. Thus, a variety of methods for the preparation of ketones have been developed. However, to the best of our knowledge, direct addition of lithium species to acyl chlorides without any additives has not yet been reported using batch reactor. Herein we report a new synthetic method for the synthesis of unsymmetrical ketones employing flow microreactor in the presence of acyl chlorides and in situ generated lithium species.

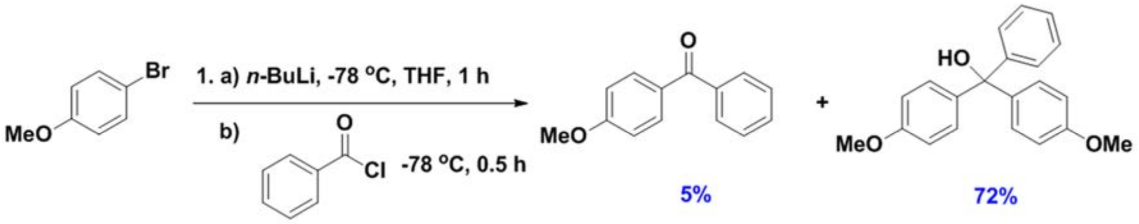
<Continuous Flow Reaction>



entry	micromixer	1 (%)	2 (%)
1	VICI	73[a] (61)[b]	19 (11)
2	YMC	71	19
3	IMM SIMM-V2	71	18

a. GC yield b. Isolated yield

<Batch Reaction>



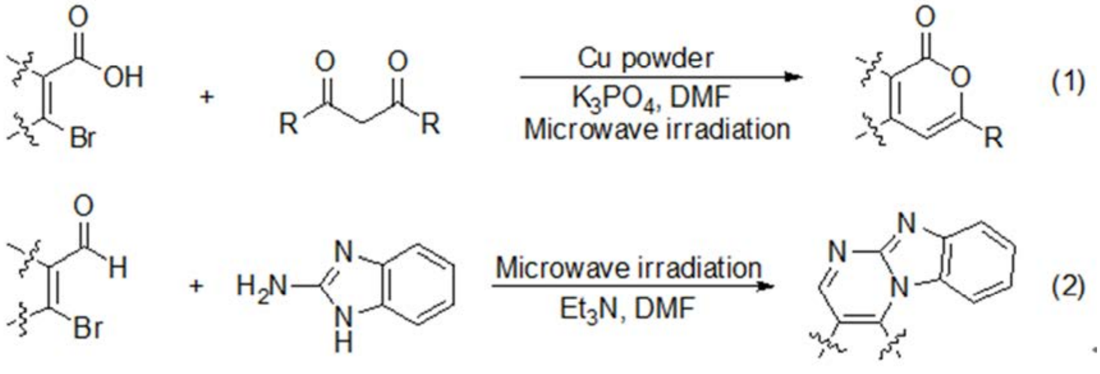
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-829**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Microwave-AssitedSynthesis of 2H-Pyran-2-ones and Benzimidazo[1,2-a]pyrimidine from β-Bromo-α,β-unsaturated carboxylic acids and Aldehydes

HOSONLONG JIAOYANG 유재명 양병우 윤일철 조찬식*

경북대학교 응용화학과

β-Bromo-α,β-unsaturated carboxylic acids were coupled and cyclized with 1,3-diketones in DMF by microwave irradiation in the presence of a catalytic amount of copper powder and a base to give the corresponding 2H-pyran-2-ones in good to high yields (eq 1).β-Bromo-α,βunsaturated aldehydeswere coupled and cyclized with 2-aminobenzimidazoles by microwave irradiation in the presence of a base and magnesium sulfate to give the corresponding benzimidazo[1,2-a]pyrimidines in good yields (eq 2).



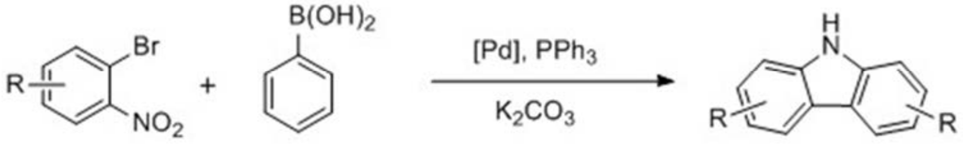
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-830**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Carbazoles via Tandem Cross-Coupling/Reductive Cyclization

구득영 우상국[1,*]

울산대학교 자연과학대학 화학과 [1]울산대학교 화학과

The carbazole core appears in a large number of biologically active natural products, pharmaceuticals and functional organic materials. So, the development of efficient synthetic routes to both core structures with a variety of substitution patterns is a current major objective in organic synthesis. We report highly efficient synthetic method of carbozole that is tandem Suzuki-Miyaura cross-coupling and reductive Cadogan cyclization of o-bromonitrobenzenes and aryl boronic acids (Figure 1). This reaction is carried out by triphenylphosphine and potassium carbonate under catalyzed by a palladium acetate(II).



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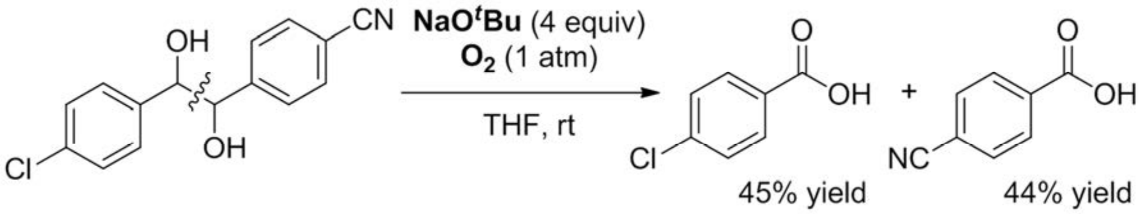
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-831**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Transition metal-free, chemoselective oxidative cleavage reactions of *vic*-1,2-diols to di-carboxylic acids with NaO^{t}Bu under oxygen atmosphere

김동완 양정운*

성균관대학교 에너지과학과

The development of transition-metal-free, chemoselective reactions is one of the most important and fundamental tasks in organic synthesis, as it contributes significantly to green chemistry practices. We have developed a transition-metal-free, oxidative cleavage reaction of *vic*-1,2-diols to carboxylic acids with NaO^{t}Bu under oxygen atmosphere. We also demonstrated how to scale-up experiments without organic extraction and chromatographic technique. The present protocol is an eco-friendly alternative to a conventional transition-metal-based method.



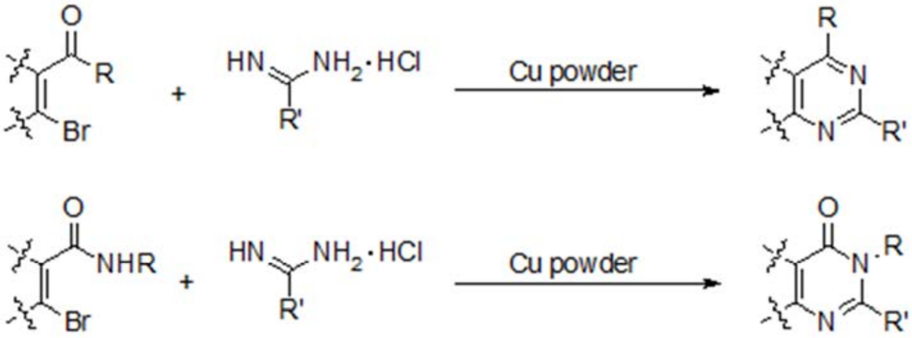
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-832**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper Powder-Catalyzed Coupling and Cyclization of β-Bromo-α,β-unsaturated Ketones and Amides with Amidine Hydrochlorides Leading to Pyrimidines and Pyrimidinones

JIAOYANG HOSONLONG 유재명 양병우 윤일철 조찬식*

경북대학교 응용화학과

β-Bromo-α,β-unsaturated ketones and amides were coupled and cyclized with amidine hydrochlorides in DMF in the presence of copper powder and a base to give the corresponding pyrimidines and pyrimidinones, respectively, in good yields.



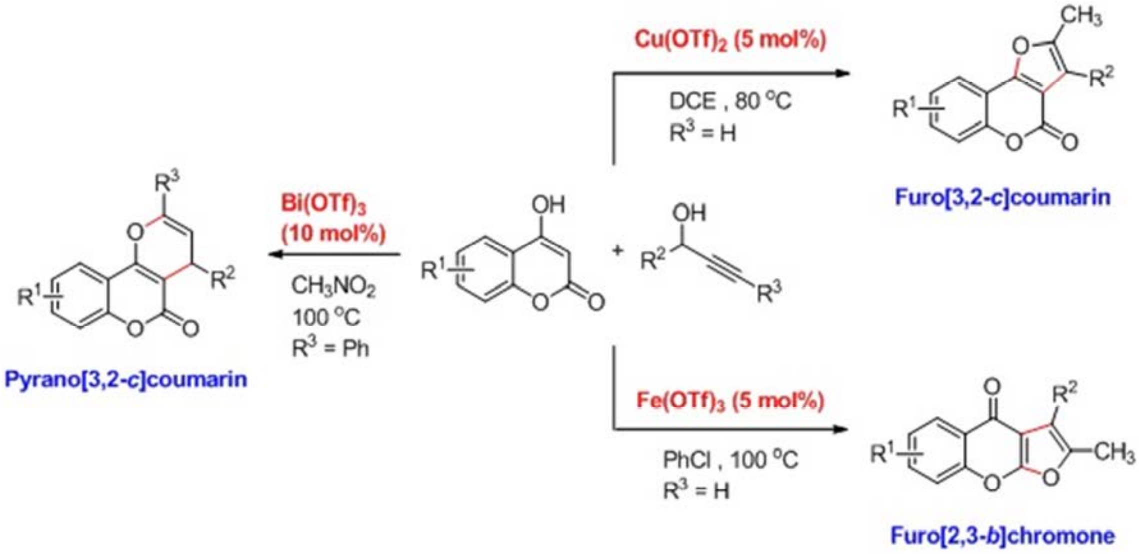
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-833**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel synthesis of furo[3,2-*c*]coumarins, furo[2,3-*b*]chromones and pyrano[3,2-*c*]coumarins via tandem propargylation/cycloisomerization switched by different metals

김재현 이구연*

강원대학교 생명건강공학과

The furan structure is a ubiquitous subunit in a variety of bioactive natural products and synthetic materials, including agrochemicals and pharmaceuticals. Thus, the developmentof efficient and concise synthetic methods that allow access to functionalized furan derivatives, and particularly furan fused heterocyclic compounds, remains an important taskin modern organic chemistry. Coumarins are an extremely important family of heterocyclic compounds owing to their presence in a large variety of biologically active substances and their use as valuable agents for pharmaceuticals and fine chemicals. Over the past several decades, synthesis and screening of coumarin compounds for drug discovery has been a vital subject of constant interest in organic and medicinal chemistry.We described three tricyclic oxygen containing heterocycle synthesis, where an arene both an alcohol and an alkyne functionality underwent three distinct pathways catalyzed by different metal salts. Starting from 4-hydroxycoumarin and propargyl alcohol derivatives, furo[3,2-*c*]coumarins was accomplished by a Cu(II) salts, while furo[2,3-*b*]chromones could be accessed via a Fe(III) salts. Pyrano[3,2-*c*]coumrains also was accomplished by a Bi(III) salts. This method provides a flexible and efficient route to substituted furocoumarins, furochromones and pyranocoumarins respectively.


Cu(OTf)₂ (5 mol%)
DCE , 80 °C
R³ = H
Furo[3,2-c]coumarin
Bi(OTf)₃
(10 mol%)
CH₃NO₂
100 °C
R³ = Ph
Pyrano[3,2-c]coumarin
Fe(OTf)₃ (5 mol%)
PhCl , 100 °C
R³ = H
Furo[2,3-b]chromone
OH
R¹
R²
R³
CH₃
O
+

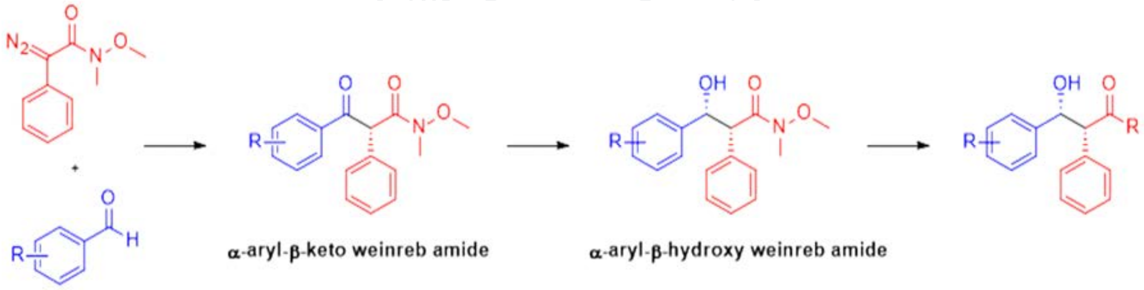
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-834**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Catalytic Asymmetric Roskamp Reaction of Weinreb Amide Diazo Compound Using Oxazaborolidinium Ion

신성호 백은희 강병철 강기태 정현실 김태형 류도현*

성균관대학교 화학과

We have developed a catalytic asymmetric Roskamp Reaction of Weinreb Amide Diazo Compound with aromatic aldehydes, which produces a-aryl-b-keto Weinreb amides in high yields and high enantioselectivities. Stereoselective reduction is proceeded sequentially to produce a-aryl-b-hydroxy Weinreb amide which can be used for various acyl derivative synthesis. This two-step reaction gives another method of asymmetric aldol product synthesis. We expect to synthesize natural products through our method.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-835**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and fluorescence properties of Rhodamine B containing Phenothiazine derivatives

손문수 장승현*

대구대학교 화학과

In this research, we have synthesized the compound 1, 2 from rhodamine B containing phenothiazine derivatives. The synthetic routes for the phenothiazine derivatives and rhodamine B derivatives are outlined in scheme 1. The imine reaction of two derivatives were synthesized. The structures of all reaction products were confirmed by ^{1}H-NMR, FAB-Mass. New compounds were found selectivity for metal cation by fluorescence titration using various metal cations.

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발표코드: **ORGN.P-836**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Luminescent Properties of Poly (9-(3-Vinyl-phenyl)-phenanthrene)

양가람 이하윤 김승호 신환규 이재현 강석우 박종욱*

가톨릭대학교 화학과

Recently, interest of polymer light-emitting diode (PLED) fabricated from conjugated polymer has augmented because PLED has advantage property that is well-suited to flexible lighting and solution processed device. In this presentation, we suggest a new polymer host based on phenanthrene, poly(9-(3-Vinyl-phenyl)-phenanthrene) (PVPP). It can be easily synthesized through simple synthetic methods which are Suzuki and Wittig reactions. From NMR data, vinyl group protons were disappeared and aromatic protons showed broad proton peaks because of polymer characteristics. PVPP film can be obtained from spin coating with solution used by common solvent. It exhibited PL maximum value of 381nm and broad PL spectrum of 70nm FWHM value. Energy transfer smoothly occurred when the three dopants for green, red and yellow were used in PVPP.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-837**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and fluorescence properties of bis-rhodamine B derivatives

최재영 장승현*

대구대학교 화학과

We synthesized new kinds of bis type of rhodamine fluorescent sensors. Compound 1 was synthesized from rhodamine B and ethylenediamine derivative and 1,4,5,8-naphthalene tertracarboxilic dianhydride. Compound 2 was synthesized from rhodamine B and 1,3-diaminopropane derivative and 1,4,5,8-naphthalene tertracarboxilic dianhydride. Synthesis, fluorescence properties will be discussed. These synthesized compounds were confirmed by ^{1}H-NMR, FAB-Mass and selectivity, complexation of metal measured in the fluorescence spectrum.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-838**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Ester via Copper-Catalyzed Aerobic Coupling of Thiols and Alcohols

임승연 장혜영[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

The esters are widespread in nature and are widely used in industry. Esters comprise most naturally occurring fats and oils, which are fatty acid esters of glycerol. Various methods have reported for one-pot and direct conversions of alcohols to esters by using ruthenium, iridium, palladium and gold complexes. Compared to the utilization of expensive metal complex, we reported a low-cost complex, copper(II) chloride-catalyzed aerobic cross-coupling of thiols and alcohols for the synthesis of esters. By utilizing this protocol, a variety of thiols and alcohols participate in the oxidative esterification to form esters in good yields.

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발표코드: **ORGN.P-839**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed synthesis of Vinylic Alkoxyamines starting from Propargyl Alcohols and TEMPO

강예원 장혜영[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

The syntheses of various types of alkoxyamines are in common practice due to its wide application in the controlled radical polymerization and radical-mediated addition/cyclization of alkenes. Among the various methods for the synthesis of alkoxyamines, the most common are 1) reactions of nitroxide radicals with carbon-centered radicals, 2) α-oxyamination of carbonyl compounds, 3) oxoammonium addition to alkenes, 4) Meisenheimer rearrangement of all N-oxides. In this study, we reported the first example of non-activated alkynes of propargyl alcohols participating in the reaction with TEMPO to afford vinylic alkoxyamines. To probe the reaction mechanism, a series of control experiments were also conducted.

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-840**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper-Catalyzed Wittig Olefination Using Thiols

이찬 **장혜영**[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

In our previous study, the oxidation of thiol by using copper catalyst to form thioaldehyde as an intermediate has been proved by the mechanism study. Based on this results, the copper-catalyzed wittig olefination using thiols was proposed. And various thiols and wittig reagents reacted under aerobic conditions to provide olefins in good yield.

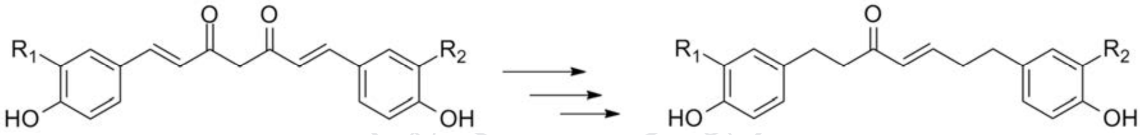
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-841**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of diaryheptanoids from curcuminoids in turmeric(Curcuma longa)

경영수* **<u>김남수</u>[1]** **박정열[2]** **노태섭[1]** **임홍규[3]**

강릉원주대학교 화학과 [1]강릉대학교 → 강릉원주대학교로 교명 변경됨(2009.3.1) 화학신소재학과 [2]한밭대학교 산학협력단 [3]강릉원주대학교 화학신소재학과

Aromatic diarylheptanoid compounds such as hirsutenone were synthesized from three curcuminoids in Curcuma longa Linn grown in Korea. We also synthesized diarylheptanoids from acetylacetone.



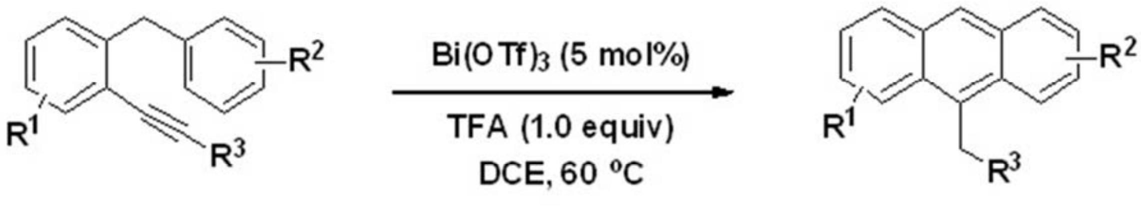
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-842**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

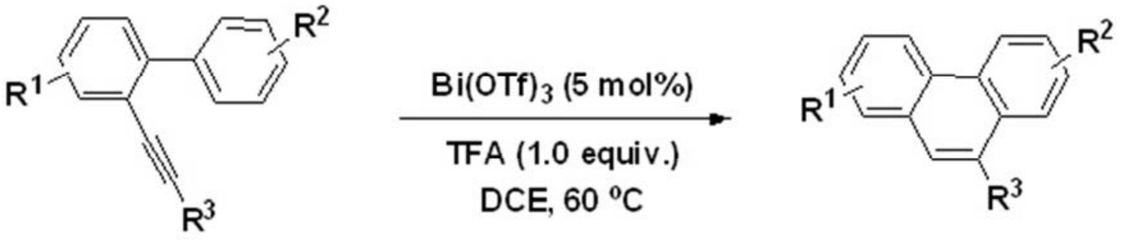
A Simple and Efficient Synthesis of Anthracenes via Bismuth-Catalyzed Cyclization of o-Alkynyldiarylmethanes

최혁 박정민 이구연*

강원대학교 생명건강공학과

Functionalized anthracene derivatives are important structure for potential therapeutics and polymeric materials. The synthesis of anthracenes has been mainly realized by a Lewis acid induced Bradsher-type reaction from diarylmethanes, but it often suffers from limited substrate scope, harsh reaction conditions, competitive reactions, and low yields. Therefore, novel approaches, especially those with high flexibility, efficiency, and good modularity, are highly demanded for its construction. Herein we have developed a concise method for the preparation of anthracenes from o-alkynyldiarylmethane catalyzed by Bi(OTf)3. A variety of substituted anthracenes were obtained from o-alkynyldiarylmethane in the presence of 5 mol% Bi(OTf)3 and 1 equiv. of TFA at 60 oC. This strategy provides a flexible and efficient route to substituted anthracenes and phenantrenes.





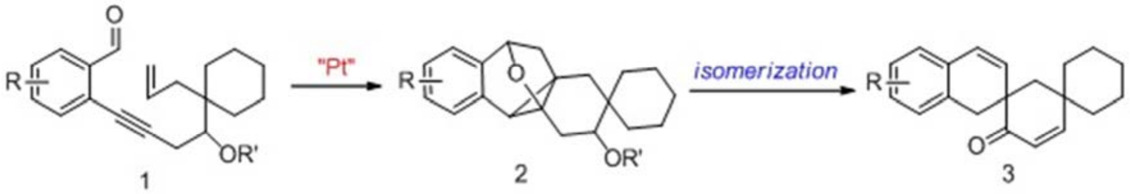
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-843**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Formation of polycyclic Spiranes via Pt-cyclization

김소영 오창호*

한양대학교 화학과

Spirane compound has a unique structure and is a important material in pharmaceutical and fine chemistry. We have developed an efficient synthesis for a variety of polycyclic Spirane derivatives. The key precursors 2 were prepared from 2-(4-(1-allylcyclohexyl)but-1-ynyl)benzaldehyde derivatives 1 via Pt-cyclization, and 3 were formed by TsOH-catalyzed isomerization in a good yield. The general scheme is shown as follows.



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

Development of Fluorescent Chemosensor for Anion with Bipyridine Derivative

심남연 남계춘*

전남대학교 화학과

On account of the important roles of anion in biological, clinical, environmental, catalysis, and chemical processes, the selective and efficient recognition of anion is an area of growing interest in supramolecular chemistry. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. In particular, the studies of chemosensors toward fluoride anion are quite intriguing because of its beneficial effects in human physiology. Therefore, developments of reliable sensors for fluoride ion are needed for environment and human health care. In most cases, fluorescent sensors involve photo physical changes such as photo induced electron transfer, photoinduced charge transfer, metal-to-ligand charge transfer to fluorescent chemosensors. We report here two novel chemosensors to a specific optical response to F-with coumarine and pyreneamidebipyridine derivatives.Binding properties were investigated by UV-vis spectroscopy, 1H-NMR and color changes and fluorescence analysis.

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발표코드: **ORGN.P-845**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Direct reductive amination of aldehydes using Hantzsch ester and S-Benzyl isothiouronium iodide as organocatalyst

이하늬 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

S-benzyl isothiouronium iodide has been successfully developed as a novel class of noncovalent organocatalyst for the direct reductive amination of aldehydes. A wide range of aldehydes as well as amines were found to give the expected products in moderate to excellent yields and short reaction times. The isothiouronium catalyst has certain valuable charateristics such as high hydrogen-bonding propensity and the ability to be recovered and reused.

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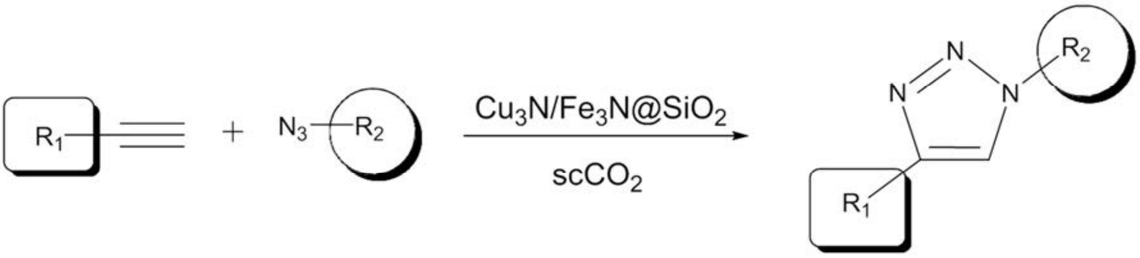
발표코드: **ORGN.P-846**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Efficient Synthesis of 1,4-disubstituted-1,2,3-triazoles using Mesoporous-supported Cu(I) catalyst in $scCO_2$

민지은 안소연 이규형[1] 허남회[1] 김학원[2,*]

경희대학교 화학과 [1]서강대학교 화학과 [2]경희대학교 응용화학과

The azide-alkyne Huisgen 1,3-dipolar cycloaddition, or click reaction is an effective way to make connections between structures that bear a wide variety of functional groups and important method for the synthesis of 1,2,3-triazoles. Especially, Cu(I)-catalyzed click reaction in water and organic solvent have been studied well and reported. We have investigated the mesoporous silica-supported copper nitride catalyzed click reaction(1) in supercritical carbon dioxide ($scCO_2$), considered as a sustainable, environmentally benign, green solvent, in the absence of amine additive. In this presentation, we will describe highly efficient $Cu_3N/Fe_3N@SiO_2$-catalyzed click reactions with various terminal alkynes and azides in $scCO_2$ and do test solubilities of various 1,2,3-triazole products in organic solvent and $scCO_2$ to explain why a reaction in $scCO_2$ shows higher yield than one in organic solvent .



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-847**
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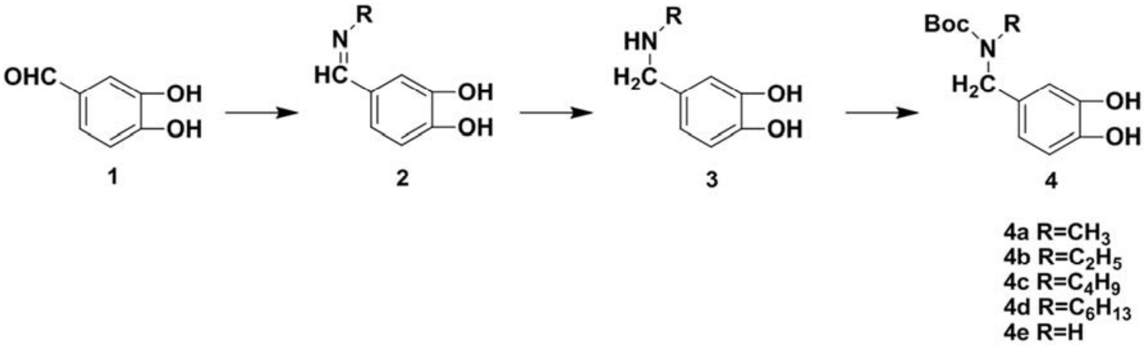
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, CO_2-solubilities and supercritical CO_2 metal extraction of catechol-containing amines as a novel CO_2-soluble chelating agent

yan xinhao 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

In present study, four new CO_2-philic catecholic amines containing non fluoroalkyl and carbamate group (Boc) on the nitrogen, as chelating agents, had been designed and synthesized from 3, 4-dihydroxybenzaldehyde by simple chemical modifications. Their solubilities and metal ion extraction ability in supercritical carbon dioxide ($scCO_2$) have been tested. The solubilities of newly synthesized compounds in $scCO_2$ were investigated by using a static analytical method at temperature from 313 K to 333 K and pressure range of 70-140 bar[1]. All synthesized catecholic amine derivatives (4a, 4b, 4c, 4d) showed much higher solubilities in $scCO_2$ than the corresponding 3, 4-dihydroxybenzaldehyde at easily accessible temperatures and pressures. We found tertiary carbamates (4a, 4b, 4c, 4d) would be CO_2-philic moiety, but secondary carbamate (4e) is not CO_2-philic group. All synthesized catechol derivatives (4a, 4b, 4c, 4d) showed good or moderate extraction efficiencies for several metal ions(Cu^{2+}, Sr^{2+}, Mn^{2+}, Cd^{2+}, and Cs^{+})[2].



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-848**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cationic water-soluble fluorescent probe with 15 crown-5 for potassium ion detection

최혜진 우한영[1,*]

부산대학교 인지메카트로닉스공학과 [1]부산대학교 나노과학기술대학 나노융합공학과

수용액에서 칼륨 이온을 검출하기 위하여 준 선형의 에너지 주게-π-받게-π-주게 구조를 가지는 1,4-bis(styryl)benzene 기반의 구조를 디자인 및 합성하고 광학적 특성 분석 및 칼륨이온 검출에 관한 연구를 수행하였다. 칼륨 이온과 특이적으로 결합하기 위하여 크라운 에테르 (crown ether)) 그룹을 π 공액 구조에 도입하였다. 또한 수용성을 높이기 위해 곁사슬 말단에 이온 그룹을 치환하였다. 새롭게 디자인된 본 형광 탐침은 우수한 수용성을 보이며 물에서 약 5.7×104M-1cm-1 정도의 높은 몰 흡광 계수와 31.1%의 형광 양자 효율을 보였다. 합성된 저 중합체는 칼륨과 1:1 의 비율로 결합함을 관찰하였으며 탐침의 흡수와 형광신호는 칼륨 농도에 비례하여 선형적으로 감소하였다. 결과적으로 크라운 에테르 감지그룹을 포함하는 1,4-bis(styryl)benzene 구조를 형광 탐침으로 사용하여 물에서 검출한계 0.05uM 에 해당하는 높은 민감도와 우수한 선택도를 구현하였다.

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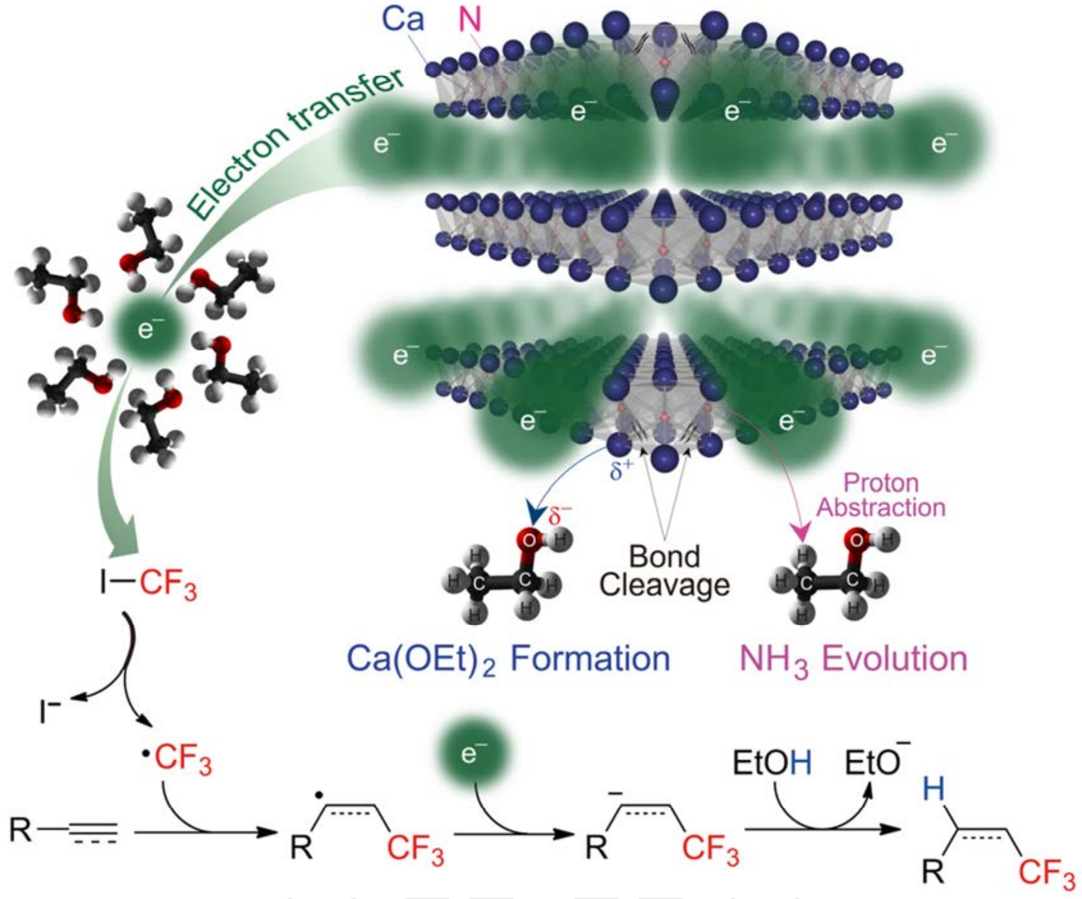
발표코드: **ORGN.P-849**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Hydrotrifluoromethylation and iodotrifluoromethylation of alkenes and alkynes using an inorganic electride as a radical generator

최성규 조은진*

한양대학교 응용화학과

We describe a simple, efficient, and environmentally benign strategy for the hydrotrifluoromethylation of unactivated alkenes and alkynes through a radical-mediated reaction using an inorganic electride, [Ca2N]+·e-, as the electron source. In the transformation, anionic electrons are transferred from [Ca2N]+·e- electrides to the trifluoromethylating reagent CF3I to initiate radical-mediated trifluoromethylation. This methodology, without need for a transition-metal catalyst, allows access to diverse hydrotrifluoromethylated and iodotrifluoromethylated products in a short reaction time. In addition, iodotrifluoromethylation of alkynes proceeds selectively upon the control of electride amount.


Ca
N
Electron transfer
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
δ⁺
δ⁻
Proton Abstraction
Bond Cleavage
Ca(OEt)₂ Formation
NH₃ Evolution
I−CF₃
I⁻
•CF₃
R
CF₃
e⁻
EtOH
EtO⁻
H

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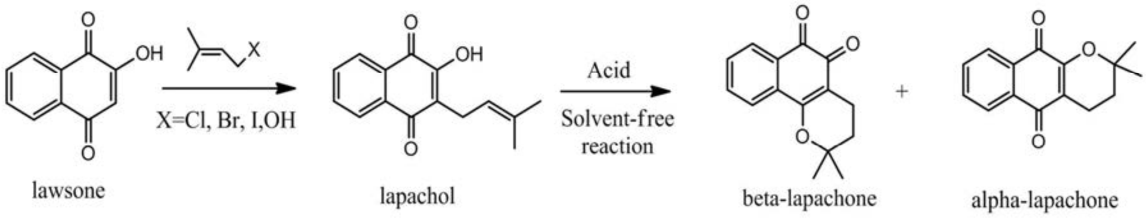
발표코드: **ORGN.P-850**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies on the solvent-free synthesis of β-lapachone through the acid-mediated intramolecular cyclization of lapachol

이현진 이고은[1] 김학원*

경희대학교 응용화학과 [1]경희대학교 일반대학원 화학과

β-Lapachone (β-LAPA), is a chemotherapeutic agent derived from the bark of the South American Lapacho tree, has recently emerged as a potent antitumor, anti-virus, anti-parasitic, and anti-inflammatory agent in vitro, and in vivo.Among previously known synthetic methods, C-prenylation of lawsone to give lapachol and the subsequent intramolecular cyclization of lapachol under strong acid condition, such as sulfuric acid and trifluoromethanesulfonic acid have been well known. However, C-prenylation of lawsone gave many side products to result in low yield and the following strong acid-mediated intramolecular cyclization yielded hazardous wastes and then it could not be suitable for industrial-scale production. Hence, in order to synthesize β-lapachone in high yield with mild, easy to handle, and environmentally-friendly reagents we have tried to develop much better and the greener process of intramolecular cyclization using recyclable solid-supported acid, such as inorganic supports(Alumina, silica, clays, zeolite) or organic supports(Polymer resins, cellulose) acid or solid acid in the absence of solvent.



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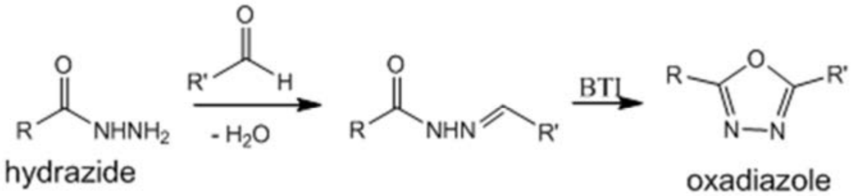
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-851**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Efficient Solvent-free Synthesis of 2,5-Disubstituted 1,3,4-Oxadiazoles and their Evaluation

노경탁 허남회[1] 김학원[2,*]

경희대학교 화학과 [1]서강대학교 화학과 [2]경희대학교 응용화학과

1,3,4-Oxadiazole is considered as very important compounds due to their biological and medicinal activities, fluorescent and corrosion inhibition properties which has led lots of efforts to develop new methodologies for the preparation of various oxadiazoles.Recently, tremendous efforts in the organic synthesis field have been devoted to reduce costs and resources consuming via environmentally benign, simple, and practical processes. In this report, a mild, general, convenient and efficient one-pot synthesis of symmetrical and unsymmetrical 1,3,4-oxadiazoles from hydrazide through N-acylhydrazones is described. Several hydrazides were efficiently grinded with various aldehydes by using ball-mill machine to give the corresponding N-acylhydrazones. Resulting N-acylhydrazones underwent a smooth BTI[bis(trifluoroacetoxy)iodobenzene]-mediated cyclization reaction in the absence of solvent to afford symmetrical and unsymmetrical 1,3,4-oxadiazoles in good yields. It would be developed for a sustainable organic synthetic process. Resulting 1,3,4-oxadiazoles have been investigated for the fluorescence properties and metal complexation. Those would be used for fluorescence chemosensor or OLED materials.



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발표코드: **ORGN.P-852**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, CO_2-solubility and supercritical CO_2 metal extraction of various 18-crown-6 ethers

오유리 김학원[1,*]

경희대학교 일반대학원 화학과 [1]경희대학교 응용화학과

Supercritical carbon dioxide(sc-CO_2) has been suggested as an environmentally benign, green solvent for heavy metal ions extraction. Due to weak solute(polar metal ions)-solvent(nonpolar CO_2) interactions, however, the direct extraction of metal ions with sc-CO_2 is not efficient. Therefore, the use of highly CO_2?soluble chelating ligands has been suggested for the successful chelation method in sc-CO_2. Those would make the CO_2?insoluble metal ions CO_2?soluble and then extractable. We have designed and synthesized novel CO_2-philic chelating ligands containing both metal binding segments, such as 18-crown-6 ether moiety and CO_2-philic segments, carbonyl and ether moieties, for more effective supercritical CO_2 metal extraction. Solubilities of synthesized 18-crown-6 ethers have been tested and explanation of the relationship between structure and solubility has been suggested. With these CO_2-soluble 18-crown-6 ethers the sc-CO_2 metal extraction (Cs^+ and Sr^{+2} etc) have been studied.

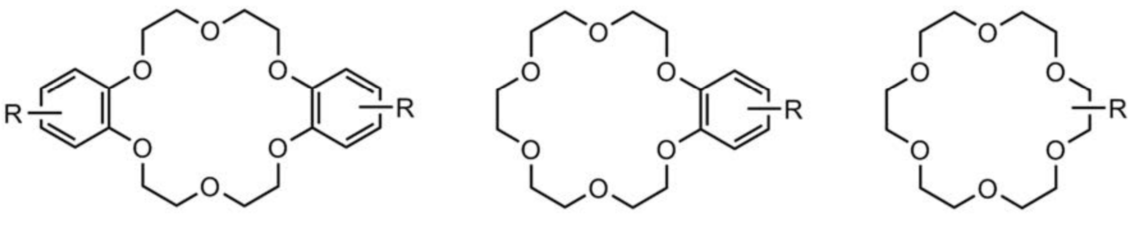

Figure 1. Various 18-crown-6 ethers
R = H, alcohol, carbonyl, etc

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발표코드: **ORGN.P-853**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Planar N-type conjugated polymers via intrachain noncovalent coulomb interactions

김지현 우한영[1,*]

부산대학교 인지메카드로닉스공학과 [1]부산대학교 나노과학기술대학 나노융합공학과

Nowadays, organic field-effect transistors (OFETs) have received significant attention because of good film forming properties, simple processability and high flexibility. To improve the intrachain planarity and interchain association, noncovalent coulomb interactions (such as hydrogen bond and dipole-dipole interactions) were incorporated in the molecular design of N-type conjugated polymers. Here we synthesized an electron-poor thiazole and benzothiadiazole based copolymer (PDTzBT) to study charge carrier transport characteristics for OFET applications. The measured number-average molecular weight (Mn) of PDTzBT was 14,000 g/mol and optical bandgap was 1.88 eV. The energy levels of the highest occupied and lowest unoccupied molecular orbitals were ?5.82 and ?3.94 eV, respectively. Here, we suggest that this thiazole and benzothiadiazole based PDTzBT is a promising building block for developing new optoelectronic n-type materials. The detailed device performance based on the polymer will be discussed further.

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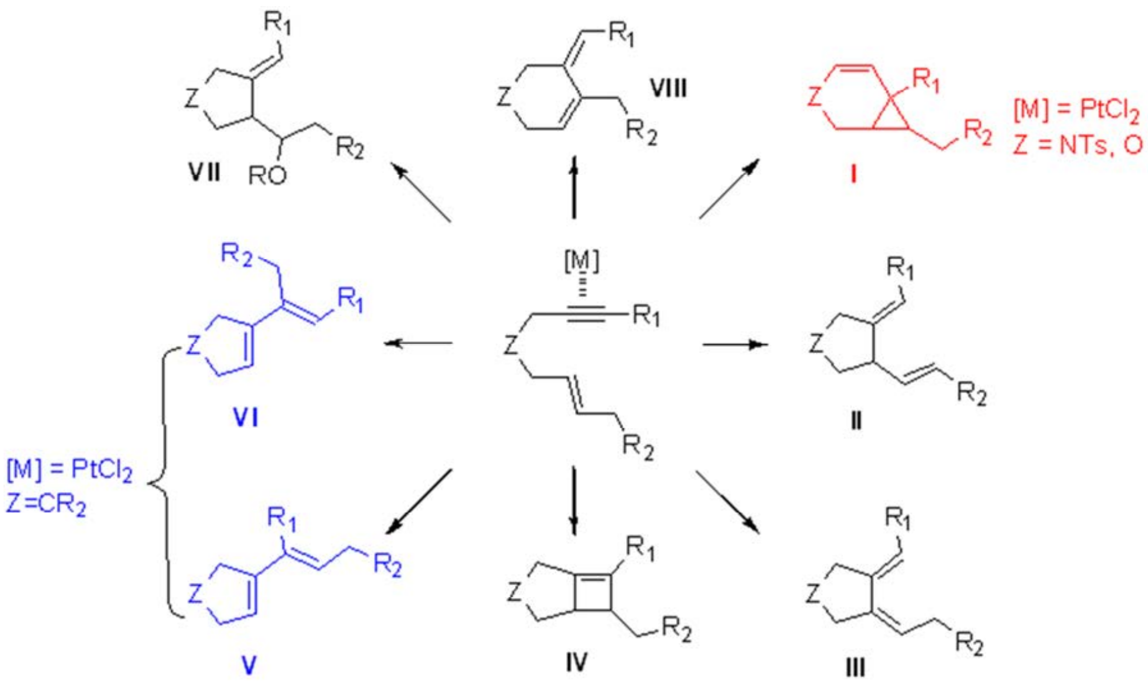
발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Investigation on the Pt-Catalyzed Cycloisomerization of 1,6-Enynes to Alder-ene type of products

박지은 강윤경*

상명대학교 화학과

Transition metal-catalyzed cycloisomerizations of enynes have been of great interest in the field of organic and organometallic chemistry as well as catalysis research. Extensive studies have provided a wide range of chemical transformations that are synthetically useful and atom economical. While Pd- and Au-catalyzed reaction of 1,6-enynes give rise to the formations of variety of products illustrated in the scheme, Pt-catalyzed one provided mainly a bicycle[4.1.0]heptenes (I) for the heteroatom-tethered substrates and single or double exo-cleavage products (V and VI) for the carbon-tethered ones. Diversity of mechanistic proposals have been suggested and part of them were underpinned by the computational analyses, the detailed background of these peculiar results have not been completely elucidated. Here, we have complete the reaction map of the $PtCl_2$-catalyzed cycloisomerization of 1,6-enyne that shows the relative energetics of virtually all possible reaction pathways by using density functional theory (DFT). We have found that the difference in reactivity of N- and C-tethered 1,6-enyne catalyzed by $PtCl_2$ catalyst stems mainly from the large destabilizations of the 6-endo-cyclization product, bicyclo[4.1.0]heptene (I), and transition state that connect these two state of C-tethered 1,6-enyne, which cause the shift of the reaction pathway toward single or double exo-cleavage products (V and VI).


R1
Z
VII
RO
R2
R1
Z
VIII
R2
Z
R1
R2
I
[M] = PtCl2
Z = NTs, O
R2
R1
Z
VI
[M]
Z
R1
R2
R1
Z
R2
II
[M] = PtCl2
Z=CR2
R1
Z
R2
V
Z
R1
R2
IV
R1
Z
R2
III

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-855**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Hg^{2+} binding-induced nanoaggregates of triazole-based amphiphilic chemoprobes in water environment

김인혜 이나은 조병기[1,*] 이은지[*]

충남대학교 분석과학기술학과 [1]단국대학교 화학과

Amphiphilic molecules based on triazole-based aromatic segment and hydrophilic tri(ethylene oxide) were easily synthesized using facile click chemistry, which act as a fluorescent turn-off Hg^{2+}-chemoprobe in an aqueous solution. Interestingly, it revealed that the metal-binding process of amphiphiles can induce the nano-assemblies even below the CMCs, and the binding stoichiometry affects the morphologies of the resultant nanostructures. The self-assembling behaviour of the amphiphiles was examined by UV-Vis and fluorescence spectroscopy. The formation of nano-aggregates was confirmed by TEM and DLS. Additionally, 1H-NMR and FT-IR experiments show the Hg^{2+}-binding mechanism and the evidence for the triazole-based amphiphile-Hg^{2+} complexes. The metal-amphiphile conjugates provide a useful and simple strategy for the detection of toxic heavy metals in aqueous medium.

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발표코드: **ORGN.P-856**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A "Light-up" silver ion sensing of peptide amphiphile nanoprobe and its biological applications

김인혜 김용재 이나은 허강무[1] 이은지[*]

충남대학교 분석과학기술학과 [1]충남대학교 고분자공학과

Herein, peptide amphiphiles consisting of a hydrophobic alkyl chain (linear for PA 1 or branched type for PA 2) and hydrophilic histidine-containing peptide, which is known to detect specific metal ions, self-assembled into nanofibers (NFs) in water with a strong aggregation tendency. Particularly, by adopting pyrene as a fluorescent probe, the self-aggregate behavior was investigated based on different optical properties between PA 1 and 2. Furthermore, PA 1 shows light-off sensing signal to Cu^{2+} while PA 2 increases the fluorescence by capturing Ag^+ in aqueous solution. Also, a considerable enhancement of fluorescence in Ag^+-NF-loaded HeLa cells was observed. In addition, the NFs of PA 2 decorated with AgNFs are shown to possess highly effective and long-term antibacterial activity against both Gram-negative and -positive bacteria. This interesting interaction between Ag^+ and PA 2 makes it possible for the biological application of cell-imaging and antimicrobial agents.

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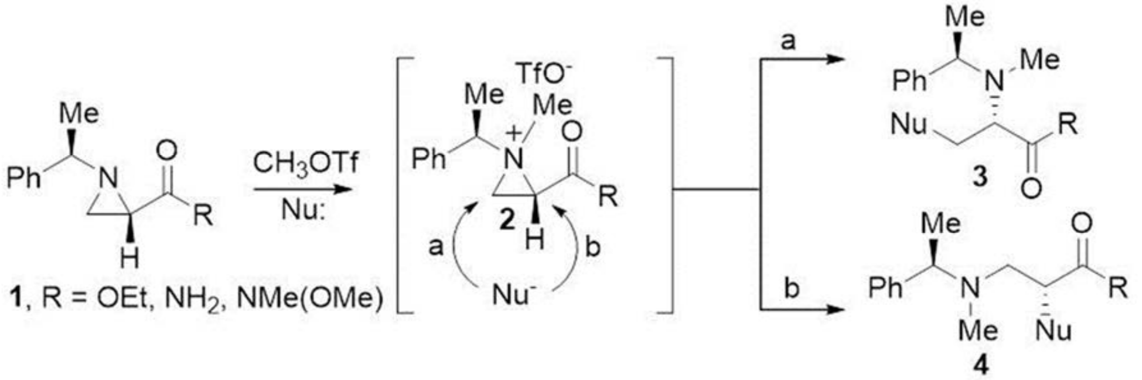
발표코드: **ORGN.P-857**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Facile Synthesis of N-Methylated Amino Acids from Chiral Aziridine-2-carboxylate

최지혜 하현준* 이원구[1,*]

한국외국어대학교 화학과 [1]서강대학교 화학과

N-methylated amino acids attract attentions due to their metabolic stability and conformational rigidity compared to their counter amino acids. Furthermore, many peptides consisted of N-methylated amino acids showed distinctive properties for the application of drug development and of novel materials. However, only limited numbers of N-methylated amino acids are commercially, most of which are quite expensive. Though various synthetic methods have been developed for the preparation of N-methylated amino acids an efficient and generally applicable protocol toward them is still needed. Recently, we reported “N-methylative aziridine ring opening reaction” of non-activated aziridines. Herein we described an efficient preparation of N-methylated amino acid by N-methylative aziridine ring opening reaction of aziridine-2-carboxylate and carboxamide with various nucleophiles including OAc$^?$, OH$^?$, $N_3^?$, CN$^?$ to yield N-methylated α- or β-amino acids.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-858**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Studies toward the C1-C10 Fragment of Madeirolide A

백인환 황성현 이철범*

서울대학교 화학부

We present studies toward the total synthesis of madeirolide A. This compound has been isolated from the marine sponge Leiodermatium sp., and has been shown to be a potent inhibitor of Candida albicans, a pathogenic fungus. Madeirolide A has a complicated structure with a 24-membered macrolactone and 16 stereocenters. The bioactivity and structural complexity make madeirolide A an attractive target for total synthesis.Our approach for synthesis is based on the assembly of four fragments. Using reductive cyclization developed from our group, three oxacycles in the compound have been envisioned to be efficiently created under novel photoredox catalysis of an iridium complex. Here we describe the introduction of the synthesis of the C1-C10 part of madeirolide A.

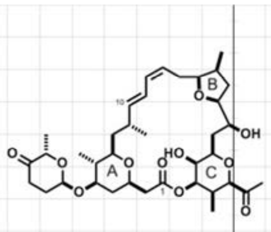


Figure 1 - Structure of Madeirolide A, Location of C1-C10 and Three Oxacycles (A~C)

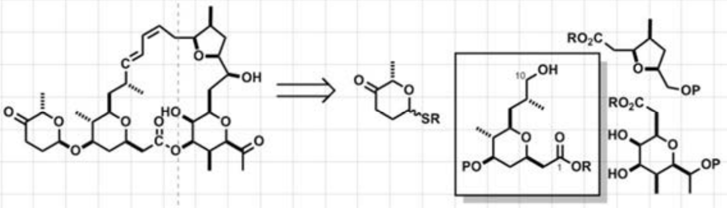


Figure 2 - Retrosynthetic Analysis of Madeirolide A and Its Four Fragments / C1-C10 Fragment Highlighted

일시: 2014년 10월 15~17일(수~금) 3일간
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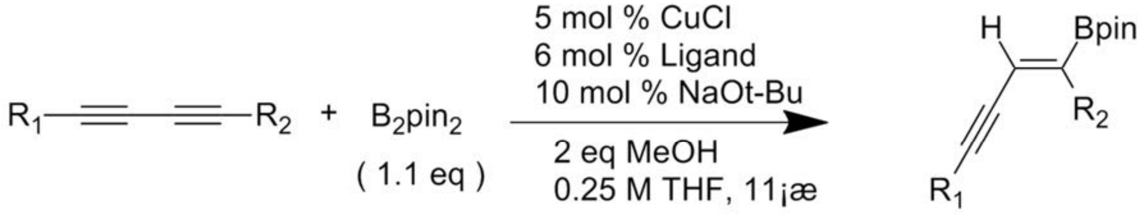
발표코드: **ORGN.P-859**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regio- and stereoselectives monoborylation of diyne compounds catalyzed by copper catalysts

<u>LI DINGXI</u> 김영은 윤재숙*

성균관대학교 화학과

Conjugated enyne compounds have received much attention because of their wide applications in organic synthesis. For example, they can be reduced to saturated hydrocarbons, oxidized to ketones, cyclized and so on. Conjugated borylenynes have a boronate group in addition, so they are more useful, because the C－B bond can be transformed to a variety of functional groups such as C－O, C－N and C－C bonds.In our current work, we investigated copper-catalyzed monoborylation of diyne compounds, which generated conjugated borylenyne compounds with high regio- and stereoselectivities. The catalytic efficiency is enhanced using monodentate phosphine ligands, and a range of diynes were borylated in good yield.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-860**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Isolation and Characterization of Cyclic dipeptides from Solid Bacterial Culture Broth (BS07)

Md.Maniruzzaman Manir 문석식* 박경석[1,*]

공주대학교 화학과 [1]농촌진흥청 국립농업과학원 농업미생물과

Bacillus vallismortis strain BS07 was originally isolated from red pepper and has been worked as an efficient plant growth promoting and diseases controlling agent. A chemical investigation of themethanolic extract of BS07 led to the isolation of several cyclic dipeptides through a series of silica gel column chromatography and preparative C-18 HPLC. Structures of cyclic dipeptides were determined by spectroscopic methods including IR, UV, HRTOFMS, and 1D & 2D NMR and conformed by synthesis. Structures of the isolates will be presented.

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발표코드: **ORGN.P-861**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantum Dot Nanolocation within the Solution-Processable P3HT-Based Hybrid Nanowire

김용재 이은지*

충남대학교 분석과학기술학과

We present simple fabrication of hybrid NWs composed of P3HT-*b*-P2VP rod-coil amphiphilic block copolymers and quantum dots via solution-state crystallization assembly. Interestingly, self-assembled P3HT-*b*-P2VP/QD hybrid NWs with highly regioregular P3HT shows a coaxial arrangement of QDs along the fibril axis. The coaxiality of QDs within the hybrid NW was controlled by varying the polymer parameters including RR values and relative block lengths. In addition, the localization of QDs within the desired domains of hybrid NWs can be controlled precisely by the surface modification of QDs. More interestingly, systematic transmission electron microscopy (TEM) revealed that dimeric QDs bridged by rod-coil block copolymers are assembled into 1D coaxial hybrid NWs by crystallization driven self-assembly.

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발표코드: **ORGN.P-862**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure confirmation of 3-*epi*-Xestoaminol C from Chiral Aziridine-2-carboxylate

최지혜 하현준* 이원구[1,*]

한국외국어대학교 화학과 [1]서강대학교 화학과

Recently, Keyzers at al. reported firstly bioassay-guided isolation of a new 1-deoxysphingoid, 3-*epi*-Xestoaminol C, isolated from the New Zealand brown alga *Xiphophora chondrophylla*. This compound as a stereoisomer of xestoaminol C show IC50 value of 19.4, 8.8 and 18.0 μM against M. tuberculosis H36Ra, HL-60 cells, and HEK cells, respectively. Any synthesis of 3-*epi*-Xestoaminol C has been not reported since its isolated from organism, structural confirmation of identified molecule through synthesis is important. We achieved efficient and asymmetric synthesis of 3-*epi*-Xestoaminol C and xestoaminol C using synthetic strategy previously developed by us to make sure the configuration of 3-*epi*-Xestoaminol C and xestoaminol C efficiently. References1. Dasyam, N.; Munkacsi, A. B.; Fadzilah, N. H.; Senanayake, D. S.; O'Toole, R. F.; Keyzers, R. A. *J. Nat. Prod.* 2014, *77*, 15192. Yun, J. M.; Sin, T. B.; Hahm, H. S.; Lee, W. K.; Ha, H.-J. *J. Org. Chem.* 2003, *68*, 7675

일시: 2014년 10월 15~17일(수~금) 3일간
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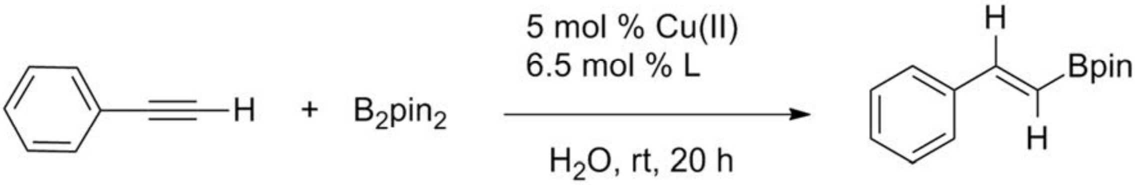
발표코드: **ORGN.P-863**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

‘On water’ β-borylation of alkynes using a Cu(II) catalyst

이혜수 이수민 이우림 윤재숙*

성균관대학교 화학과

There is worldwide interest in developing reactions in view of environmental concerns. Especially, development of reaction using water as solvent is considered environmentally important. While some studies on β-borylation of electrophilic alkenes in water have been reported, β-borylation study for alkyne is relatively less reported. Therefore, we tried to develop a methology for β-borylation of alkynes using water as a reaction medium. We screened a variety of Cu(II) catalysts, ligands and we will present our optimized conditions for the reaction.



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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-864**
발표분야: 유기화학
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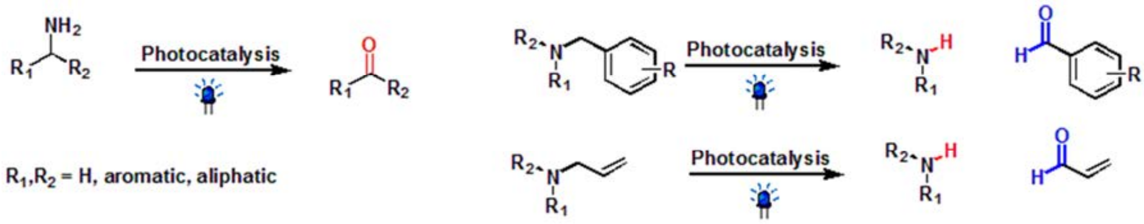
Oxidative C-N bond Cleavage by Visible Light Photoredox Catalysis and its Application to N-debenzylation & N-deallylation

<u>Naeem Iqbal</u> 조은진*

한양대학교 응용화학과

A visible light mediated method for the C-N bond cleavage has been developed. This method was applied for the conversion of a large number of different kinds of amine to their corresponding carbonyl groups. This C-N bond cleavage can be employed as a deprotecting method for N-benzyl & N-allyl moieties, which have been extensively employed as N-protecting groups. Reactions proceeded by the use of Ru(bpy)3Cl2 as the photocatalyst along with K2S2O8 as an oxidant in solvent system of H2O/CH3CN under visible light irradiation.



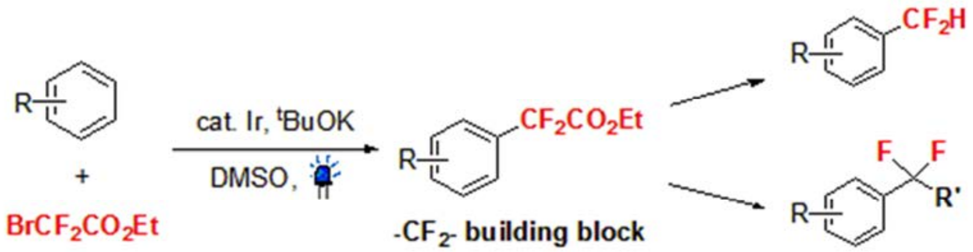
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-865**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

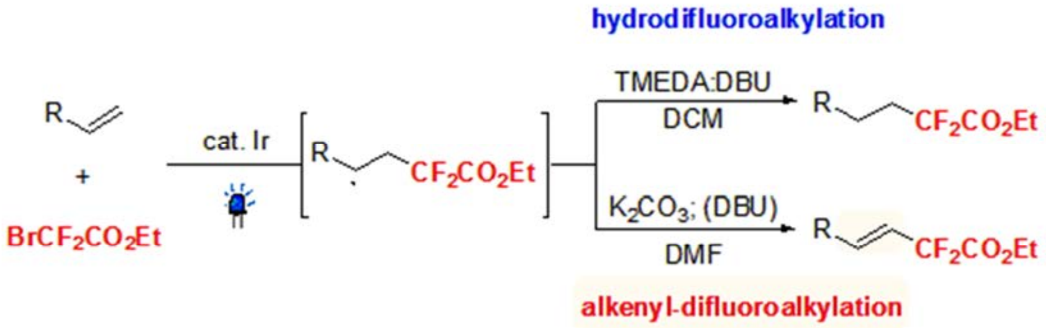
Difluoroalkylations of aromatics and alkenes

유충현 조은진[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Perfluoroalkylated compounds play important role in the pharmaceutical, agrochemical and material sciences. We present environmentally benign difluoroalkylation methods of aromatics and alkenes by visible light-driven photoredox catalysis. A variety of unactivated aromatics, including heteroaromatics, are difluoroalkylated with $BrCF_2CO_2Et$ as the CF_2R source in the presence of *fac*-[Ir(ppy)$_3$] under visible-light irradiation at room temperature. In addition, difluoroalkylated alkanes and alkenes can be produced selectively from unactivated alkenes. The choice of base is crucial in governing the chemoselectivity of the process.





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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-866**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Bassiamide from Cordyceps Bassiana

김기현 이윤미*

광운대학교 화학과

The bassiamide, a novel natural product, was recently isolated from Cordyceps bassiana, which is one of the most important species in traditional Chinese medicine. In order to examine the biological activities such as anti-cancer, anti-inflammatory, and antiviral, we envisioned the synthesis of bassiamide started from 2-hydroxymethyl-1,3-propanediol. Our synthesis involves three key transformations such as the dialkylation of dimethyl malonate, the HWE olefination for the synthesis of an amide intermediate, and N-monoalkylation.

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발표코드: **ORGN.P-867**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Cu-Catalyzed Amine Conjugate Addition to α,β-Unsaturated Olefins

김성철 이윤미*

광운대학교 화학과

Amines are an important moiety in a wide range of biologically active natural products and pharmaceuticals. Although various methods for the preparation of amine compounds have been studied, the direct addition of N-H bond to α, β-unsaturated olefins is one of the most attractive processes in terms of efficiency and atom-economy. Herein, we describe an efficient Cu catalyst system for the conjugate addition reactions of a variety of anilines to activated alkenes, affording the amine compounds with high yields.

일시: 2014년 10월 15~17일(수~금) 3일간
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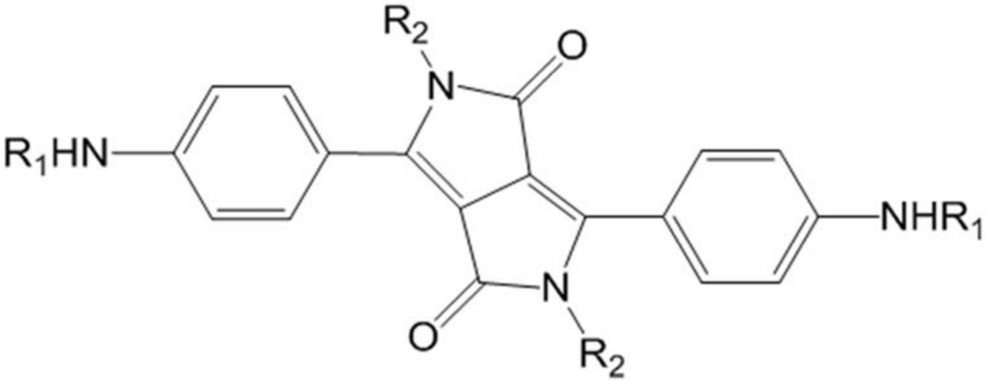
발표코드: **ORGN.P-868**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The Synthesis of 3,6-bis(4-aminophenyl)pyrrolo[3,4-c]pyrrole-1,4-(2H,5H)-diones as pigment Dispersion Synergist

김주영 강용한* 이은영

한양대학교 응용화학과

DPP Pigments were invented in the early 1980’s. These pigments are considered as very important group of synthetic pigments. They are useful in various applications because they have the property of forming numerous colors. This large range of colors is possible due to the simple selection of different constituents on the phenyl rings. The proposal of this research was to synthesize 2,5-dialkyl substituted 3,6-bis(4-aminophenyl)pyrrolo[3,4-c]pyrrole-1,4-(2H,5H)-diones and 3,6-bis(4-acylaminophenyl)pyrrolo[3,4-c]pyrrole-1,4-(2H,5H)-diones.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-869**

발표분야: 유기화학

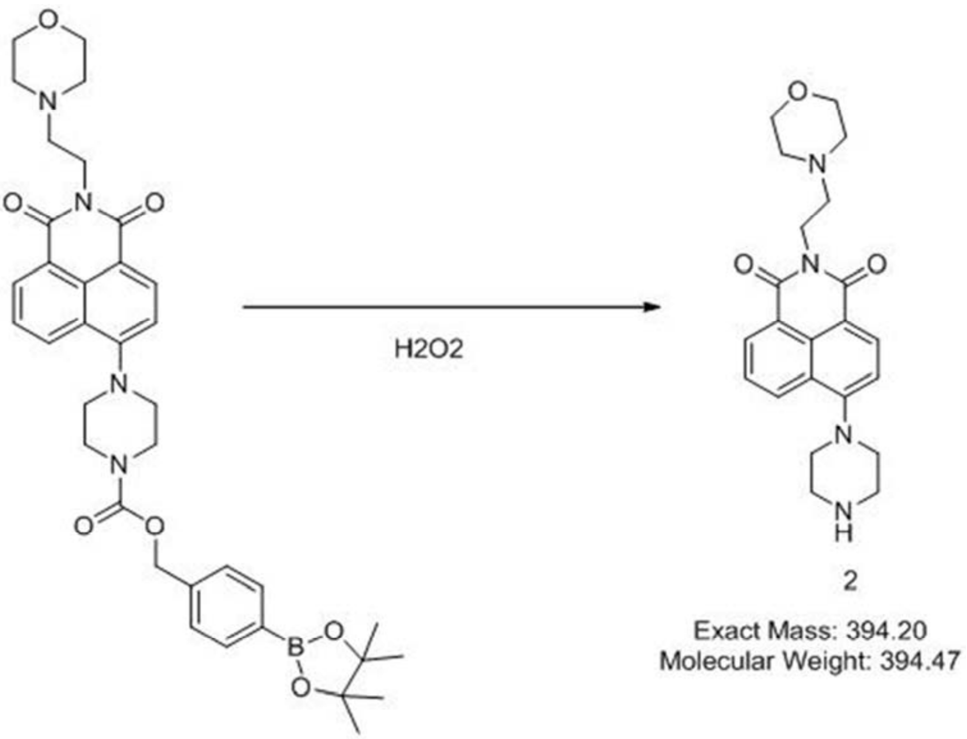
발표종류: 포스터, 발표일시: 수 16:00~19:00

New naphthalimide derivative for detection hydrogen peroxide in living cells

김진아 김다빈[1] 윤주영[2,*]

이화여자대학교 유기화학 [1]이화여자대학교 화학.나노과학과 [2]이화여자대학교 화학·나노과학과

Reactive oxygen species (ROS) play an essential role in many biological processes such as aging and immunity. However, deregulation of ROS production and/or elimination may cause pathophysiological consequences such as aging and chronic inflammatory diseases of the human. Many efforts have been focused on developing selective fluorescent probes to image ROS including H2O2. In the chemical, biological, environmental and medical sciences, detection of hydrogen peroxide (H2O2) is important. Hydrogen peroxide (H2O2) enables lysosome to detect. The cause of disease such as cancer, cardiovascular diseases and storage disorders is related to the lysosome. So, it is important to detect and image the lysosome for understanding of intracellular reaction and mechanisms.Therefore, we designed and synthesized a fluorescent probe for hydrogen peroxide (H2O2) with high sensitivity and selectivity for detection of lysosome. A new probe based on naphthalimide. When hydrogen peroxide was added to 1, probe 1 was converted to 2 and showed fluorescence. This phenomenon easily monitored in live cells. References1. Q. Xu, K. Lee, S. Lee, K. Lee, W. Lee, J. Yoon, J. Am. Chem. Soc. 2013, 135, 9944-99492. Q. Qiao, M. Zhao, H. Lang, D. Mao, J. Cui, Z. Xu, RSC Adv., 2014, 4, 25790-257943. O. S. Wolfbeis, A. Durkop, M. Wu, Z. Lin, Angew. Chem. Int. Ed. 2002, 41, 4495-4498



2
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Molecular Weight: 394.47

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Exact Mass: 654.32
Molecular Weight: 654.56

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-870**

발표분야: 유기화학

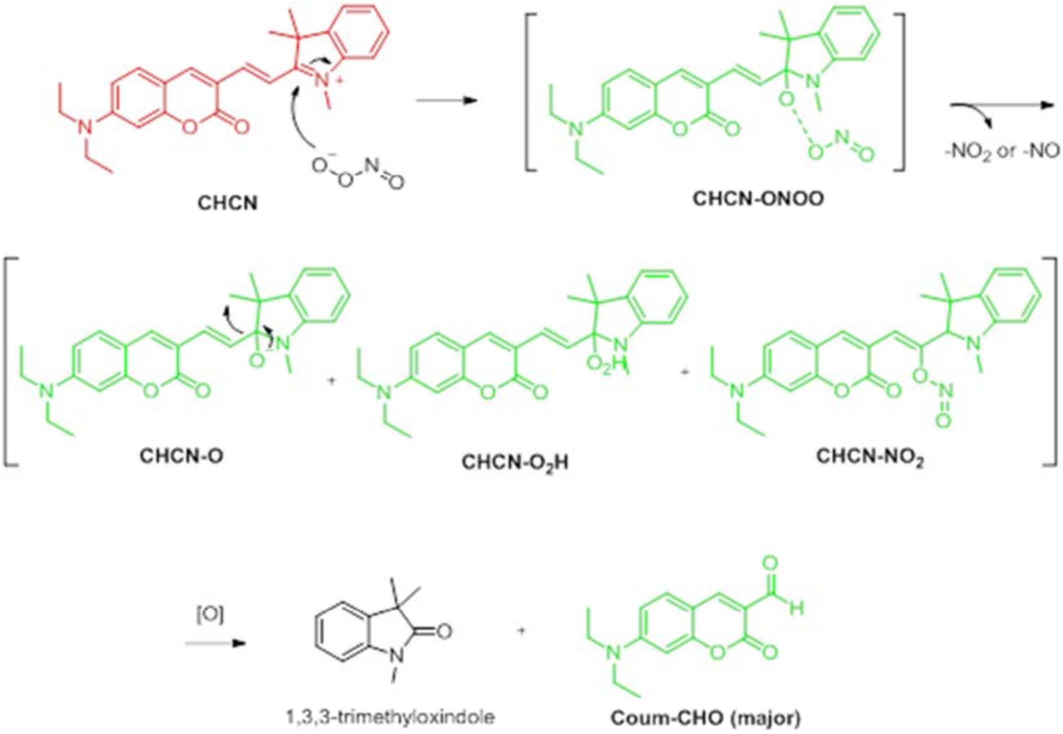
발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of peroxynitrite in a ratiometric and colorimetric manner with high sensitivity and selectivity by using a CHCN probe

백연주 zhouxin[1] 윤주영[2,*]

이화여자대학교 유기화학 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학·나노과학과

Peroxynitrite has a multiple physiological and pathological roles in cellular signaling transduction and cell damage. Therefore, the interest in developing fluorescent probe for selective detection of this reactive oxygen species has been increased these days. The red emitting probe CHCN can dedect ONOO- and CHCN is dissapeared in the presence of ONOO- and be replaced by green emission.ONOO- produced by an oxidation process reacts with CHCN and shows a dual ratiometric and colorimetric response. CHCN has appreciable cell permeability and, as a result, it is applicable to ratiometric detection of exogenous and endogenous ONOO- in living cells during phagocytic immune response. Therefore, We anticipate that, owing to their ideal properties, we can look cell imaging easily and this type of probe will find great use in explorations of the role played by ONOO- in biology. References1. Guo, Z., Park, S., Yoon, J., Shin, I., 2014. Recent progress in the development of near-infrared fluorescent probes for bioimaging applications. Chem Soc Rev 43(1), 16-29.2. Xu, Q., Lee, K.A., Lee, S., Lee, K.M., Lee, W.J., Yoon, J., 2013. A Highly Specific Fluorescent Probe for Hypochlorous Acid and Its Application in Imaging Microbe-Induced HOCl Production. Journal of the American Chemical Society 135(26), 9944-9949.


CHCN
CHCN-ONOO
-NO$_2$ or -NO
CHCN-O
CHCN-O$_2$H
CHCN-NO$_2$
[O]
1,3,3-trimethyloxindole
Coum-CHO (major)

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-871**

발표분야: 유기화학

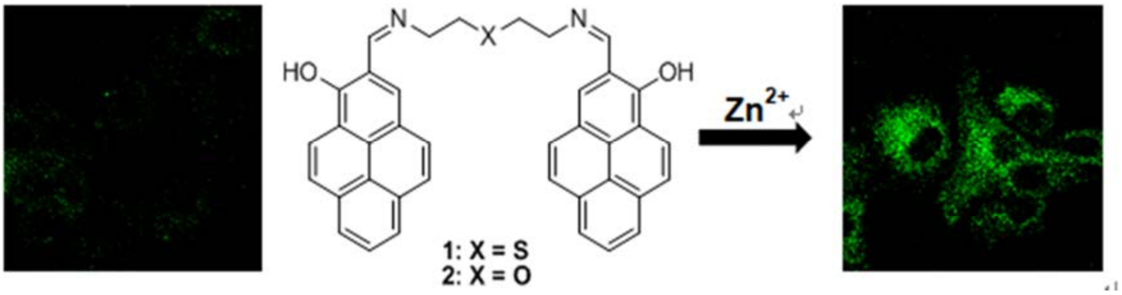
발표종류: 포스터, 발표일시: 수 16:00~19:00

The bispyrene derivatives based fluorescent probes and their bioimaging applications

<u>Hu Ying</u> 윤주영[1,*]

이화여자대학교 화학-나노과학과 [1]이화여자대학교 화학·나노과학과

Two unique pyrene derivatives (1 and 2) are reported as Zn^{2+} selective fluorescent probes, in which two pyrenes bearing imine and OH groups are connected via ether linker (1) or thioether linker (2). Upon the addition of Zn^{2+}, resulting phenolate group can induce internal charge transfer (ICT) peaks, which can cause selective turn-on fluorescence of 1 and 2 at 550 nm. Probes 1 and 2 can successfully image exogenous Zn^{2+} ions as well as free zinc ions released during apoptosis. Also we developed sensor 3-Cu (II) for detection of GSH, Complex 3-Cu (II) senses GSH and give a marked fluorescence enhancement at pH 7.4 under aqueous media. Ref.[1] Y. Hu, Y. F. Liu, G. Kim, K. M. K. Swamy, Y. Kim, S. J. Kim, J. Yoon, Dyes and Pigments. in press; [2] Z. Xu, J. Yoon, D. R. Spring. Chem. Soc. Rev 2010; 39: 1996-2006; [3] Y. Zhou, H. N. Kim, J. Yoon. Bioorg. Med. Chem. Lett 2010; 20: 125-8.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-872**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The fluorescent and colorimetric sensors for carbon dioxide detection activated by anions

이다영 이송이 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

In the present study, we prepared naphthalimide derivatives as CO_2 sensors based on fluoride or cyanide recognition. Among the various anions, these probes showed selective colorimetric and fluorescence changes with F^- or CN^-. Moreover, they can restore their original color and fluorescence after the bubbling of CO_2. In particular, one of our CO_2 sensors detects CO_2 through its reversible sol-gel transition. So these distinct "On-Off-On" changes proved that our probes can be used for this anion-activated CO_2 sensing mechanism.

Reference

1. Zhang, X.; Lee, S.; Liu, Y.; Lee, M.; Yin, J.; Sessler, J, L.; Yoon, J. *Scientific Reports*, 2014, *4*, 4593.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-873**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Detection of $ONOO^-$ by using the boronate-based sugar complex

엄지연 **xu qingling[1] 윤주영[2,*]**

이화여자대학교 화학나노과학부 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학·나노과학과

A water-soluble boronate-based fluorescent probe was used to detect the peroxynitrite($ONOO^-$) in the monosaccharides(eg. D-fructose). When the boronate probe interacts with D-fructose, the fluoroscence intensity increases, but this complex in the presence of $ONOO^-$ has very low intensity. While, ROS/RNS also led to decrease the fluoroscence intensity but decrease less than $ONOO^-$ because of protection by the internal N-B iteraction. The interaction of probe with D-fructose can protect the boronic acid to oxidation by ROS/RNS. So, the boronate-based sugar complex can reacts preferentially with $ONOO^-$. $ONOO^-$ largely influences the cell signaling and apoptosis under physiological conditions.

reference

(1)X. Sun, Q. Xu, G. Kim, S.E.Flower, J. P. Lowe, J. Yoon, J.S. Fossey, X. Qian, S. D. Bull, D. James* "A water-soluble boronate-based fluorescent probe for the selective detection of peroxynitrite imaging in living cells" Chem. Sci. 2014, DOI: 10.1039/c4sc01417k.

(2)Zhang, Q.; Zhu, Z.; Zheng, Y.; Cheng, J.; Zhang, N.; Long, Y. T.; Zheng, J.; Qian, X.; Yang, Y. J. Am. Chem. Soc. 2012, 134, 18479.

(3)Beckman, J. S.; Beckman, T. W.; Chen, J.; Marshall, P. A.; Freeman, B. A. P. Natl. Acad. Sci. 1990, 87, 1620.

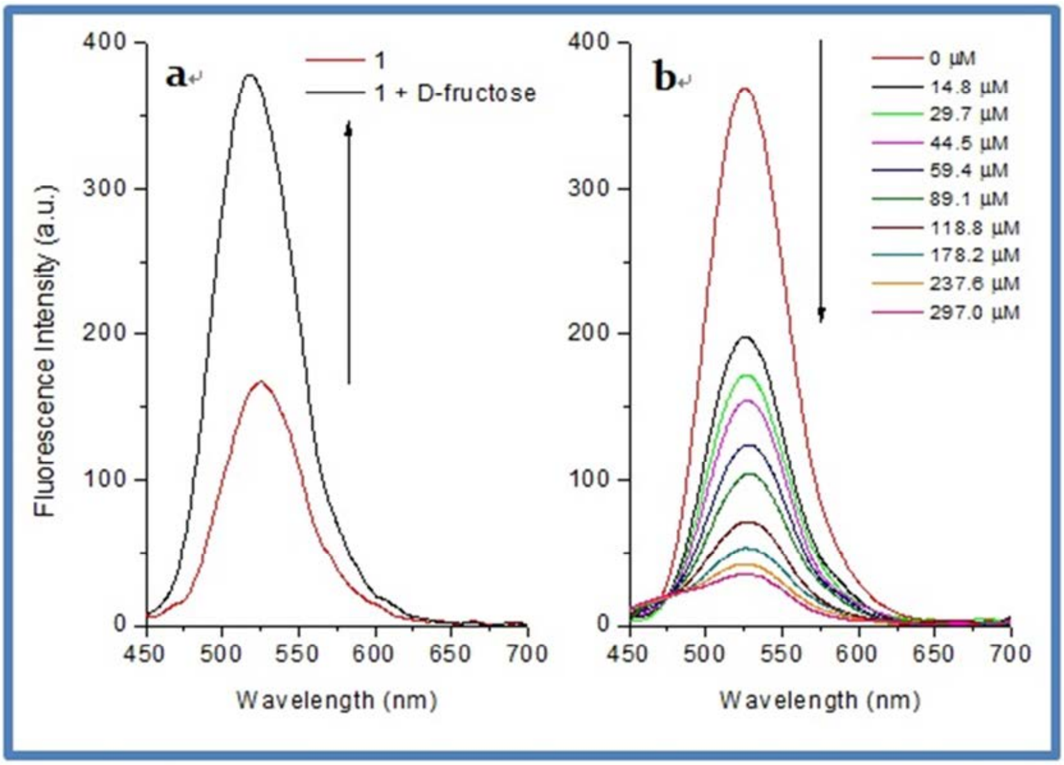


Figure 2. (**a**) Fluorescence spectra of probe **1** (2 μM) and the change on addition of D-fructose (100 mM). After addition of D-fructose, the mixtures were stirred for 10 min; (**b**) Probe **1**-D-fructose complex (probe **1**, 2 μM; D-fructose, 100 mM) with different concentrations of $ONOO^-$. After addition of peroxynitrite, the mixtures were stirred for 5 min. The data was collected in PBS buffer (1/15 M, pH 7.30) with excitation at 410 nm (Ex slit: 5 nm, Em slit: 5 nm).

일시: 2014년 10월 15~17일(수~금) 3일간
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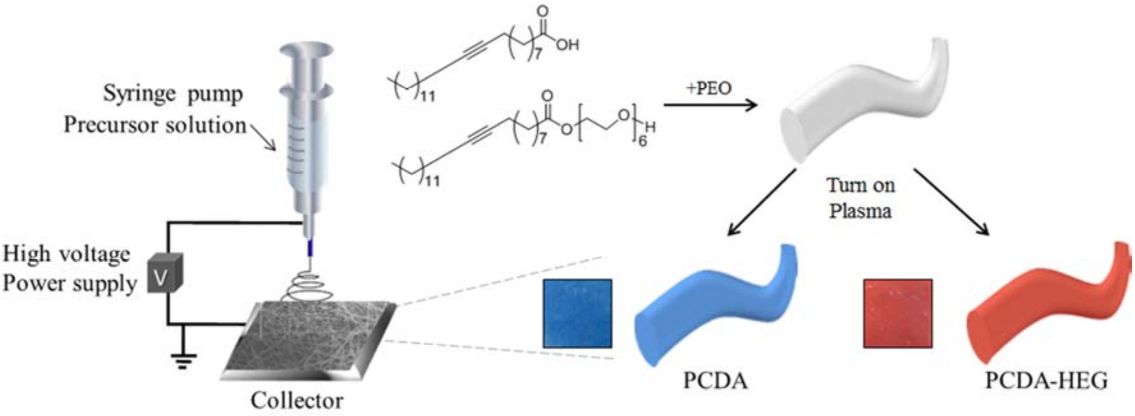
발표코드: **ORGN.P-874**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

An effective strategy to make unconventional polydiacetylenes driven by plasma induced polymerization and application of coloured patterning

이송이 김명화[1,*] 윤주영[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과 [2]이화여자대학교 화학·나노과학과

Polydiacetylene (PDA) polymers show the blue PDAs with 640 nm maximum absorption wavelength, which can display a unique color change to a red with 550 nm maximum absorption wavelength upon environmental stimulation. In addition, red-phase PDAs are fluorescent even though blue-phase PDAs are nonfluorescent, which enables PDAs to be not only colorimetric sensors but also fluorescent sensors. Common stimulations or anayltes have been temperature, pH, metal ions, anions, surfactants, other biologically important molecules, etc.Typically, PDA polymers have been prepared by UV irradiation from self-assembled diacetylene (DA) monomers. Interestingly, it has not been reported that PDAs have been obtained from plasma induced polymerization process so far. However, it should be noticed that since some new types of DAs (diacetylene monomers) would not be appropriate to produce PDA by UV irradiation due to the structural differences of head groups of DA monomers, alternative routes could be carefully considered. For example, a new diacetylene (DA) monomer bearing hexaethylene glycol (HEG) units in this study did not undergo into blue PDAs under UV radiation in both the solution state and embedded fiber. On the other hand, we found out that it was easily polymerized to produce PDAs in the form of pure HEG embedded fibers as well as the mixture fibers between HEG and 10, 12-pentacosadiynoic acid PCDA at even very short exposure of plasma for the first time. (References)S. Lee, Y. Cho, B. U. Ye, J. M. Baik, M. H. Kim, J. Yoon Chem. Commun. 2014, DOI: 10.1039/C4CC03511A S. Lee, J. Lee, M. Lee, Y. K. Cho, J. Baek, J. Kim, S. Park, M. H. Kim, R. Chang, J. Yoon Adv. Funct. Mater. 2014, 24, 3699-3705.


Syringe pump
Precursor solution
High voltage
Power supply
V
Collector
11
7
OH
O
11
7
O
O
O
6
H
+PEO
Turn on
Plasma
PCDA
PCDA-HEG

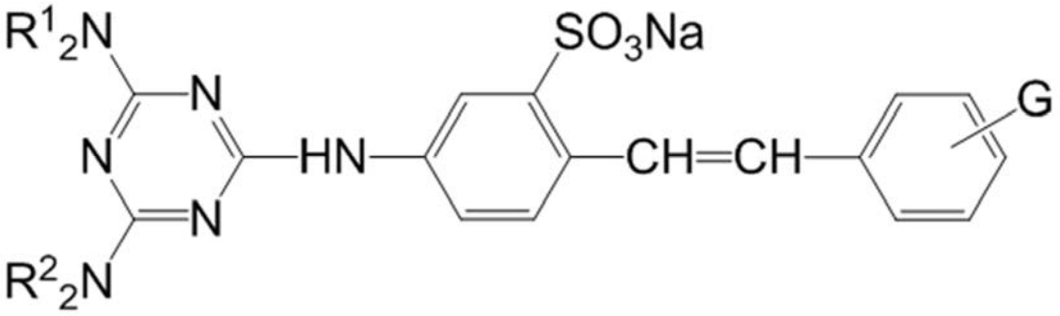
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-875**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Physical Properties of 4-Triazinylaminostilbenes as the Fluorescent Whitening Agents

김성래 강용한* 박나라

한양대학교 응용화학과

Disodium 4,4'-bis(triaznylamino)stilbene-2,2'-disulfonate derivatives are most widely used as fluorescent brighteners for the whitening of both cotton and wool. A typical fluorescent brightener absorbs light in ultraviolet ray (330~380nm) and emits visible blue lights (400~450nm). In this research, a series of non-symmetrically substituted triazinylaminostilbene derivatives were synthesized. For the synthesis of asymmetric stilbene fluorescent brighteners, the key intermediates, sodium 4-amino- stilbene-2-sulfonate derivatives, were prepared by reacting sodium 4-nitrotoluene-2-sulfonate with various aldehydes then followed by the reduction of nitro group. 4-(2,6-Dichloro-1,3,5-triazinyl)-aminostilbene-2-sulfonate was obtained from the reaction of sodium 4-aminostilbene-2-sulfonate derivatives with cyanuric chloride (CNC). Without isolating the intermediate, two remaining chloro groups were substituted with two kinds of amines.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-876**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of a Novel Material Related with OLED

박민주 노영리 강훈민 천민경 송동진 이상경*

경상대학교 화학과

The heterocycle which has eight membered ring was designed and synthesized. The compound was synthesized under Suzuki and Stille coupling reaction condition. The obtained compound was confirmed by FT-IR, 1H-NMR, 13C-NMR spectroscopy. The thermal properties of material were measured by thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). As a result, the material showed good thermal stability. In this presentation, we will report for the development of synthetic method, special optical character and electrochemical properties of the synthesized compound.

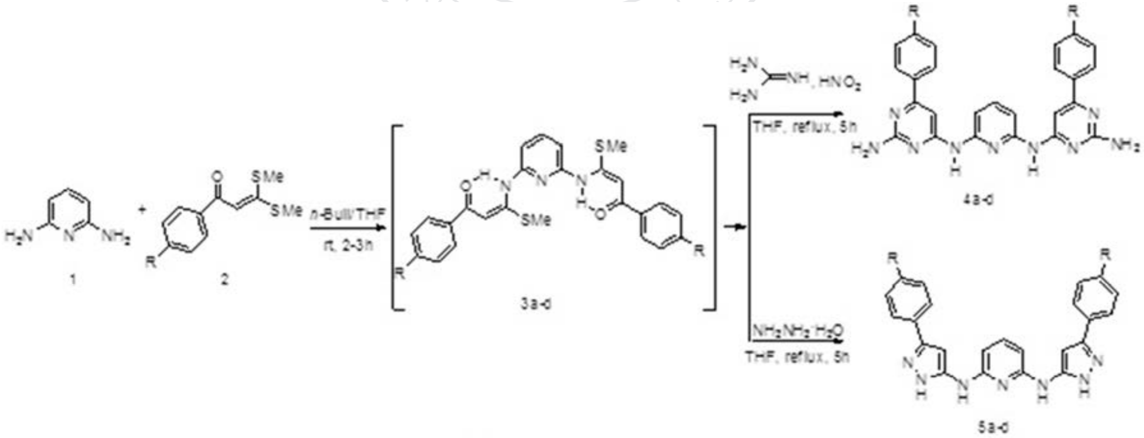
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-877**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Regioselective Synthesis of Polyaza Pyrimidines and Polyaza Pyrazolesunder One-Pot Multicomponent Reaction Conditions

천민경 송동진 강훈민 박민주 이상경*

경상대학교 화학과

Convenient methods of synthesis of novel polyaza pyrimidines and polyaza pyrazoles have been described in this report. The synthetic method is based on one-pot, three-component cyclocondensation of α-oxoketene dithioacetals, 2,6-diaminopyridine, and guanidine/hydrazine. Polyaza S,N-acetals have been generated in situby treating α-oxoketene dithioacetals with 2,6-diaminopyridine in the presence of n-butyllitium, which were subsequently treated with guanidine nitrate and hydrazine hydrate to afford polyaza pyridines and polyaza pyrazoles, respectively.



[2,3,4,5] a, R=H; b, R=Cl; c, R=Me; d, R=MeO

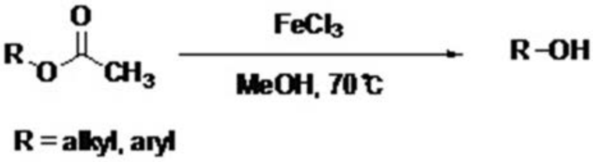
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-878**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A mild and efficient deacetylation using $FeCl_3$ as a catalyst under neutral condition

김상현 윤태일 전흥배*

광운대학교 화학과

A number of methodologies for the deacetylation have been reported, because the deacetylation is one of the most popular reactions in the protection-deprotection area of organic synthesis. However, many of those were performed under basic or acidic conditions. We recently have studied the reactions of various acetates with $FeCl_3$ as a catalyst. As a result, we could obtain the corresponding alcohols in excellent yields (>90%) when alkyl and aryl acetates were treated with 10 mol% $FeCl_3$ in methanol at 70℃. This protocol should be a very useful reaction in organic synthesis because of the easy operation, mild condition, and high generality of substrates.



일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-879**

발표분야: 유기화학

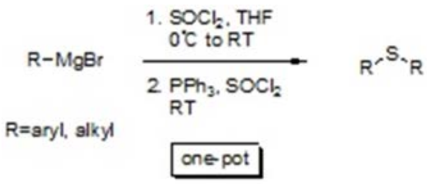
발표종류: 포스터, 발표일시: 수 16:00~19:00

An efficient diaryl and dialkyl sulfides using Grignard reagents and $SOCl_2$

정희선 전홍배*

광운대학교 화학과

Because of the valuable applications in the field of synthetic organic chemistry, a number of methodologies have been studied for the synthesis of organic sulfur compounds. Recently, we have studied the reaction using Grignard reagents and thionyl chloride for the synthesis of dialkyl sulfides or diaryl sulfides. A variety of Grignard reagents were treated with thionyl chloride in THF at 0℃ to room temperature to yield sulfoxides, which were reacted with triphenylphosphine and additional thionyl chloride in THF at room temperature in one-pot. As a result, we could obtain the symmetrical dialkyl sulfides or diaryl sulfides in good yields. This protocol should be a very useful reaction in organic synthesis because of the easy operation and mild condition.



일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-880**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative Iminium Catalysis/1,5-Hydride Transfer/Cyclization Sequences: Enantioselective Synthesis of Ring-Fused Tetrahydroquinolines

서창원 김대영*

순천향대학교 화학과

The development of C-C bond formation via C-H bond activation has become an area of intense interest in synthetic organic chemistry. Such reactions offer practical methods for the construction of structurally complex and biologically active organic molecules with atom- and step economy. The first organocatalytic enantioselective intramolecular oxidative iminium catalysis and 1,5-hydride transfer/ring closure reaction is described. The feature of this research is a one-pot transformation of 3-arylprop-2-en-1-ol derivatives into tetrahydroquinolines using environmentally benign Ru(VII)-catalyzed aerobic oxidation and highly efficient internal redox reactions. The ring-fused tetrahydroquinoline derivatives were obtained in high enantioselctivities.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-881**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric Synthesis of Tetrahydroquinolines via Saegusa-type Oxidative Enamine Catalysis/1,5-Hydride Transfer/Cyclization Sequences

서창원 김대영*

순천향대학교 화학과

Enantioselective organocatalytic synthesis of tetrahydroquinolines has been achieved via Saegusa-type oxidative enamine catalysis/1,5-hydride transfer/cyclization sequences. The feature of this research is a one-pot transformation of 3-arylaldehydes into tetrahydroquinolines using environmentally benign catalytic Saegusa oxidation and highly efficient internal redox reactions. The synthetically useful tetrahydroquinoline derivatives were obtained in moderate yields and high levels of enantioselecitities.

일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-882**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enantioselective conjugate addition of 3-fluorooxindoles to vinyl sulfone: an organocatalytic access to chiral 3-fluoro-3-substituted oxindoles

김이슬 김대영*

순천향대학교 화학과

Oxindoles are widely present in natural products and bioactive molecules, and oxindoles bearing a 3-fluorinatedquaternary stereogenic center are structural motifs that have important applications in the pharmaceutical industry. We wish to report an organocatalytic conjugate addition of prochiral 3-fluorinated oxindoles to vinyl sulfones. In the presence of bifunctional tertiary amine-thiourea catalysts, 3-fluoro-3-substituted oxindole adducts were obtained in excellent yields and with high enantiomeric excesses.

일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **ORGN.P-883**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Asymmetric Synthesis of 3-Chlorooxindoles Bearing AdjacentQuaternary-Tertiary Centers

정현정 김대영*

순천향대학교 화학과

Oxindoles bearing a chiral quaternary center at C3 make up the core of many natural products and pharmaceuticals. These compounds are used as building blocks in alkaloid synthesis and, in many cases, as starting materials in medicinal chemistry. In this presentation, we wish to report a novel methodology for the synthesis of 3,3-disubstituted 3-chlorooxindoles via a conjugated addition of 3-chlorooxindoles to nitroolefins under organocatalytic conditions. High levels of diastereoselectivity and enantioselectivity were observed, with the high yields. Both electron-donating and electron-withdrawing groups were well tolerated at the aromatic ring of nitroalkenes as well as the heteroaromatic substituents.

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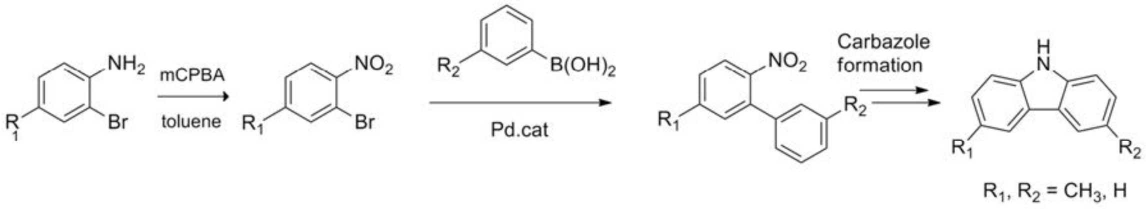
발표코드: **ORGN.P-884**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of carbazoles using heterogeneous Pd catalyst on reverse phase silica gel in water : Key intermediate of carbazole derivatives for OLED

백정현 shabbir saira 반재영[1] 이학준*

한양대학교 응용화학과 [1]한양대학교 과학기술대학 / 응용화학과

Carbazole derivatives are widely used for Organic Light-Emitting Diode. Typical key intermediates of carbazole derivatives are expensive. In this study, We tried to synthesize carbazoles efficiently using heterogeneous Pd catalyst on reverse phase silica gel in water.



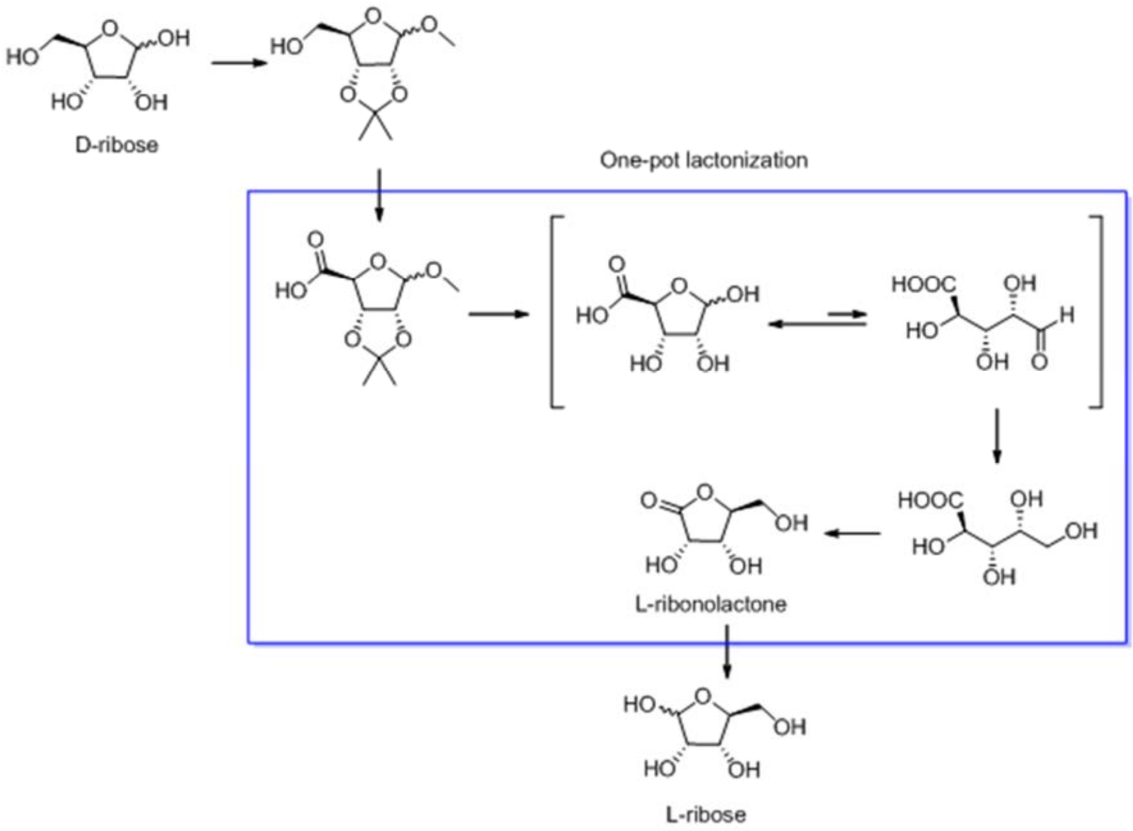
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-885**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of L-ribose from D-ribose by One-pot lactonization

반재영 안현석[1] 이학준[2,*]

한양대학교 과학기술대학 / 응용화학과 [1]한양대학교 바이오나노학과 [2]한양대학교 응용화학과

L-ribose can be used for the synthesis of L-nucleosides as a potent antiviral material. Therefore, there is a need for the development of more efficient methods of L-ribose synthesis. We demonstrated the synthetic method for the preparation of L-ribose from D-ribose using cheaper reagents and mild reaction conditions in overall four steps including one-pot lactonization as a key step.


D-ribose
One-pot lactonization
L-ribonolactone
L-ribose
HOOC
OH
HO
H

일시: 2014년 10월 15~17일(수~금) 3일간
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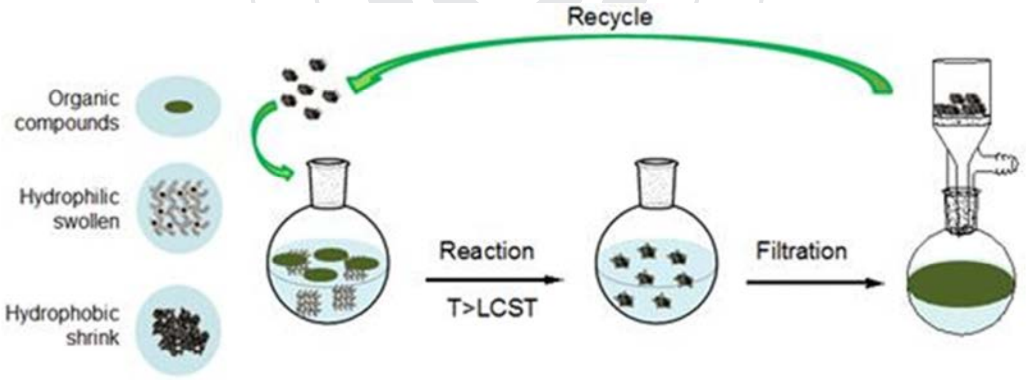
발표코드: **ORGN.P-886**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

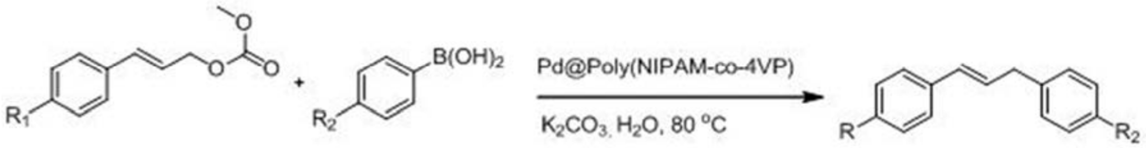
Pd Catalyst Immobilized on PNIPAM-co-4-VP Hydrogel : Carbon-Carbon Coupling Reaction of Allylic carbonate in Water

이용우 안현석 이신영 이영은 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

We present here the Tsuji-Trost reaction with various allylic carbonates and aryl boronic acids using reusuable Pd catalyst in water. Pd catalyst on poly(NIPAM-co-4-VP) hydrogel was prepared and characterized by XPS, ICP-MS, DSC, etc. The catalyst showed excellent reactivity and recyclability.





일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-887**
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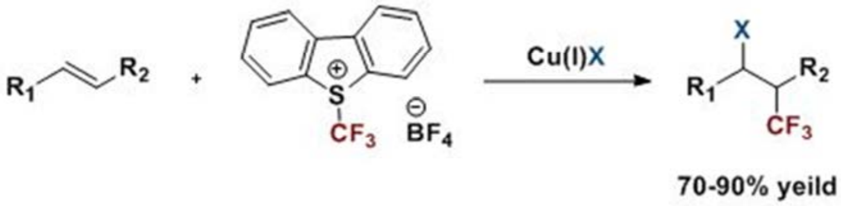
발표종류: 포스터, 발표일시: 수 16:00~19:00

Copper(I) mediated trifluoromethyl-halogenation of alkenes

하늘

과학기술연합대학원대학교(UST) 의약및약품화학과

A highly practical reaction for the trifluoromethyl-halogenation of alkene has been developed with copper(I) halide. Formation of C-CF3 bond could be enhanced lipophilicity and bioavailability in vivo and the substituted halogen is feasible to further modification. In the presence of Copper(I) halide and Umemoto’s reagent, an addition reaction was conducted to introduce halogen and CF3 group. Copper(I) halide can be used as a source of halogenation and handled it easily. This methodology provides variety of trifluoromethyl-halogenated alkenes.



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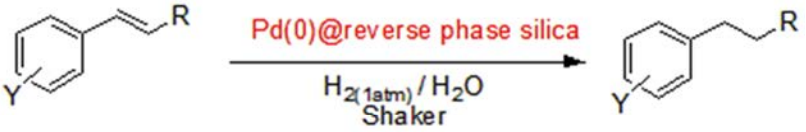
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-888**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Green Hydrogenation Reaction in Water Using Pd on Reverse Phase Silica Gel

이신영 고성현[1] 이학준[1,*] 안현석

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Reverse phase catalyst system was developed for hydrogenation reactions in water. The catalyst was synthesized by anchoring 2,2'-bipyridine-4,4'-dicarboxylic acid ligand on commercially available 3-aminopropyl-functionalized silica gel, followed by Pd metal dispersion. Reactivity of these catalysts was tested for hydrogenation of various aryl substituted α,β-unsaturated carbonyl compounds in aqueous medium under a hydrogen atmosphere (1 atm). The reverse phase silica catalyst has the advantages of excellent yields and catalyst recyclability.



Y = -H, $-CH_3$, -OH, $-OCH_3$
R = -COOH, $-CH_3C(COOH)$, $-COOCH_3$, $-CH_2OH$, -CHO

일시: 2014년 10월 15~17일(수~금) 3일간

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발표코드: **ORGN.P-889**

발표분야: 유기화학

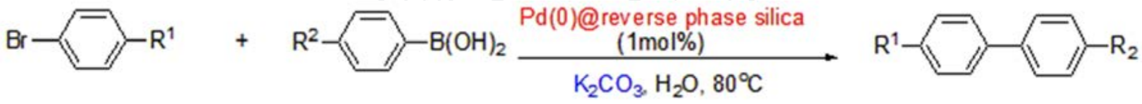
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of an Efficient Pd catalyst on Reverse Phase Silica Gel for Green Chemistry: The Suzuki-Miyaura Cross Coupling Reaction in Water

이신영 이학준[1,*] 안현석

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

We prepared an efficient heterogeneous palladium catalyst in accordance with green chemistry using reverse phase silica gel. The catalyst was characterized by XPS, ICP-MS, TEM, etc. Using the catalyst, we got excellent yield and recyclability for the Suzuki-Miyaura cross coupling reaction in water. Catalytic activity was improved by the nonpolar interactions between the reverse phase silica gel and organic reagents in water.



R_1= -H, -NH_2, -OH, -OCH_3, -CH_3, -NO_2, -CN, -CO_2CH_3,-$COCH_3$, -CHO,

R_2= -H, -CH_3, -OCH_3, -Cl, -NO_2, -CO_2CH_3

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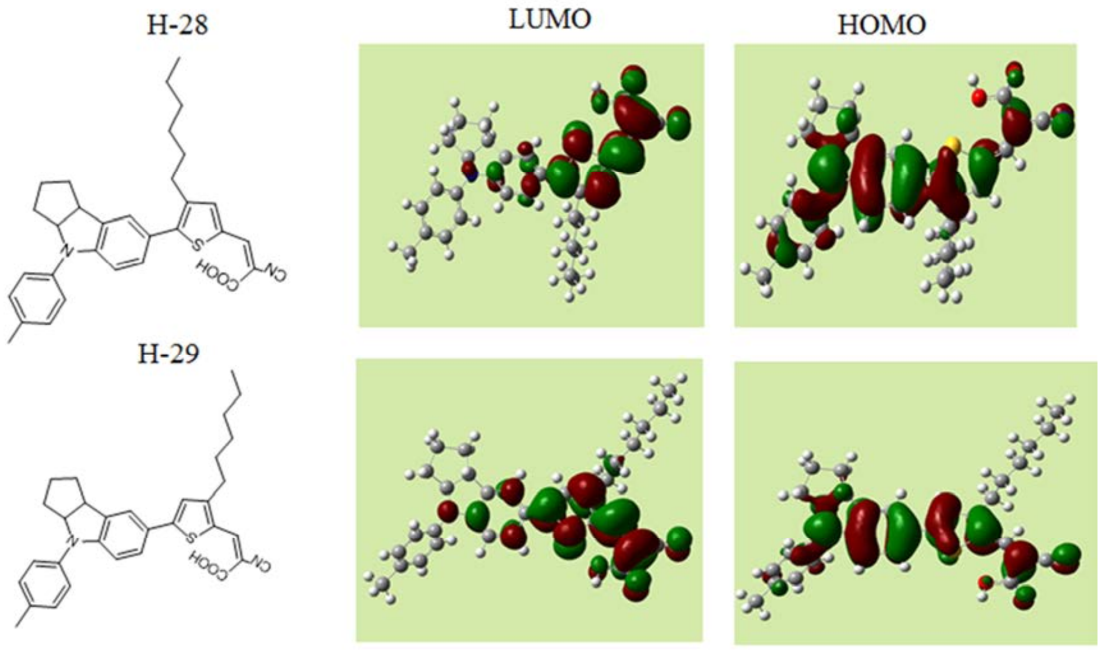
발표코드: **ORGN.P-890**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

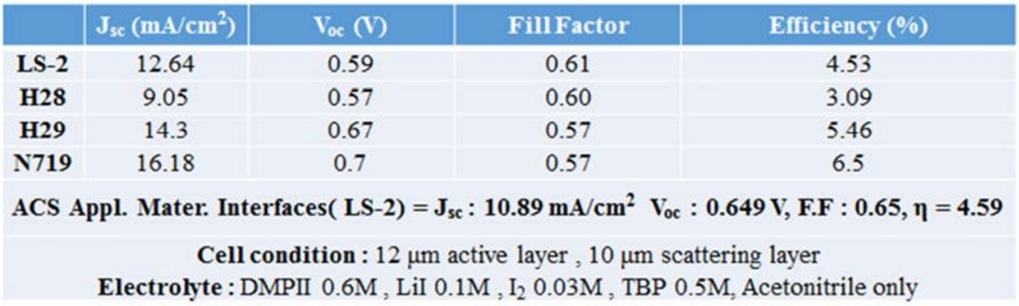
Molecular Engineering of Indoline Based Organic Sensitizers Using Hexyl Thiophene

김광명 홍종인*

서울대학교 화학부

Dye-sensitized solar cells (DSSCs) are under intensive investigation because of the cost-effectiveness and flexibility of devices. In 1999, such cells employing ruthenium complexes as sensitizers have achieved power conversion efficiency (η) over 11% under standard global air mass of 1.5.Meanwhile, metal-free organic dyes, usually with an electron donor?π bridge?electron acceptor (D? π ?A) configuration, have been actively pursued due to low material costs, easy synthesis, high molar extinction coefficients, and environmental friendly materials with respect to classical ruthenium dyes.In the past decade, many kinds of organic dyes with such configuration have been explored for DSSCs. It has been well known that one can improve device performance of DSSCs by facilitating electron injection and suppressing charge recombination. This can be done by controlling the assembly morphology of sensitizers on the TiO2 surface. Introduction of alkyl chains to the dye skeleton based on thiophene or its derivative has proved to be an effective method to improve the DSSC performance since they can not only prevent dye aggregation but also diminish the charge recombination between electrons and electron acceptors in the electrolyte.Herein, we report the design and synthesis of two new organic dyes with n-hexyl (H28 and H29) substituted at the spacer part, and their use as sensitizers in DSSCs. Compared to H28 (with alkyl chains at the acceptor position of dye), the JSC of H29 (with alkyl chains at the donor position of dye) was enhanced significantly from 9.05 to 14.3 mA cm?2, and VOC also increased from 570 to 670 mV due to the position of the incorporated alkyl chains. Details on the difference in the device performance between H28 and H29 will be discussed from the structural viewpoint.





	J_{sc} (mA/cm^2)	V_{oc} (V)	Fill Factor	Efficiency (%)
LS-2	12.64	0.59	0.61	4.53
H28	9.05	0.57	0.60	3.09
H29	14.3	0.67	0.57	5.46
N719	16.18	0.7	0.57	6.5

ACS Appl. Mater. Interfaces(LS-2) = J_{sc} : 10.89 mA/cm^2 V_{oc} : 0.649 V, F.F : 0.65, η = 4.59

Cell condition : 12 μm active layer , 10 μm scattering layer
Electrolyte : DMPII 0.6M , LiI 0.1M , I_2 0.03M , TBP 0.5M, Acetonitrile only

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발표코드: **ORGN.P-891**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Properties of Conjugated Polymers utilizing Tetrafluorophenylene for Organic Photovoltaics

한가람 서홍석*

부산대학교 화학과

Recently fluorinated polymers have clearly demonstrated improved short circuit current (Jsc) and fill factor (FF) in BHJ devices in comparison with those of the nonfluorinated polymer-based devices. To study more these effects, we introduced 1,4-dibromotetra-fluorobenzene unit, which is a new strong electron withdrawing unit, adjacent to a electron rich unit. We synthesized new conjugated polymers utilizing tetrafluorophenylene; HS-5477, HS-5478, HS-5479, and HS-5480 by Suzuki and Stille polymerization. The UV-vis absorption onset of four polymers was at around 700 nm and their optical band gaps were about 1.60 eV. HOMO energy levels of four polymers were at around 5.5 eV, and their LUMO energy levels were at about -3.8 eV, corresponding to the electrochemical band gap of around 1.6 eV. Among these polymers, HS-5480 showed the greatest device performance with Voc of 0.71 V, Jsc of 8.68 mA/cm2 and FF of 0.44, giving the power conversion efficiency of 2.71%.

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발표코드: **ORGN.P-892**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Photovoltaic properties of novel electron deficient unit 2,2-bithiophene-3,3-dicarboximide-based D?A type copolymer

한가람 서홍석*

부산대학교 화학과

The novel electron deficient moiety unit, 4H-dithieno[3,2-c:2’,3’-e]azepine-4,6(5H)-dione, was utilized and prepared for the synthesis of the conjugated alternating polymers containing electron Donor and Acceptor (D-A) pair for Bulk Heterojunction (BHJ) solar cells. The dithienoazepinedione, bithiophene imide (BTI) group, is a stylish electron deficient unit as it demonstrates strong electron-withdrawing disposition, and planar structural design. The polymer with benzodithiophene(BDT) unit and linear dodecyl-BTI unit substituted with 2-octyldodecyl side chain was synthesized using Stille polymerization to construct P1. The novel polymer P2 was synthesized by Suzuki polymerization of carbazole, thiophene as electron rich units, and linear octyl-BTI unit as electron deficient unit to increase conjugation length. Both polymers exhibited thermal stability with glass transition temperature and excellent solubility. The spectra of P1 and P2 solid films show absorption bands with maximum peaks at P1:395, 538 P2:380, 491 nm and the absorption onsets by 652 and 634 nm, akin to band gaps of 1.90 eV, 1.96 eV, likewise. The best device with P1: PC71BM in ODCB with 2% DIO showed VOC of 0.97 V, JSC of 3.06 mA/cm2, and FF of 0.49, which yielded PCE of 1.49%. and the P2:PC71PM (1:2) showed VOC of 0.84 V, JSC of 2.48 mA/cm2, and FF of 0.36, which yielded PCE of 0.76%

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발표코드: **ORGN.P-893**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Newly Synthesized Conjugated Polymers using Tetrafluorophenylene for Organic Solar Cells

한가람 서홍석*

부산대학교 화학과

In recent years, bulk hetero-junction organic solar cells have been studied because lightweight, low-cost, solution-processability and flexibility. In this literature, our group demonstrate strong electron withdrawing units on an electron-deficient backbone based on 1,4-dibromotetrafluorobenzene unit. Recently our group has synthesized a copolymer which exhibit strong electron-withdrawing character, a planar architecture, and high solubility. In this work, tetrafluorophenylene unit was used in order to construct copolymers for organic photovoltaics and it exhibited large electron and hole mobilities. Tetrafluorophenlene unit has more advantage of decreasing steric encumberance than other acceptor units. Benzodithiophene (BDT) and dithieno-benzodithiophene (BDTT) were selected here as the initial donor monomers because those have high solubilizing characteristics, low-bandgap. Moreover, the fluorine affects morphology resulting blends of polymer donors and fullerene acceptors that are regarded as key requisite determining the PCE of the OPV devices. In conclusion, this polymer that have highest performance showed VOC of 0.75 V, a JSC of 11.80 mA/cm2, and FF of 0.59, giving the PCE 5.22%.

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발표코드: **ORGN.P-894**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Small molecules are made of phenanthrothiadiazole, benzimidazole and benzodithiophene for bulk heterojunction photovoltaic cells

한가람 서홍석*

부산대학교 화학과

Recently, bithiophenes are known a center aromatic ring was chosen as a subject, because the planar benzodithiophene (BDT) unit has made π-π stacking which is good for improving mobility, and the thiophenes display weaker steric hindrance and lead to smaller dihedral angles with neighboring monomers. A new D-A small molecules having benzodithiophene as the electron rich units have synthesized in organic solar cells with phenanthrothiadiazole (PT) by an electron deficient units. The DBDTPT (HS-5465) and DBDTMBI (HS-5483) were synthesized using Stille coupling reaction and estimated in OPVs. The band gaps of DBDTPT and DBDTMBI are shown 361 nm and 603 nm, respectively. HOMO and LUMO of DBDTPT and DBDTMBI were presented at -5.46 eV,-3.65 eV and -5.84 eV and -3.84 eV . The small molecules have good thermal stability. The device including DBDTMBI with PCBM (3:7) displayed a PCE value of 0.28%.

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발표코드: **ORGN.P-895**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of alkoxy-MBI containing for photovoltaic application

한가람 서홍석*

부산대학교 화학과

A novel electron-deficient unit, PTDOMBI have been designed and synthesized with thiophene and carbazole to Stille and Suzuki polymerization. DOMBI unit, the sulfur at 2-position of BT unit was changed with dialkyl replaced carbon and dioctyloxy groups were established at 5,6-position of MBI unit. DOMBI is still continue to progress 1,2-quinoid type with two alkyl groups on the carbon which replaced the sulfur of BT. Additionally, dioctyloxy groups on 5,6-position will advance the absorption at the longer wavelength region. We demonstrated that PTDOMBI thin films showed broad absorption region from 350 to 800 nm. The absorption maximum onset at 775 nm in the range for optical band gap of 1.60 eV. The devices comprising PTDOMBI with PC71BM exhibited VOC of 0.58 V, JSC of 4.03 mA/cm2, FF of 0.32 and resulted power conversion efficiency of 0.76%.

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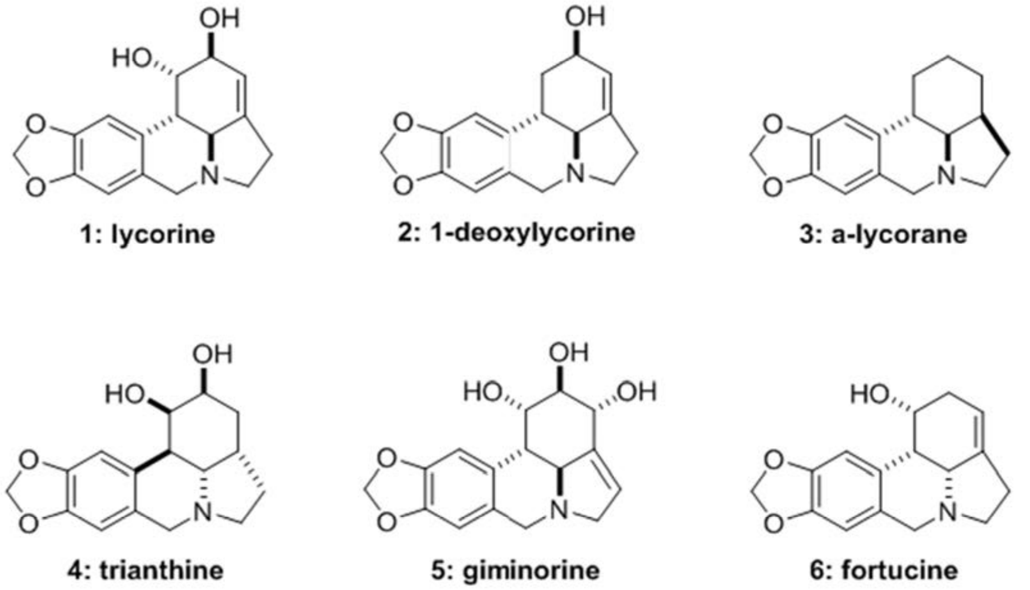
발표코드: **ORGN.P-896**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total synthesis of (±)-lycorine via Diels - Alder reaction of3,5-dibromo-2-pyrone

신형섭 박용규 조천규*

한양대학교 화학과

Lycorine (1) is a toxic crystalline alkaloid present in various amaryllidaceae plant species that include lycoris, pancratium, narcissus, galanthus, zephyanthes, and haemanthus. Arising from norbelladine in its biosynthesis, lycorine has the pyrrolo[*de*]phenanthridine framework that is common to many other congeneric natural compounds (Figure 1). It has a wide variety of important biological activities range from 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 is our path-finding effort that affords the eventual synthesis of (±)-lycorine.



1: lycorine

2: 1-deoxylycorine

3: a-lycorane

4: trianthine

5: giminorine

6: fortucine

Figure 1. pyrrolo[de]phenanthridine-type natural alkaloids.

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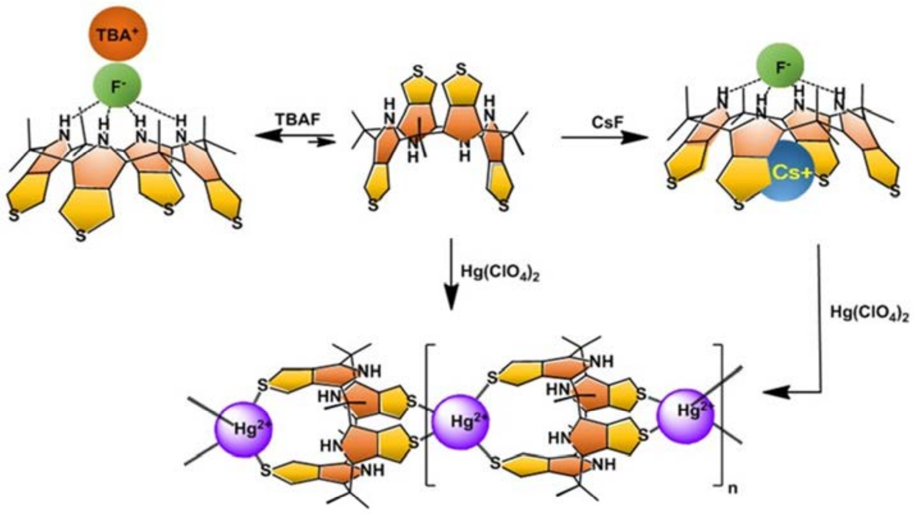
발표코드: **ORGN.P-897**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Calix[4]pyrrole-Based Amphiphilic Receptor Displaying Split Personality For Ion Recognition

이창희* **SAHAINDRAJIT**

강원대학교 화학과

Calix[4]pyrroles which are fused with tetrahydrothiophene have been synthesized and characterized. The ion binding study of the synthesized hosts displayed very interesting properties. The deep cavity, cation binding pocket which was created by anion binding shows different selectivity depending on the nature of applied cations. For example, the cone conformation resulting upon the pre-complexation with fluoride anion, forms stable ion-pair complex with cesium cation. The cesium cation is thought to be bound to the deep inside the cavity by cation-pi interaction. On the other hand, the mercury(II) ion form stable donor-acceptor complex with the sulfur atom. The ion binding studies confirmed that the synthesized receptors form stable complexes with various metal salts in organic media. The binding affinities and spectroscopic changes upon ion binding will be presented.



TBA+
F-
TBAF
CsF
Cs+
Hg(ClO4)2
Hg(ClO4)2
Hg2+
NH
HN
S
n

일시: 2014년 10월 15~17일(수~금) 3일간
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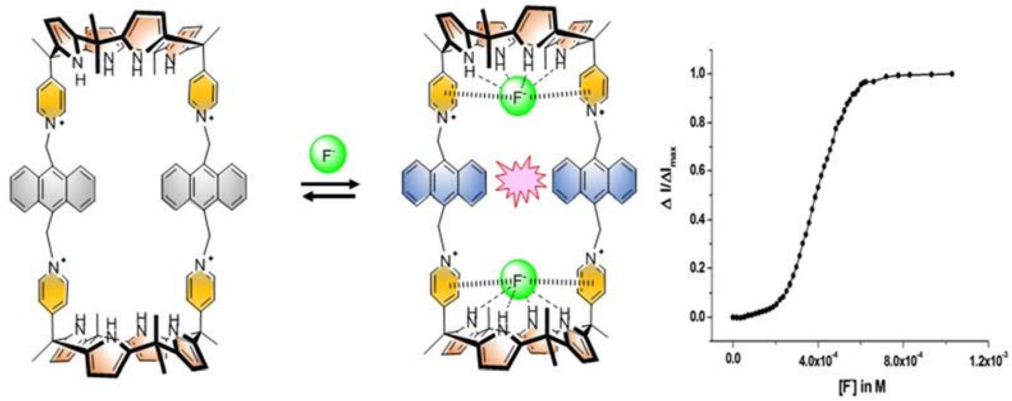
발표코드: **ORGN.P-898**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Turn-on Type, Non-Linear Allosteric Regulation of Anion Binding by Tetracationic Calix[4]pyrrole Homodimer

이창희* **SAHAINDRAJIT**

강원대학교 화학과

A covalently coupled, capsular tetra-cationic calix[4]pyrrole bearing fluorescent anthracene linkers has been synthesized and characterized. The designed receptor displayed exclusive binding with fluoride anion accompanying with large enhancement of fluorescence. The two identical binding sites which are suitable in accommodation of fluoride anions exhibit highly cooperative binding property. The receptor displayed exceptionally high affinity toward the fluoride anion due to the allosteric binding behaviour. The clean sigmoidal binding isotherm clearly indicate the positive allosteric binding of the designed host.



N
H
N·
F⁻
Δ I/ΔI$_{max}$
1.0
0.8
0.6
0.4
0.2
0.0
0.0
4.0x10⁻⁴
8.0x10⁻⁴
1.2x10⁻³
[F] in M

일시: 2014년 10월 15~17일(수~금) 3일간

장소: 광주 김대중컨벤션센터

발표코드: **ORGN.P-899**

발표분야: 유기화학

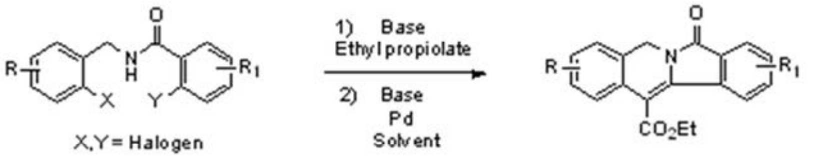
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic study of isoindolinone anuulation using Micheal-Heck-reaction intramolecular cyclization

이복진 홍길표 김건철*

충남대학교 화학과

The stydy of isoindolinone anuulation was accomplished in a sequence reaction based on the tandem Heck reaction. In this process, Micheal-Heck-Heck reaction follwed by cyclization was attempted to synthesize the fused isoindolinone derivative.



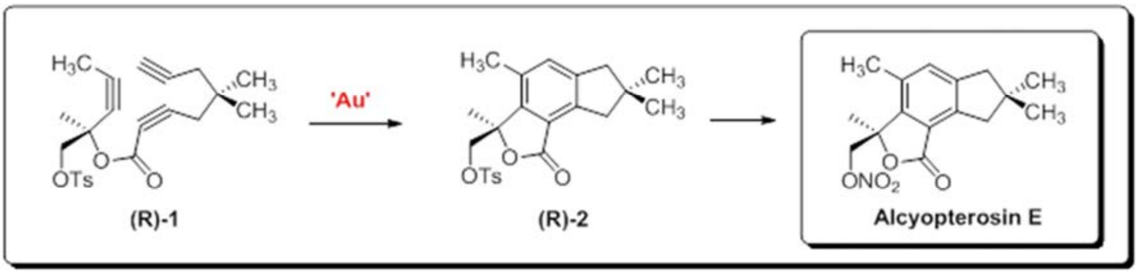
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-900**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total synthesis of the marine illudalane sesquiterpenoid alcyopterosin E

유진 오창호*

한양대학교 화학과

The central six-membered ring unit in the illudalane sesquiterpene is attractive targets in natural product synthesis. The alcyopterosins is a unique set of marine illudalanes isolated from the sub-Antartic deep sea soft coral Alcyonium paessleri. Among these, alcyopterosin E showed cytotoxicity toward the human larynx carcinoma cell line. This compound can be synthesis by the intramolecular version of the transition metal-catalyzed [2+2+2] alkyne cycloaddition. The synthesis of (R)-1 started with the syntheses of diyne acid and propargylic alcohol. After gold-catalyzed intramolecular [2+2+2] cycloaddition, it is formed the tricycle core (R)-2. Finally, synthesis of alcyopterosin E was completed by nucleophilic displacement of the tosyl against a nitrate ester functionality.



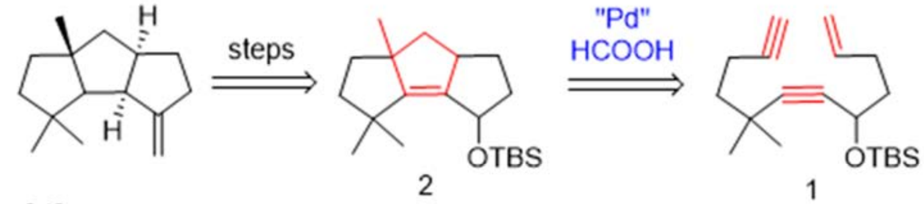
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-901**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Total synthesis of Triquinane Natural Products : Use of Pd-Catalyzed Cycloreduction

고은비 오창호*

한양대학교 화학과

Pd-catalyzed cycloreduction of enediynes affording the [m,5,n]-tricyclic compounds indeed proceeds with high levels of chemo- and stereo-selectivities. And Pd-catalyzed cycloreduction of enediynes is accompanied by a significant increase in structural complexity. Many alcohol derivatives of Capnellene have demonstrated potential as a chemotherapeutic agent with antibacterial, anti-inflammatory and anti-tumor properties. Because of these reasons, capnellene has been targeted for synthesis by numerous investigators. We used this method to synthesize triquinane natural product, (±)-Ceratopicanol and we are applying this enediyne cycloreduction method to $\Delta^{9,12}$-capnellene synthesis. Our synthesis involves Pd-catalyzed cycloreduction of enediyne 1 in order to construct the tricyclic framework 2.



$\Delta^{9,12}$-Capnellene

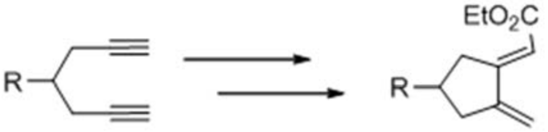
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-902**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed cycloaddition of hepta-1,6-diyne

오부근 오창호*

한양대학교 화학과

The development of efficient cyclization for 5-membered carbocycles has been a major challenge in organic synthesis due to a variety of biologically active natural products. In previous researches, palladium-catalyzed cycloadditions of various substrates such as 1,6-diene, 5-allen-1-ynes and haloene-ynes have been accomplished for 5-membered ring formation by each unique condition. Herein, we have developed the palladium-catalyzed cyclizations of hepta-1,6-diyne by using a catalytic amount of additives.



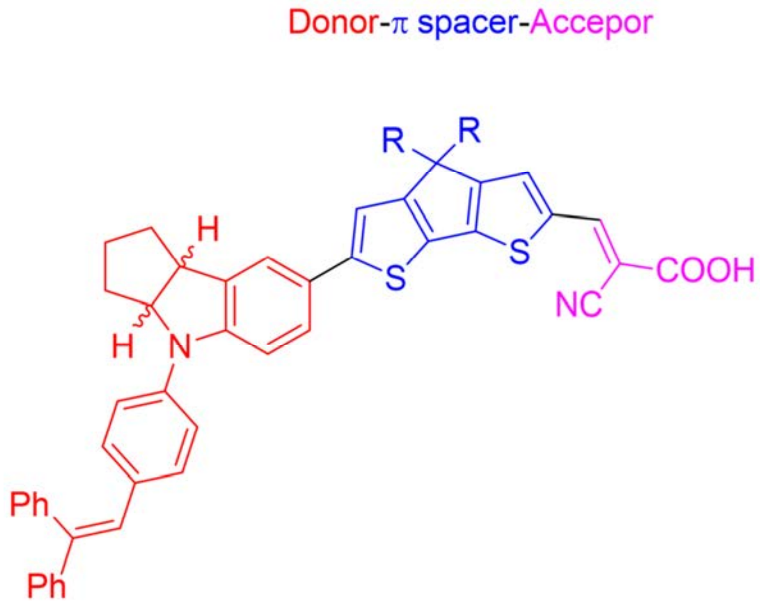
일시: 2014년 10월 15~17일(수~금) 3일간
장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-903**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The effect of cyclopentadithiophene derivates in dye-sensitized solar cells

정현실 **JINMINGYU** 강병철 김태형 강기태 심수용 신성호 백은희 류도현*

성균관대학교 화학과

Metal-free organic dyes exhibit many virtues, such as low cost, being environmental friendly, as adjustable structure, and a competitive efficiency.1 In D-π-A organic dyes, cyclopentadithiophene and its derivates have served as π-conjugated spacers successfully. Here reports three new cyclopentadithiophene organic dyes with different methylene units, consisting of indoline donor and cyanoacetic acceptor, have been synthesized and applied in dye-sensitized solar cells (DSSCs). The organic dye RHI-2 shows the best performance: a short-circuit photocurrent density (Jsc) of 17.9 mA cm-2, an open-circuit photovoltage (Voc) of 730 mV, and a fill factor (FF) of 0.65, which corresponds to a power conversion efficiency (PCE) of 8.47%, under the concentration of dyes is 5 mM in chloroform mixed 1 drop MeOH with 0.1 mM CDCA at AM 1.5 simulated sunlight. This research will pave a way for further molecular design and mechanism study of D-π-A structured organic dyes.



RHI-1 R = C_7H_{15}

RHI-2 R = $C_{12}H_{25}$

RHI-3 R = $C_{16}H_{33}$

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발표코드: **ORGN.P-904**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid metal free oxidative cyclization using chloramine T for the synthesis of benzo[4,5]imidazo[1,2-a]pyridine derivatives

이미정 정유진 박진균*

부산대학교 화학과

Benzo[4,5]imidazo[1,2-a] pyridines have been recognized as important building blocks for the biologically active compounds and organo electronic materials. Therefore, many synthetic methods are available including palladium catalyzed cyclization , copper catalyzed oxidative cyclization, photo catalyzed cyclization, and metal free cyclization reactions. However, most of known methods require relatively long reaction time, high temperature. Our initial effort toward mild reaction found cyclization of aminopyridines using oxidants. After screening of various oxidants and solvents, we found chloramine T in HFIP gave desired product within one minute. Further details will be provided in the poster.

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발표코드: **ORGN.P-905**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Study of Diimides and Dyads Containing Naphthalene Moiety

김성식* **T. Majima**[1]

전북대학교 화학과 [1]*Osaka University*

Synthesis of a series of diimides and dyads containing naphthalene is described. Diimides such as pyromellitic diimide, naphthalene diimide and related compounds were prepared. Several types of other diimides were linked to the common unit, i.e., naphthalenediimide, using phenyl bridge. Phthalimide and naphthalimide were also introduced in the dyads system for comparison of their photophysical properties. Spectroscopic properties of the diimides and dyads were investigated.

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발표코드: **ORGN.P-906**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Quantitative analysis of hydrogen peroxide using fluorescent nanoparticles

김형섭 최낙원[1,*] 박명환[*] 박두한[*]

삼육대학교 화학과 [1]한국과학기술연구원(KIST) 바이오마이크로시스템연구단

Reactive oxygen species(ROS), including hydrogen peroxide(H_2O_2) known to generate free radical, has important roles in cell signaling and homeostasis. However, the excessive production of ROS may result in many diseases such as cancer, heart disease, stroke, and neurodegenerative disease. To date, fluorescence analysis in combination with a ROS-sensitive fluorescence probe is generally used as a detection method of ROS. Here, we have synthesized poly(urethane acrylatenonionmer)(PUAN) nanoparticles with the H_2O_2-sensitive fluorophore that is chemically conjugated to the nanoparticle matrix. We measured of H_2O_2 levels quantitatively by estimating ratiometric fluorescence intensity of our H_2O_2-sensing nanoparticles. Our nanoparticles have the potentialfor 1) multiple sensing of biomolecules of interest, and 2) active targeting to specific cell types such as cancer cells.

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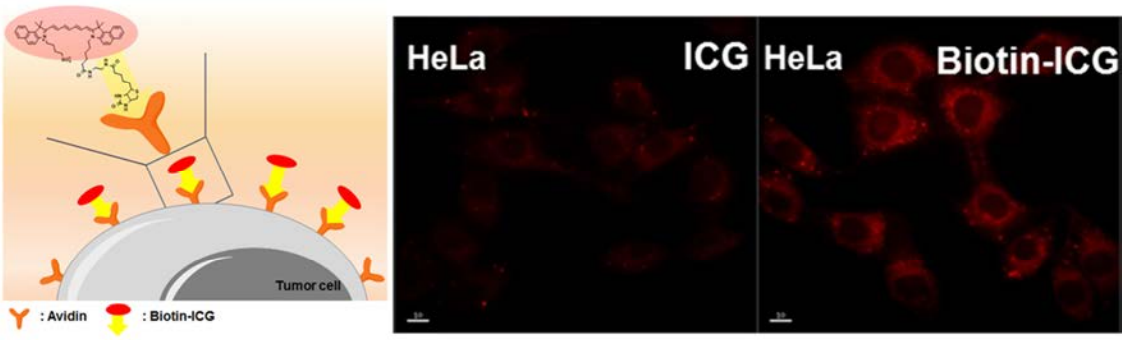
발표코드: **ORGN.P-907**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Target Specific Imaging of Cancer Cells Using The Biotin-Indocyanine Green (Biotin-ICG) Conjugate

엄수진 김종승* 정효성 권보미 박소연 김원영

고려대학교 화학과

In clinical practice, the major method to treat cancer is surgical resection. In that sense, precise spatial discrimination between cancer and healthy tissue is the main issue. To reach this goal, image guided cancer surgery using near-infrared (NIR) fluorescence has emerged as attractive approach. Among NIR fluorophores, which provide advantages of improved contrast and deep tissue penetration, only indocyanine green (ICG) is approved by FDA for clinical use. However, ICG is limited by a lack of target specificity. Herein, we present the design, synthesis and contrast efficacy of a novel tumor targeted NIR contrast agent, Biotin-Indocyanine green (Biotin-ICG), which can specifically target the cancer cell. The intracellular uptake experiments prove that the targeting efficacy of the Biotin-ICG was more effective than that of free ICG in biotin receptor-positive HeLa tumor cells. Furthermore, the results from cell viability tests also confirm that Biotin-ICG did not show any cytotoxicity. Therefore, Biotin-ICG is expected to be a suitable contrast agent for surgical image guidance.



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장소: 광주 김대중컨벤션센터
발표코드: **ORGN.P-908**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Central Thienothiophene and lateral Fluorenyl based Organic Thin Film Transistor Compounds; Synthesis and Characterization

SHAIK BAJI 윤순병 노영리 장용주 이다현 이상경*

경상대학교 화학과

Organic semiconductors have many advantages over the inorganic semiconductors such as control of molecular structures by varying HOMO and LUMO energy levels for mobility optimization, high ?exibility, low cost of materials fabrication, ease for large area processing and compatibility with ?exible substrates. Thus OTFTs have several applications in active matrix display, RIF tags and smart cards etc. In order to exhibit good charge mobility, compounds should have well conjugation and well molecular arrangement in the thin film. Thienothiophene and fluorenyl based compounds designed and synthesized. The alkyl chains of fluorenyl facilitated good solubility. The optical, thermal and electrochemical properties of the compounds were determined. The compounds have shown good thermal and electrochemical stability. Based on these results, we can expect OTFTs prepared by using these materials can be exhibit high mobility.

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발표코드: **MEDI.P-909**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development and Optimization of AlphaScreen Assay for Identification of IRAK-4 Inhibitors

이성호 **HONG VICTOR SUKBONG***

계명대학교 화학과

The interleukin-1 receptor-associated kinases (IRAKs) consisting of IRAK-1, 2, M, and 4 are serine/threonine kinases that regulate Toll-like receptor (TLR) and interleukin-1 (IL-1) signaling pathways. Among IRAK family members, IRAK4 has been widely studied as a potential therapeutic target for treatment of immunological disorders. Here, we report on the development and optimization of an amplified luminescent proximity homogeneous assay (Alpha) technology for screening small-molecule modulators of IRAK-4. In this method, biotin-labeled phosphopeptides are captured on donor and acceptor beads, yielding Alpha signals. The AlphaScreen assay method for IRAK-4 kinase allows us to carry out high-throughput screening and enables identification of novel inhibitors for drug development.

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발표코드: **MEDI.P-910**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development and Optimization of a Fluorescence Polarization Assay to Identify SGK Kinase Inhibitors

김정은 이진호 **HONG VICTOR SUKBONG**[*]

계명대학교 화학과

Serum and glucocorticoid-inducible kinases (SGKs) consisting of SGK1, 2, and 3 are serine-threonine kinases that are activated in response to growth and survival factors. SGKs regulate cell growth, survival and proliferation as well as sodium, potassium, and chloride channels. Thus, SGKs are emerging as novel targets for therapy in cancer, diabetes, and stroke and a compound controlling the activity of SGKs can be useful in treating those diseases. Here, we report on the development and optimization of an immobilized metal ion affinity-based fluorescence polarization (IMAP) method for SGK in a 384-well assay format. In this method, FITC-labeled phosphopeptide yields high fluorescence polarization values due to slow rotation. The apparent Km values for ATP were determined to be 60 uM, 125 uM, and 40 uM for SGK1, SGK2, and SGK3, respectively. The IMAP FP assay was further validated by determining IC50 values for staurosporine.

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발표코드: **MEDI.P-911**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Aminoquinazolinylurea Derivatives and Their Antiproliferative Activities against Bladder Cancer Cell Line

김정훈 정은임[1] 최정훈 유경호[2,*]

한양대학교 화학과 [1]고려대학교 화학과 [2]한국과학기술연구원(KIST) 화학키노믹스연구센터

Bladder cancer is a common malignancy with over 70,000 estimated new cases and 14,000 deaths per year in USA. In western countries, around 90% of bladder tumours are transitional cell carcinoma, with rare cases of squamous cell carcinoma and adenocarcinoma. Their conventional treatment involves surgical resection and intravesical chemo- or immunotherapy. Despite advances in the surgical and medical treatment, there have only been limited improvements in disease-specific mortality rates over the past decades.The purpose of this study is to develop the potent compounds for the treatment of bladder cancer. A series of aminoquinazolinylurea derivatives with a novel hinge moiety were designed and synthesized. And their *in vitro* antiproliferative activities against RT112 bladder cancer cell line were tested. These compounds exhibited potent antiproliferative activities. The study for the mode of action is in progress.

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발표코드: **MEDI.P-912**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Quinoline & Quinolon derivatives as potents inhibitions of WT-TTR aggregation

정지만 최성욱[1,*]

충남대학교 신약전문대학원/신약개발학원 [1]충남대학교 신약개발학과

Transthyretin (TTR) is homotetrameric protein composed of four 127-amino acid β-sheet-rich subunits. TTR transports both the thyroid hormon thyroxin (T4) and holo-retinol binding protein in the blood and cerebrospinal fluid(CSF). In the blood, more than 99% of the T4 binding sites within TTR are unoccupied because of the presence of two other T4 carrier proteins, thyroid binding globulin and albumin.TTR fibril formation requires the rate-limiting tetramer dissociation and monomer misfolding of TTR. Small molecules stabilize the tetramer ground state of TTR over the dissociative transition state, imposing native state kinetic stabilization and consequently inhibiting TTR amyloidosis.There are two symmetrical T4 binding sites for ligands in each tetrameric TTR. Quinoline and Quinolon based small molecules synthesized in the study can bind to T4 binding sites. We are evaluated their ability to inhibit TTR amyloidosis using stagnant acid-mediated turbidity assay.

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발표코드: **MEDI.P-913**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development and Optimization of LanthaScreen TR-FRET Activity Assay for Small Molecule Inhibitors of AXL Kinase in a 384-Well Format

김송이 **HONG VICTOR SUKBONG**[*]

계명대학교 화학과

AXL belongs to a family of TAM (Tyro-3, Axl, Mer) receptor tyrosine kinases. It has been reported that AXL plays an important role in tumor progression, invasion, metastasis and chemoresistance. Thus, AXL kinase is a potential therapeutic target for many human cancers including various hematological malignancies and many solid cancers. Here we describe the development and optimization of a LanthaScreen TR-FRET (Time-Resolved Fluorescence Resonance Energy Transfer) kinase assay in a 384-well format, designed to identify inhibitors of AXL. A LanthaScreen TR-FRET assay uses fluorescein-labeled peptide substrate as acceptor fluorophore and a terbium chelate-labeled anti-phosphotyrosine specific antibody as a donor fluorophore. Upon excitation of terbium at 340 nm, the TR-FRET signal was measured as a ratio between the terbium donor emission at 495 nm and the fluorescein acceptor emission at 520 nm. In addition, we developed and validated a panel of four LanthaScreen TR-FRET kinase assays (Mer, Tyro3, Met, Ros1) for the selectivity profiling of AXL inhibitors.

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발표코드: **MEDI.P-914**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Structure-based optimization and biological evaluation of some pyrazole derivatives as potent ROS1 kinase inhibitors

alsaneamohamedmahmoudibrahimattia **박병선[1] 태진성[1] 이소하[2,*]**

과학기술연합대학원대학교(UST) Medicinal Chemistry [1]연세대학교 화학과 [2]한국과학기술연구원 (KIST) 화학키노믹스연구센터

A series of rationally designed ROS1 tyrosine kinase inhibitors with phenyl bipyridinyl pyrazole scaffold was synthesized and screened. The scaffold itself has showed an exclusive selectivity profile over ROS1 closely related kinases, ALK and c-Met. The objective was to further explore the structure-activity relationships (SAR) of the phenyl bipyridinyl pyrazole core structure, and to improve its ROS1 inhibitory potency. The rational of this current study is to explore the nature of the proposed binding site for the pyrazole NH substituents. Careful selection of pyrazole NH substituent groups along with their regioisomers were considered. Eleven compounds of this series were synthesized and screened against ROS1 kinase. Nine compounds exhibited high degree of potency, IC50 values of 21-79.5 nM. The other two remaining compounds 6d and 6e showed IC50 values of 159 and 1300 nM, respectively. A detailed structure activity relationship (SAR) of phenyl bipyridinyl pyrazole scaffold has been finally well established and the virtual screening strategy, through molecular docking, has been performed for this type of ROS1 kinase inhibitors and the docked poses along with the activity data have gone in consistent with SAR specifications.

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발표코드: **MEDI.P-915**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, synthesis and screening of new 4,5'-bipyrimidine and 2,3'-bipyridine derivatives as ROS1 kinase inhibitors

selimahmedzakariaabdelazem 박혜미[1] 최기항[1] 이소하[2,*]

과학기술연합대학원대학교(UST) Biological Chemistry [1]고려대학교 화학과 [2]한국과학기술연구원 (KIST) 화학키노믹스연구센터

A hypothetical model predicting the required essential features for ROS1 inhibitory activity was developed based on our previous studies. To test this model validity, novel 4,5'-bipyrimidin and 2,3'-bipyridine derivatives has been designed, synthesized and screened against ROS1 kinase. The target compounds could be synthesized on 3-4 steps according to compounds. The structures of the newly synthesized compounds have been confirmed on 1H-NMR and 13C-NMR. Four out of the tested compounds showed good to moderate ROS1 kinase inhibitory activity. The most active compound has IC50 of 330 nM. Through this set of new compounds, we could test the validity of the postulated model.

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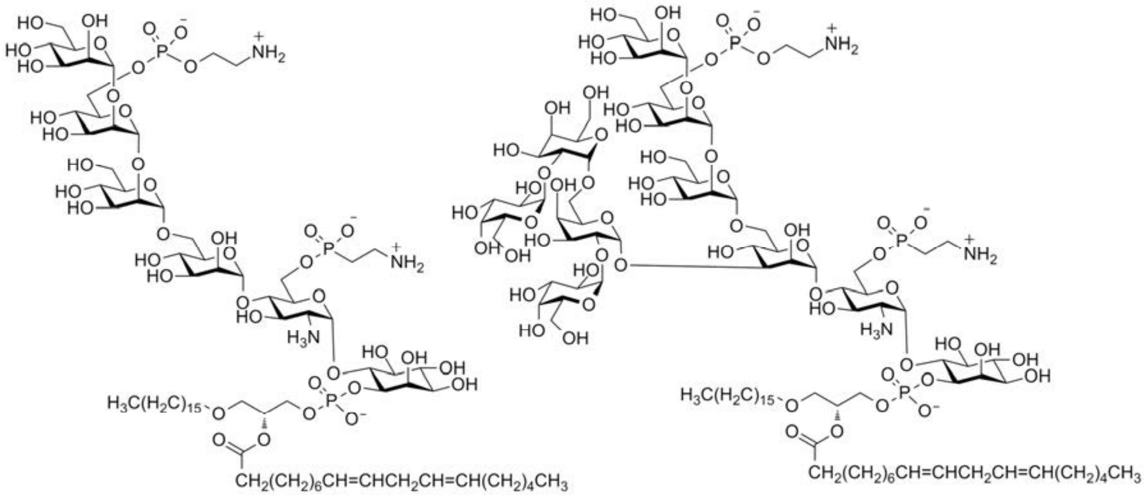
Synthesis of Bioactive Glycosylphosphatidylinositols (GPIs) from *Trypanosoma cruzi (T.cruzi)* using an Innovative Protecting Group Strategy

이보영 Daniel Varon Silva Peter H. Seeberger*

Max Planck Institute of Colloids and Interfaces, Germany

The important role in numerous biological and pathological events of glycosylphosphatidylinositols (GPIs) and GPI-anchored molecules and the difficult isolation has attracted the interest to their chemical synthesis. It has been reported that a GPI fraction of *Trypanosoma cruzi (T. cruzi)* trypomastigote mucins, the etiological agent of Chagas disease, revealed extraordinary proinflammatory activities, comparable to those of bacterial lipopolysaccharide. In the case of the GPI anchor of *T. cruzi*, as the presence of unsaturated fatty acids in the lipid moiety was not compatible with the use of benzyl ethers as permanent O-protecting groups, a novel O-protecting group is positively necessary. Also, as biological activity of the GPI anchor of *T. cruzi* was associated with D-galactose branches along the glycan core, it is in need the chemical synthesis of GPI anchor of *T. cruzi* to study the bioactivity. The building blocks of the GPI anchor of *T. cruzi* would be designed utilizing naphthyl methyl (Nap) ethers, *p*-methoxybenzoyl (*p*-MeOBz) esters, acid- and fluoride-labile protecting groups. The synthetic strategy would be relied on the use of trichloroacetimidate as glycosyl donors and on late-stage phosphorylation after the assembly of the glycan core.



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Cell surface polysaccharide: from Virulence Factor to Synthetic Vaccine for the Haemophilus influenzae type b (Hib)

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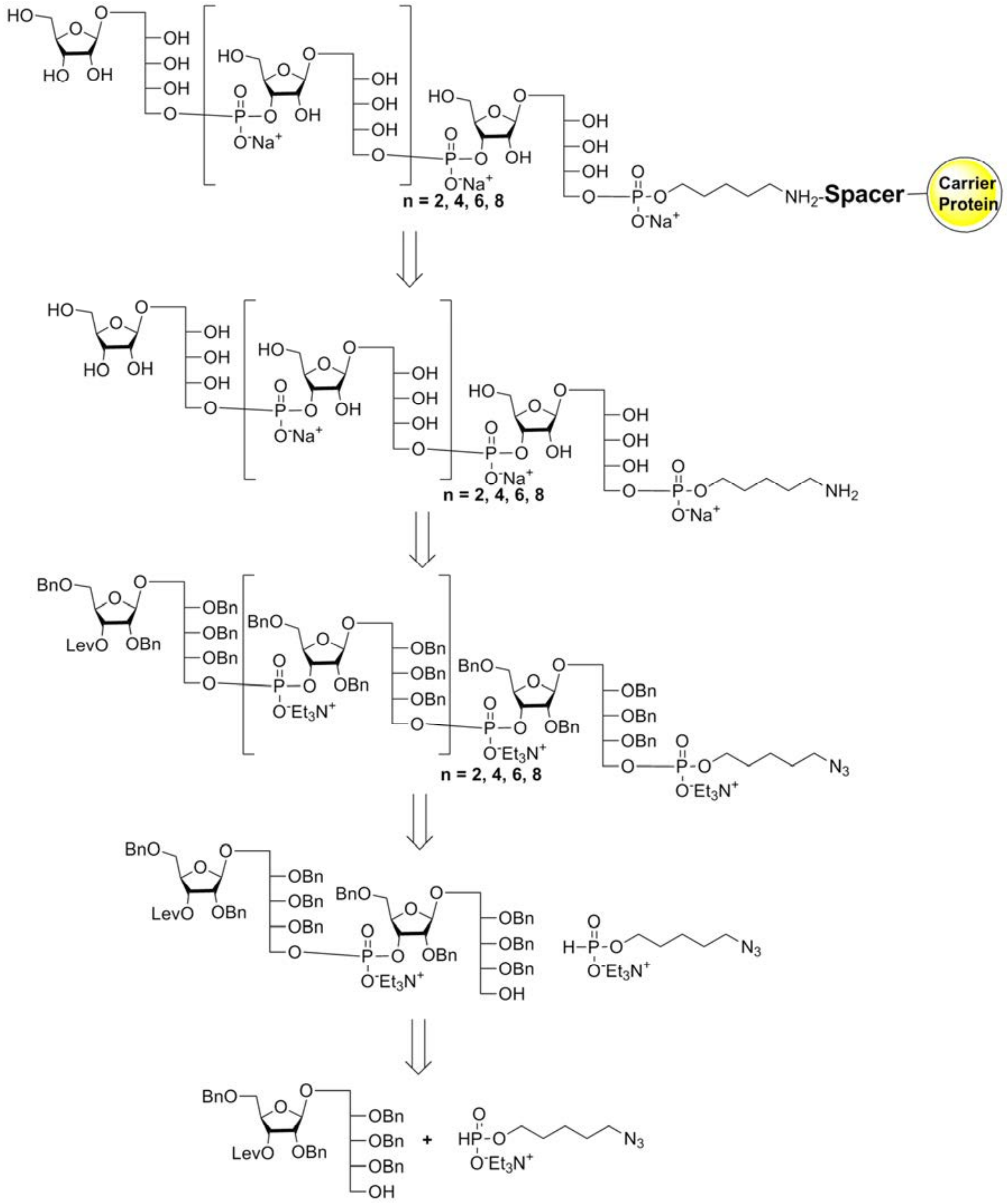
Max Planck Institute of Colloids and Interfaces Department of Biomolecular Systems, Vaccine group [1]*Max Planck Institute of Colloids and Interfaces Department of Biomolecular Systems*

Haemophilus influenzae type b (Hib) is a serious human health problem worldwide, being responsible of a variety of diseases including meningitis, pneumonia and other diseases of the respiratory tract especially in children under the age of 5. It has been shown that a vaccine against these diseases can be prepared using either the capsular polysaccharide polyribosyl-ribitol phosphate (PRP) or its oligosaccharide fragments coupled to a carrier protein. The isolation and purification of Hib-PRP and conjugation of such Hib-PRP to proteins are difficult to standardize, and moreover, these processes may cause chemical rearrangements within the Hib-PRP. In practical terms this would mean that variation in composition must be controlled for new vaccine containing these Hib-PRP. On the other hand, well-defined chemical synthesis have several advantages: Hib-PRP could be reproducibly produced and efficiently conjugated with protein and cost-efficient. So far synthetic Hib-PRP candidates reported consist of a range of monomeric units per oligosaccharide antigen.The aim of our studies was solution phase synthesis of Hib-PRP oligosaccharides from tetramer to decamer. The ribitol unit of the Hib-PRP that can be possible to large scale reaction was prepared from commercially available D-ribose. The initiation and propagation units were prepared by glycosylation of protected D-ribose with protected ribitol. To elongate chain of the Hib-PRP oligosaccharide, the initiation and elongation units were combined using H-phosphonate coupling reaction with block synthesis. Finally, the specialized ribose-phosphate amine linker is attached to the tetramer to decamer using H-phosphonate coupling reaction. The Hib-PRP oligosaccharides are being utilized to develop vaccine candidates.


n = 2, 4, 6, 8
NH2-Spacer
Carrier Protein
n = 2, 4, 6, 8
n = 2, 4, 6, 8

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Synthesis of curcumin mimics with substituted triazolyl groups and their sensitization effect of TRAIL against brain cancer cells

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Glioblastoma multiforme (GBM) is one of the most aggressive forms of human malignant brain tumor and has a high mortality rate. Therefore, there is an urgent need for new chemo-therapeutic strategies to effectively treat GBM. In this respect, tumor necrosis factor (TNF)-related apoptosis-inducing ligand (TRAIL) seems to be a promising drug because TRAIL induces apoptosis in cancer cells without inducing the apoptosis of normal cells. However, many cancer cells have a resistance to treatment with TRAIL, so we need to discover novel sensitizer that can increase the anticancer activity of TRAIL to be able to use in clinical trial. Recently, we synthesized a novel curcumin mimic libraries with substituted triazolyl groups and discovered the curcumin mimics have a strong sensitization effect of TRAIL without any or with only slight cytotoxicity. Based on the preliminary structure?activity relationships, the curcumin mimic library substituted triazol groups will be a promising template for developing novel TRAIL sensitizers as anticancer agents in the future.

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Synthesis of dibenzazepine lactam derivatives via a sequential Pd-catalyzed amination and aldol condensation

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We have developed a sequential Pd-catalyzed amination and aldol condensation reaction for the synthesis of dibenzazepine lactam derivatives in good to excellent yields. This protocol employs 4-amino-2-methylisoindolin-1-one and 2-(2-bromophenyl)-1,3-dioxolane as coupling partners under microwave irradiation.

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2-Aminobenzimidazole derivative as potent and selective BACE1 inhibitors for the treatment of Alzheimer's disease

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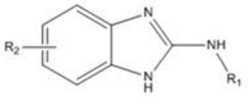
한국화학연구원 의약화학연구센터 [1]과학기술연합대학원대학교(UST) 의약 및 약품화학 [2]한국화학연구원 화학물질연구단

BACE 1 (b-secretase), a key enzyme in the process of amyloid precursor protein (APP) into neurotoxic Ab? peptide, is considered a promising therapeutic target for the Alzheimer's Disease (AD). Here, we reported the synthesis and inhibitory activity of 2-aminobenzimidazole derivative as BACE 1 inhibitors



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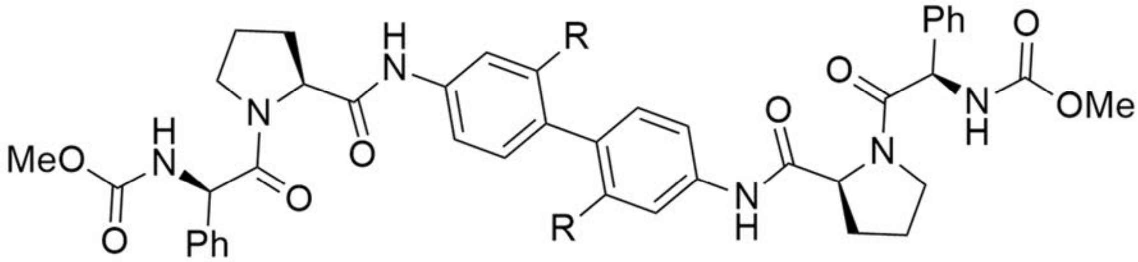
발표종류: 포스터, 발표일시: 수 16:00~19:00

Potent Inhibitors for Hepatitis C Virus NS5A: Studies on the Benzidine Core Variation

배일학 유영수 선민경 김병문*

서울대학교 화학부

Hepatitis C virus (HCV) belongs to the hepacivirus genus in the Flaviviridae family as a single stranded RNA virus (50 nm in size) and its infection often leads to serious diseases such as liver cirrhosis followed eventually by hepatocellular carcinoma. HCV RNA consists of structural and nonstructural proteins. Especially, several non-structural proteins (NS2, NS3, NS4A, NS4B, NS5A and NS5B) involved in the reproduction of HCV are of great importance for new therapeutic target identification. However, current standard of anti-viral therapy has been the combination of pegylated interferon-α with ribavirin (Peg-IFN/RBV), until a recent addition of the HCV protease inhibitors, Boceprevier and Telaprevir. However, even with the protease inhibitors, sustained virologic response for genotype 1 is still about 60~80%. Therefore development of effective anti-HCV drug candidates is urgently needed. Here we report the discovery of a series of extremely potent HCV NS5A inhibitors based on the benzidine prolinamide skeleton. Taking a simple synthetic route, we developed a novel inhibitor structure, which allows easy modification, and through optimization of the benzidine core structure, we identified BMK-20313, BMK-20613, and BMK-20713 with highly potent anti-HCV activities. Especially, BMK-20313 is nontoxic and anticipated to be an effective HCV drug candidate.



Type 2a: EC_{50} = 0.01 nM, G-1b: EC_{50} = 0.007 nM

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Design and synthesis of MELK (maternal embryonic leucine zipper kinase) inhibitor

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과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 의약화학 연구센터 [3]한국화학연구원 신물질연구단

Maternal embryonic leucine zipper kinase (MELK) belongs to the SNF1/AMPK family that has been implicated in stem cell renewal, cell cycle progression, cytokines, mRNA splicing and apoptosis. MELK is considered to be a promising drug target for anticancer because overexpression and hyperactivation of MELK is correlated with several human cancers and associated with poor prognosis in breast cancer and glioblastoma patients. In this study, we are reporting the design, synthesis, and evaluation of new compounds as MELK inhibitors. New compounds were designed based on the structure of hits from HTS and crystal structure of enzyme.

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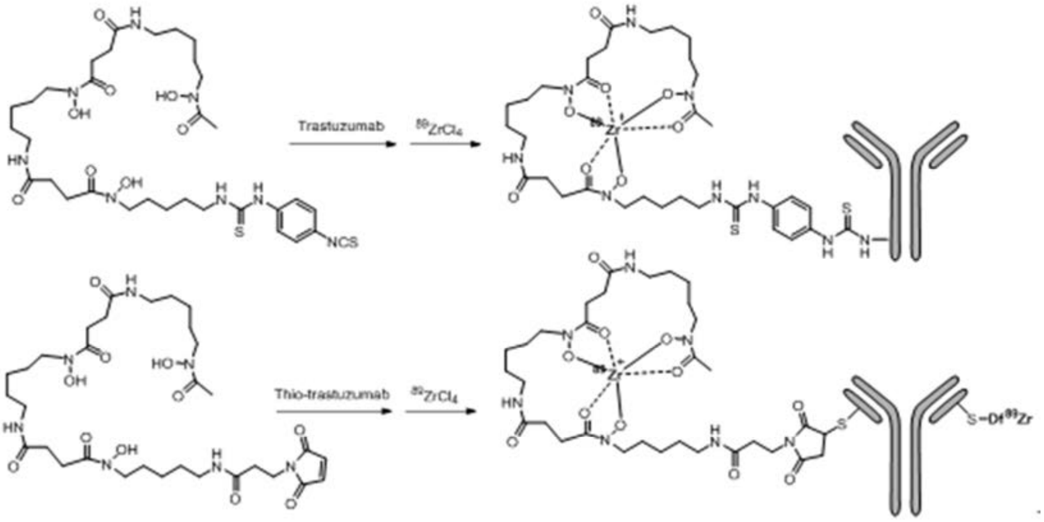
Synthesis of 89Zr-labeled trastuzumab and thio-trastuzumab for immunoPET

이지웅 신운철[1] 박지애[2] 이교철[3] 안광일[4] 김정영[3,*]

고려대학교 보건과학 [1]연세대학교 의공학과 [2]한국원자력의학원 분자영상연구부 핵의학연구팀 [3]한국원자력의학원 방사성의약품연구팀 [4]한국원자력의학원 방사성의약품 개발실

Object: 89Zr (t1/2 = 78.41 h, Eγ = 511, 908 KeV) is a positron-emitting radioisotope, which has known as well-suited radioisotope for use in a monoclonal antibody based imaging agent for immunoPET. In this study, we report the preparation of 89Zr-labeled trastuzumab and thio-trastuzumab for research and clinical application, with the chelation by 89Zr chloride and derivatives of desferrioxamine.Materials and Methods: Desferrioxamine-p-SCN (Df-Bz-NCS) and deferrioxamine-maleimide (Df-maleimide) were purchased from Macrocyclics (Dallas, TX, USA). The mAb trastuzumab was purchased from Roche(Schweiz), and thio-trastuzumab was obtained from professor Hyo-Jeong Hong group (Kangwon National University). The radioisotope 89Zr was produced by domestic purification system and KIRAMS using medical cyclotron (50 MeV, Scantronix). The conjugates of Df-trastuzumab and Df-thio-trastuzumab were prepared with Df-Bz-NCS and Df-maleimide under basic aqueous solution (pH 8-9) at room temperature, respectively. The conjugates purified by PD-10 column were mixed with dried 89Zr chloride. 89Zr-labeled conjugates were purified and concentrated by Amicon ultra centrifugal filter.Result: The preparation step and time of 89Zr-labeled conjugates was shorted as 4 steps within 2 hours. 89Zr-labeled conjugates showed the highly radiochemical purity of over 98%, and were very stable until 7 days by the analysis of radio-ITLC method. In particular, the radio-labeled conjugates were exhibited the highly stability in both PBS buffer and mouse serum.Conclusion: We optimized the preparation of two 89Zr-labeled conjugates, 89Zr-Df-Bz-NCS-trastuzumab and 89Zr-Df-thio-trastuzumab, as highly efficiency from the production of 89Zr to radiolabeling method.


Trastuzumab
89ZrCl4
Thio-trastuzumab
89ZrCl4
NCS
S-Df-89Zr

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of Novel Monoamine Oxidase B Inhibitorsfor Parkinson's Disease Therapy

송효정 박기덕[1,*]

연세대학교 생명공학과 [1]한국과학기술연구원(KIST) 뇌의약연구단

Hyo Jung Song,[1,3] Ji Won Choi,[1,3] Min Ho Nam,[2,4] Bo Ko Jang,[1,5] Seul Ki Yeon,[1,3] Eun Ji Ju,[1,3] Min Kyung Ko,[1] Yong Gu Kang,[1] Justin Lee,[2,*] Ki Duk Park[1,*]*[1]Center for Neuro-Medicine, [2]Center for Neural Science, Korea Institute of Science and Technology; [3]Department of Biotechnology, College of Life Science and Biotechnology, Yonsei University; [4]Department of Pathology, College of Korean Medicine, [5]Department of Fundamental Pharmacentical Science, College of Pharmacy, Kyung Hee Univerisity, Seoul*Parkinson’s disease (PD) is the second most common neurodegenerative disease and is caused by neurodegeneration of dopaminergic neuronal cells in substantia nigra pars compacta, resulting in a significant loss of dopamine (DA). Current symptomatic treatment for PD is mainly dopamine replacement therapy. One of main approaches in PD treatment is the inhibition of monoamine oxidase B (MAO-B), responsible for the metabolism of DA in the brain. In this study, we synthesized a novel series of amide derivatives as reversible MAO-B inhibitor and tested for their MAO-B and MAO-A inhibitory activities. Among them, compound 10 showed most potent and selective MAO-B inhibitory activity (IC50 human MAO-B 42 nM, >10,000-fold selective versus MAO-A) and good reversibility compared with Selegiline, well-known irreversible MAO-B inhibitor. In addition, compound 10 significantly protected DAergic neurons from cytotoxic damage and attenuated the PD-associated motor deficits in MPTP induced mouse model of PD. In conclusion, we present a novel amide compound with a therapeutic potential for PD.

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Naturomimetic Approach Method를 이용한 생리활성 아릴나프탈렌 락톤 리그난 천연물의 SAR연구Ⅰ

김태정 정규혁[1] 최필주 김영석[1] 함정엽[*]

한국과학기술연구원(KIST) 강릉분원 [1]강릉원주대학교 화학신소재학과

아릴나프탈렌락톤은 다양한 식물군에서 발견되는 리그난류 천연물로 암을 비롯하여 염증, HIV, 뇌질환, 골다공증 등에서 다양한 유효 활성을 나타내는 것이 보고되고 있다. 이 중 대표적으로 손꼽히는 천연물로 다이필린, 저스티시딘류, 실리나프탈렌류 및 타이와닌류 등이 있으며, 이들은 나프탈렌락톤(naphtho[2,3-*c*]furan-1(3*H*)-one)을 중심골격으로 유사한 구조를 가지고 있다. 그러나 이러한 유사 구조를 가지고 있음에도 불구하고 치환기의 위치나 종류에 따라 전혀 다른 생리활성이 발현되어 현재까지 여러 화합물에 대한 연구 내용이 논문이나 문헌을 통해 보고되고 있다. 한편, 아릴나프탈렌락톤 리그난류 천연물은 많은 유기합성 그룹의 연구를 통해 전합성이 달성되어 있으나 현재까지 보고된 모든 방법이 아릴기(-Ar)를 합성 초기단계에 도입하는 방법으로 다양한 유도체화를 통한 SAR 연구를 수행하기에는 비효율적이다. 이에 본 연구진은 아릴나프탈렌락톤 리그난류 천연물의 중심골격인 나프탈렌락톤을 합성 초기단계에 구축한 후, 마지막에 여러 가지 아릴기를 도입하는 Naturomimetic Approach Method 를 이용하여 천연물을 비롯한 다양한 유도체를 효율적으로 합성하는데 성공하였다. 또한, 각각의 화합물에 대한 생리활성을 측정하여 현재 시판되고 있는 항암제 VP16 및 Taxol 과 유사 또는 뛰어난 활성을 나타내는 유효물질을 도출하는데 이르렀다. 본 포스터발표에서는 상기의 연구내용에 대해 상세히 보고하고자 한다.

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Naturomimetic Approach Method를 이용한 생리활성 아릴나프탈렌 락톤 리그난 천연물의 SAR연구Ⅱ

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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 Method 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 최근에 진행했던 생리활성 아릴나프탈렌락톤 리그난 천연물의 활성증대를 위한 SAR 연구 내용에 대해 보고하고자 한다.

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Hybrid PET-Ultrasound Dual-modality Probe : [Cu-64]ATSM Loaded Phase-shift Perfluorocarbone Nanodroplets

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Object: Multifunctional nanocarrier studies have been reported ultrasound?activated perfluorocarbon (PFC) nanodroplets which can be phase-shift by ultrasound inertial cavitation in recent years. The purpose of this study is to develop a dual-modality contrast agent incorporating perfluorocarbon and [Cu-ATSM] for hybrid PET-ultrasound imaging. Methods: Acoustic PFC nanodroplets were fabricated by perfluoropentane (PFP) with phospholipids (PLs) solution consisting of DPPC and DPPA. [Cu-64]ATSM was encapsulated into micellar monolayer of UCAs due to hydrophobic property. Nanodroplets including PFP and [Cu-64]ATSM was controlled in size by extrusion through 100 nm polycarbonate filter. The PET images of nanodroplets (PLs-PFC-[Cu-64]ATSM) were obtained by a small animal PET/CT scanner (InveonTM, Siemens). Ultrasound images were obtained by ultrasound image scanner (Sonoace Pico, Medison). Small animal PET-CT image of the nanodroplets (PLs-PFC-[Cu-64]ATSM) was obtained by directly intratumoral injection into U87MG xenograft nude mouse. Result: PET images in vitro of the nanodroplets were observed as hot spot in the bottom of green tube, while [Cu-64]ATSM in same tube has a wide distribution without a specific hot spot. ROI mean activity of nanodroplets was increased to 280% in lower area than only [Cu-64]ATSM, and were also showed strongly contrast-enhanced ultrasound images. The nanodroplets was showed more low uptake of about 71 % than only [Cu-64]ATSM in liver PET images of U87MG tumor model. Conclusion: This study was aimed at development of biocompatible nanodroplets encapsulated [Cu-64]ATSM and PFP in size controlled micelle (80-100 nm). [Cu-64]ATSM loaded PFC nanodroplets is expected to contribute hybrid PET-ultrasound technology as a potential dual imaging agents.

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Synthesis and Biological Evaluation of Novel Modulators for Amyloid beta-induced Mitochondrial Dysfunction for the Treatment of Alzheimer’s Disease

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Although the mechanism of Alzheimer’s disease (AD) pathogenesis is largely unknown, the role of mitochondrial amyloid beta (Aβ) has been highlighted in the pathophysiology of AD. Aβ is produced from transmembrane amyloid precursor protein (APP) by sequential actions of β- and γ-secretase. And Aβ is implicated in the pathogenesis of AD by its interaction with cyclophilin D (CypD), which is a component of mitochondrial permeability transition pore (mPTP). CypD, Adenin nucleotide translocator (ANT), Voltage-dependent anion channel (VDAC), and the 18 kDa Translocator proetein (TSPO) 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 TSPO can be an effective therapeutic strategy in mPTP blocking. Based on the pharmacophore-based virtual screening, we identified novel scaffolds KKPN0001, and the synthesis and biological evaluations of those compounds were performed. The newly synthesized KKPT compounds were biologically evaluated in vitro and in vivo. Their mPTP blocking activities were evaluated by a JC-1 assay, measuring the change of mitochondrial membrane potential. Also the maintenance of cell viability and mitochondrial function was evaluated by MTT assay, ATP assay, and ROS assay. The biological data from those assays showed the improvement in symptoms of AD by novel KKPT compounds. Thus, the optimization of novel modulators for Aβ-induced mitochondrial dysfunction is now in progress.

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Novel anticancer quinolines with selective TrKA inhibitory activity

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A novel series of 2,5-disubistituted quinolines (10 final compounds) has been synthesized to explore their antitumor activity.. All the target compounds were evaluated for their antiproliferative effect against three cancer cell lines (MCF7, HCT116 and SKBR3) by MTT assay. The most potent compound 1i was selected to be tested over a panel of 60 cancer cell lines at a single dose concentration of 10 uM at NCI. It exhibited promising mean growth inhibitions and therefore was further tested at five-dose testing mode to determine its GI50, TGI and LC50 over the 60 cell lines. It exhibited potent antitumor activity with submicromolar GI50 value against some cell lines. Moreover, compound 1i was tested against a kinase panel (48 kinase) at 10 uM and showed selective inhibition 96% against TrKA with IC50 of 2.5 uM.

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Hit discovery of potent Hsp90 inhibitors and structure-based optimization

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Heat shock protein 90 (Hsp90) is an ATP-dependent chaperone that is responsible for the folding, activation, and stabilization of numerous client proteins. Hsp90 has become an attractive therapeutic target in cancer research. Many Hsp90 client proteins play significant roles in six essential hallmarks of cancer cell, including Akt, Raf-1, mutant p53, Cdk4, VGEF, MET and HIF-1α. The therapeutic potential of targeting Hsp90 may be best appreciated by simultaneously attacking the six hallmarks of cancer cells. Accordingly, the inhibition of Hsp90 function promotes ubiquitin-dependent proteasomal degradation of its client proteins, which can eventually lead to cell death. Besides, Hsp90 is expressed at 2-10 fold higher levels in tumor cells than their normal cells.As part of our ongoing efforts to discover small molecules targeting N-terminal ATP-binding pocket of Hsp90, we had performed a structure-based drug design (SBDD) of small molecule inhibitors against Hsp90. Designed inhibitors were synthesized and their antitumor activities were evaluated. Here, we report our effort to develop therapeutic agents against Hsp90 in cancer. Further lead optimization and preclinical development of synthesized compounds are underwent.

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Her-2/neu **타이로신 키나아제의 억제제로서 [^{123}I]iodoemodin의 합성 및 평가**

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Emodin (1,3,8-trihydroxy-6-methylanthracene-9,10-dione)은 다중고리 방향족 안쓰라퀴논 화합물로서 항종양 활성을 포함하는 다양한 생물학적 성질을 가지고 있다. 안쓰라퀴논 화합물들은 항암제로서 유방암세포의 *HER-2/neu* 타이로신 키나아제의 발현을 억제한다는 보고가 되어져 있어, 에모딘 화합물에 I-123 을 표지하여 *HER-2* 수용체에 대한 억제제로서 유방암의 진단 및 치료에 사용 가능할 것으로 보여진다. I-123 의 표지는 Emodin 을 DMF 에 녹인 후, 200 μL 를 취해 [^{123}I]NaI solution (159MBq/100μL)과 산화제로서 chloramines T 를 넣어 실온에서 10 분간 교반 하였다. [^{123}I]emodin 화합물은 역상-고성능 액체 크로마토그래피로 분리?정제하여 사용 하였으며, 유방암세포에 대한 생물학적 평가는 유방암을 발현시키는 MCF-7 과 *HER-2* 수용체가 과발현 되어있는 SK-BR-3 세포주를 대상으로 실시하였다. In vitro, 세포섭취도 평가는 세포주를 well 당 1×10^{5}cells 씩 접종하여 24 시간 배양 후 진행 하였으며, [^{123}I]emodin 은 well 당 235KBq/240μL 씩 주사한 후 15 분, 30 분, 60 분, 120 분 간격으로 주사된 방사능량 (ID%)으로 나타내었다. 시간이 증가함에 따라 세포섭취도 결과는 HER-2 수용체가 과발현 되어있는 SK-BR-3 에서 좀 더 우수한 세포섭취도 결과를 나타냈다. In vivo, 마우스 생체내 분포도 실험은 SK-BR-3 종양이 이식된 balb/c 마우스를 대상으로 1.11MBq/100μL [^{123}I]emodin 을 꼬리 정맥 주사하여 60 분 후 장기를 적출하였으며, 장기 무게당 방사능량 % (%ID/g)으로 나타내었다. 대장, 위, 혈액, 간, 종양, 심장, 종양의 순으로 높은 분포도를 나타내었다. 안쓰라퀴논 화합물인 emodin 에 방사성동위원소인 I-123 을 높은 수율로 표지 하였으며, *HER-2* 수용체에 대한 [^{123}I]emodin 의 우수한 친화력을 확인 함으로서 유방암의 진단 및 치료제로서 사용 가능할 것으로 보여 진다.

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Discovery of Hsp90 inhibitors from natural product and its analogues

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Kava(*Piper methylsticum*) is a native plant traditionally used as a medicine and social drink in the South Pacific islands, including Fiji, Vanuatu and Western Samoa. Flavokawain, one of chalcone component isolated from kava extract, has been reported to exhibit strong anti-proliferative effects against several cancer cell lines.Hsp90 is an ubiquitous molecular chaperone protein, which accounts for 1-2% of the cytosolic protein under non-stressed conditions. Hsp90 plays an important role in regulating maturation and stabilization of many oncogenic proteins in six essential hallmarks of cancer, including EGFR, Her2, Met, Akt, Raf, HIF-1 and MMP2. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways.Non-small cell lung cancer(NSCLC) is the most common type of lung cancer and that is responsible for 85% of lung cancer patients. Despite several EGFR inhibitors have been developed in the treatment of NSCLC, the clinical efficacy of EGFR inhibitors in NSCLC is limited by the development of drug-resistance through the mutation of EGFR and the overexpression of Met. Considering both EGFR and Met are client proteins of Hsp90, to block Hsp90 protein folding machinery may be best suited to overcome the resistance form EGFR mutation and Met amplification.In this study, we discovered that a natural product, flavokawain its analogues disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer(H1975). The result suggested that flavokawain and its analogues could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

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Clicked Synthesis of Purpurinimide Derivatives for Photodynamic Therapy

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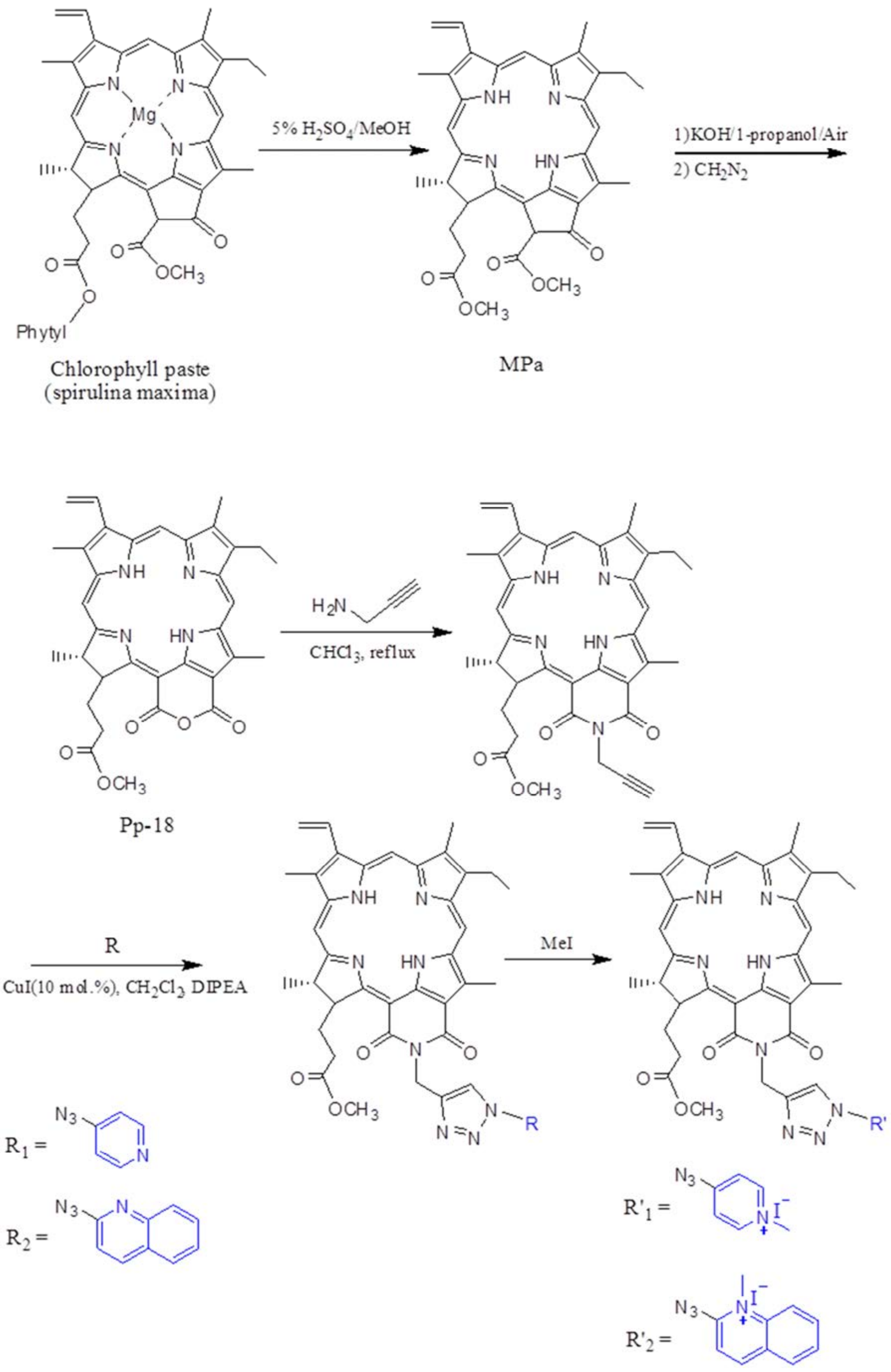
Photodynamic therapy (PDT) is based on the accumulation of a photosensitizer (PS) in tumors, for which given exposure of light at an appropriate wavelength generates reactive oxygen species (ROS, e.g.singlet oxygen) that results in tissue destruction.Photodynamic study for various functional groups (about shift of wavelength of maximum absorption and biological efficiency) will cause the more convenience about the prediction and control of the photodynamic properties of PS.In this study, purpurinimide methyl ester derivatives were synthesized using N-propargyl-purpurinimide methyl ester as starting material. The derivatives were synthesized by 1,3-dipolar cycloaddition of N-propargyl-purpurinimide methyl ester containing a terminal triple bond and azide derivatives containing various functional groups. The click reaction, which was carried out using 10 mol% of copper(I) iodide in dichloromethane with an addition of diisopropylethylamine (DIPEA).Each derivative was characterized by 1H-NMR and IR spectroscopies for structure determination, configurations and functional groups.For photodynamic effect of the derivatives, bioassays were investigated by MTT assay against A549 and HeLa cell lines, and shift of wavelength of maximum absorption assays was determined by UV-vis spectroscopy.And then, each photodynamic result was compared with previous studies for cationic chlorins.


Chlorophyll paste
(spirulina maxima)
Phytyl
Mg
5% H_2SO_4/MeOH
MPa
1)KOH/1-propanol/Air
2) CH_2N_2
Pp-18
H_2N
$CHCl_3$, reflux
R
CuI(10 mol.%), CH_2Cl_3 DIPEA
MeI
OCH_3
R
R'
R_1 =
R_2 =
R'_1 =
R'_2 =
N_3
I^-

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Comparison of the optical activity of MPPa-Oxime derivative and HPPH

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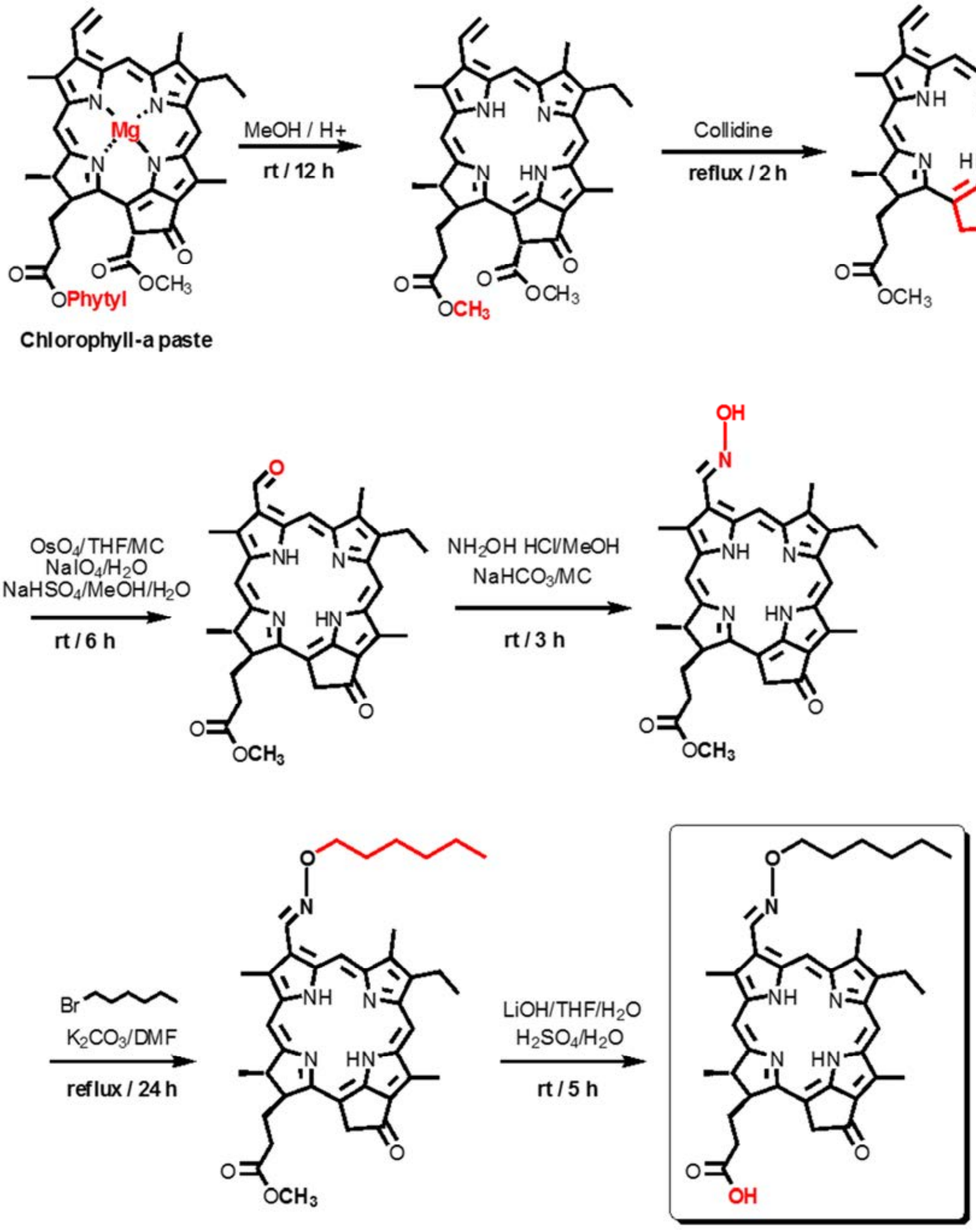
C3-ethynylated chlorophyll derivative was increases the maximum absorption wave length of the UV spectrum through the various substitutions. we are manufactures HPPa- oxime derivative with similar the structure of HPPH generally known, and compare maximum absorption wavelength.


Mg
Phytyl
Chlorophyll-a paste
MeOH / H+
rt / 12 h
Collidine
reflux / 2 h
OsO_4/ THF/MC
$NaIO_4/H_2O$
$NaHSO_4/MeOH/H_2O$
rt / 6 h
NH_2OH HCl/MeOH
$NaHCO_3$/MC
rt / 3 h
Br
K_2CO_3/DMF
reflux / 24 h
LiOH/THF/H_2O
H_2SO_4/H_2O
rt / 5 h
NH
N
HN
O
OH
OCH_3

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Synthesis of Novel Asymmetric Hepatitis C Virus (HCV) Inhibitors for the Treatment of Hepatitis C Infection

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Hepatitis C Virus (HCV), a positive strand RNA virus, causes serious disease such as cirrhosis, liver failure and liver cancer. NS5A is one of the HCV non-structural proteins and has a critical role of the viral replication. NS5A inhibitors have potential ability to bind across the NS5A dimer interface and allow NS5A dimers to rigid spherical form, then dimers are shuttled to lipid droplet surface, consequently prevent from forming new viral replication complex. Daclatasvir, highly potent NS5A inhibitor which is now in phase III, has subnanomolar EC50 in genotype 1 and symmetric structure. However, treatment with Daclatasvir quickly induce the mutation at domain I. Based on the structure of the HCV NS5A inhibitor Daclatasvir, a series of novel asymmetric NS5A inhibitor candidates were designed, synthesized, expected to solve the mutation problems and improve potency. We plan to demonstrate the compounds inhibitory potency by in vitro virus replicon assay.

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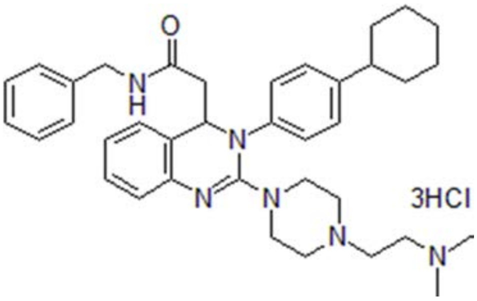
Suppression of cell proliferation and induction of apoptosis in human lung adenocarcinoma A549 cells by T-type calcium channel antagonist

손주미 주동준 이재열*

경희대학교 화학과

The anti-proliferative and apoptotic activities of new T-type calcium channel antagonist, BK10040 on human lung adenocarcinoma A549 cells were investigated. The MTT assay results indicated that BK10040 was cytotoxic against human lung adenocarcinoma (A549) and pancreatic cancer (MiaPaCa2) cells in a dose-dependent manner with IC_{50} of 2.25 and 0.93 μM, respectively, which is ca. 2-fold more potent than lead compound KYS05090 despite of its decreased T-type calcium channel blockade. As a mode of action for cytotoxic effect of BK10040 on lung cancer (A549) cells, this cancer cell death was found to have the typical features of apoptosis, as evidenced by the accumulation of positive cells for annexin V. In addition, BK10040 triggered the activations of caspases 3 and 9, and the cleavages of poly (ADP-ribose) polymerase (PARP). Moreover, the treatment with z-VAD-fmk (a broad spectrum caspase inhibitor) significantly prevented BK10040-induced apoptosis. Based on these results, BK10040 may be used as a potential therapeutic agent for human lung cancer via the potent apoptotic activity.



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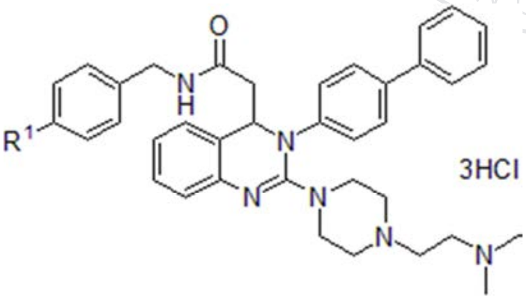
발표종류: 포스터, 발표일시: 수 16:00~19:00

Anti-cancer effect of T-Type Calcium Channel Blockers on Human Pancreatic MIA PaCa-2 Carcinoma Xenografts

변준석 주동준 이재열*

경희대학교 화학과

Two piperazine-containing 3,4-dihyroquinazolines (BK10007S/8S) have been synthesized, based on ourprevious work on the synthesis and antitumoral activity of 3,4-dihyroquinazolines. After evaluating them forT-type calcium channel blocking effect and *in vitro* anti-cancer effect, they were profiled for acute and repeat dose toxicity (40 mg/kg, 2 weeks) to BALB/c mice. BK10007S/8S were further *in vivo* evaluated against human pancreatic MIA PaCa-2 carcinoma in BALB/$c^{nu/nu}$ nude mice, which exhibited 54 and 61% tumor growth inhibition through 57-day oral administration of 2 mg/kg of body weight, respectively.



BK10007 S, R =F
BK10008 S, R=OCH3

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Solid-phase Synthesis of Drug-like 2-Amino/amido-1,3,4-oxadiazole and 1,3,4-thiadiazole Derivatives via Reagent-based Regioselective Cycilzation of Thiosemicarbazide Intermediate

양승주 JUVEKARVINAYAK Puttavva meti 공영대[*]

동국대학교 화학과

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

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Scaffold hopping and Synthesis of Arylethynyl-subsititued-bicyclic heteroaromatic compounds as Trasnglutaminase 2 inhibitor Design and Optimization

김나연 공영대*

동국대학교 화학과

High levels of Trasnglutaminase 2 (TGase 2) have an effect on various diseases. Specially, TGase 2 inhibitor may become a very effective treatment for cancer. We have identified the anticancer effect of GK-13, 2-(phenylethynyl)-3-(2-(pyrrolidin-1-yl)ethoxy)quinoxaline, which is associated with its inhibition against TGase 2. In line of a scaffold hopping strategy, we developed a novel scaffold of pyrido[2,3-b]pyrazine and thienopyrazine through the modification of GK-13 which was a lead compound in previous studies. Some of the pyrido[2,3-b]pyrazine and thienopyrazine derivatives was shown to hold promise for use as potential therapeutic small-molecules in cancer treatment through the inhibition of the TGase 2 activity. Especially, compared to GK-13, GK-428(N,N-dimethyl-3-((3-(phenylethynyl)thieno[3,4-b]pyrazin-2-yl)oxy)propan-1-amine) and GK-921 (3-(phenylethynyl)-2-(2-(pyrrolidin-1-yl)ethoxy)pyrido[2,3-b]pyrazine) showed a higher prospect as an TGase 2 inhibitor. Furthermore, we carried out the docking study of GK-13, GK-428 and GK-921 to provide a rational explanation for the active sites of the Transglutaminase 2 structure.

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A Solid-Phase Parallel Synthesis of Drug-like 1,3,4-Thiadiazole Analogues via Desulfurative Cyclization of Thiosemicarbazide Intermediate

최지혜 양승주 이은실[1] 공영대[*]

동국대학교 화학과 [1]동국대학교 의약화학연구실

Solid-phase combinatorial chemistry has hold its place an extremely powerful techgnique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. And five-membered ring heterocyclic compounds usually serve as the core components of many substances that possess a wide range of interesting biological activities. In a preceding study, 1,3,4-oxadiazole analogues shown potent biological activity in Wnt signaling pathway which has been regulate cell proliferation, differentiation and morphogenesis. In this respect, we have a interest in synthesis both 1,3,4-oxadiazole and 1,3,4-thiadiazole as a bioisostere. However, we couldn't obtain 1,3,4-thiadiazole analogues selectively in our previous study. In this research, we has established another synthetic method to synthesize 1,3,4-thiadiazole analogues on the solid-phase. And substitution reactions with some electrophiles such as alkyl halide and acid chloride generate N-alkylamino and N- acylamino-1,3,4-thiadiazole libraries.

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An efficient Solid-phase Parallel Synthesis of N-Substituted-2-aminobenzo[d]thiazine Derivatives on a BOMBA Resin

김은미 임수정 곽세훈 공영대[*]

동국대학교 화학과

Recently, heterocyclic compounds analogues and their derivatives have attracted strong interest in medicinal chemistry due to their biological and pharmacological properties. The small and simple benzo[d]thiazine nucleus possesses numerous biological properties like - antitumor, cardiovascular, neurodegenerative pathologies, antiproliferative activity. These activities are also possessed by its substituted derivatives as well. Also solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. A efficient solid-phase methodology has been developed for the synthesis of N-acyl, and N-sulfonyl-2-aminobenzo[d]thiazine derivatives. These core skeleton 2-aminobenzo[d]thiazine resins undergo functionalization reaction with various electrophiles, such as acid chlorides, and sulfonyl chlorides to generate N-acyl, and N-sulfonyl-2-aminobenzo[d]thiazine resins, respectively. Finally, 2-aminobenzo[d]thiazine derivatives are then generated by cleavage of the respective resins under trifluoroacetic acid (TFA) in dichloromethane (DCM).

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Synthesis of a Novel *N*-five-membered-heterocycle-*N*',*N*"-disubstituted-guanidine Derivatives as a *S*-nitrosoglutathion Reductase Inhibitor

이지형 최용문[1] 서진호 공영대[*]

동국대학교 화학과 [1](재)경기과학기술진흥원 연구개발팀

Asthma is a common chronic inflammatory disease of the airways characterized by variable and recurring symptoms, reversible airflow obstruction, and bronchospasm. GSNO is an endogenous bronchodilator that relaxes the bronchial smooth muscles and causes dilation of bronchi and bronchioles. The protective role of GSNO in airways has been supported by the observation that the level of GSNO was lower in asthmatic airways compared to that in normal physiology and that restoration of GSNO levels correlated with attenuation of both bronchoconstriction and inflammation in animal models of experimental asthma (Blonder et al., 2014; Que et al., 2009). These results implicate GSNO metabolism as a target for therapeutic intervention of asthma.And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In that regard, we concentrated our effort to construction of a novel small organic drug-like lead compound without side-effect of existing anti-inflammatory drugs. As a result, we synthesized *N*-five-membered-heterocycle-*N*',*N*"-disubstituted-guanidine derivatives via heterocyclic thiourea intermediate with various aromatic amines.

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SYNTHESIS OF NOVEL SULFONYLHYDRAZIDE DERIVATIVES AND THEIR INHIBITORY ACTIVITY OF PGE2 PRODUCTION IN RAW 264.7 MACROPHAGE CELLS

김민주 이재열* 주동준

경희대학교 화학과

Inflammatory processes are implicated in 25% of all cancers and chronic inflammation has been shown to promote the growth of malignant tissues. Indeed, prostaglandin E2 (PGE2) has been identified as a key mediator of pain and inflammation and is overexpressed in various cancers. Definitive evidence suggests that PGE2 is the dominant prostaglandin involved in the growth of tumors associated with colon, lung, breast, head, and neck cancers. In search of novel PGE2 inhibition small molecules with the capacity to reduce cellular levels of PGE2 without affecting in vitro COX-2 activity, our group has recently reported a series of sulfonylhydrazide derivatives with interesting biological profiles. A series of novel sulfonylhydrazide derivatives were synthesi-zed and biologically evaluated for the inhibitory activities on LPS-induced PGE2 production in RAW 264.7 macrophage cells via intensive SAR study on unique sulfonylhydrazide scaffold. Among the compounds investigated, 1-(4-benzyloxyphenoxycarbonyl)-1-phenyl-2-(4-chlorophenyl)sulfonylhydrazide (MPO-0063) showed a strong inhibitory activity of PGE2 production (IC50 = 3.42±0.15 nM) from LPS-induced RAW 264.7 cells and its inhibition mechanism was elucidated using in silico docking studies.

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The 3D-QSAR approach for 5-(biphenyl-2-yl)-1*H*-tetrazole derivatives as angiotensin Ⅱ receptor type 1 (AT_1) antagonists

이선희 이재열*

경희대학교 화학과

As a development strategy for backups of Fimasartan (1), a comparative molecular similarity indices analysis (CoMSIA) of a set of sixty-five 5-(biphenyl-2-yl)-1*H*-tetrazole derivatives has been performed to find out the pharmacophore elements for angiotensin Ⅱ receptor type 1 (AT_1) blockade. The most potent compound containing pyrimidin-4(3*H*)-one ring, Fimasartan (1) was used to align the molecules. As a result, we obtained 3D-QSAR model which provided good predictivity for both the training set (q^2 = 0.846, r^2 = 0.975) and the external test set (r^2_{pred} = 0.980). This model would guide the design of backups for Fimasartan (1), a launched oral antihypertensive agent.

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Evaluation of iodoemodin for inhibition of breast cancer

박정훈 김보람 허민구 양승대*

한국원자력연구원 방사선기기연구부

Emodin(3-methyl-1,6,8-trihydroxyanthraquinone)은 대황, 하수오 등의 뿌리에서 추출되는 anthraquinone 천연물로서 항암 및 항염 등 다양한 생리활성을 가지며 세포분화를 관여하는 tyrosine kinase 을 억제시키는 효과가 있다. 특히, 유방암에 과발현되어 있는 HER-2 수용체를 특정적으로 억제시키는 저해제로서의 항암효과를 나타낸다. 본 연구에서는 형광면역법을 통해 일반적인 유방암을 발현시키는 MCF-7 대해 iodoemodin 과 emodin 의 세포섭취도를 비교하였고, 이 두 약물을 넣어 세포의 morphology 의 변화를 통해 세포가 사멸하는 것을 확인하였다. Iodoemodin 의 합성은 emodin 을 DMF 에 녹인 후, NaI 와 chloramin T 를 1 시간 동안 교반하여 하였다. Ammonium-acetate 와 methanol 을 이동상으로 역상-고성능액체크로마토그래피(RP-HPLC)법을 이용하여 iodoemodin 을 분리하였으며, H1-NMR 과 FT-IR 을 이용하여 분자구조를 확인하였다. 유방암 세포인 MCF-7 을 2000, 1000, 5000 씩 black 96 well plate 에 넣어 5% CO2, 37℃에서 24 시간동안 성장시켜 각각의 well 에 0.625uM 의 두 약물을 넣고 시간별로 (15 분, 30 분, 60 분, 120 분)로 phosphate buffered saline (PBS)으로 두 번씩 세척 후, 형광을 측정하였다. 그 결과, Emodin 은 60 분에서 형광의 세기의 가장 강하게 나타났고, iodoemodin 은 120 분에서 형광이 강하게 나타났으며, 형광의 세기는 두 물질이 비슷하게 나타났다.또한, MCF-7 의 morphology 를 확인하기 위해, 2×105 개 1ml 씩 24 well plate 에 넣어 5% CO2, 37℃에서 24 시간동안 성장시켜 각각의 well 에 2.5uM 의 iodoemodin 을 넣고 24, 48 시간 후, 세포의 morphology 를 현미경을 이용하여 관찰하였다. 그 결과, 시간이 지날수록 세포의 morphology 가 동그란 모양을 띄며 사멸하는 것을 확인하였다.

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Discovery of KR-36676 as a novel and oral active urotensin-II receptor antagonist

임채조* 김성환[1] 이규양

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Urotensin-II is a vasoactive cyclic peptide which was originally isolated from fish spinal cords and is widely expressed in several peripheral tissues including cardiovascular system. The urotensin-II ligand binds to a class of G protein-coupled receptor known as GPR 14 or the urotensin receptor (UT). The activation of the urotensin-II receptor (UT) as G protein-coupled receptor by binding of U-II exerts various cardiovascular effects in the peripheral vasculature, heart, skeletal muscle, pancreas and kidney. As the based on the previous results of UT function on biological and pharmaceutical study, UT would be a promising target for treatment of cardiovascular diseases, especially heart failure. In continuing our efforts to discover novel and potent UT antagonists, we recently identified a series of benzoxazinone derivatives, which exhibited potent UT binding activity. Among those compounds, KR-36676 showed highly potent UT binding activity. In addition, this compound exhibited good human and rat microsomal stability, no CYP inhibition and good in vivo PK profiles. The details synthesis, toxicity, in vivo PK profile and physicochemical property of KR-36676 will be discussed.

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Discovery of KR-36996 as a novel and oral active urotensin-II receptor antagonist

임채조* **장주영**[1] **이규양**

한국화학연구원 대사증후군치료제연구센터 [1]*과학기술연합대학원대학교(UST) 한국화학연구원 /의약및약품화학*

The urotensin-II ligand (U-II) is known as one of the most potent vasoconstrictor. The activation of the urotensin-II receptor (UT) as G protein-coupled receptor by binding of U-II exerts various cardiovascular effects in the peripheral vasculature, heart, skeletal muscle, pancreas and kidney. As the based on the previous biological and pharmacological study, UT would be a one of the most promising therapeutic target for treatment cardiovascular diseases, especially heart failure. As a part of our drug discovery projects on the development of novel and potent UT antagonists, we previously found that variously substituted benzothiophenyl amide scaffold exhibited potent UT binding activity. Further extensive and systematic SAR investigation leads to the identification of KR-36996, which showed highly potent UT binding acitivity. This compound also exhibited good human and rat microsomal stability, no CYP inhibition and good in vivo PK profiles. The details synthesis, toxicity, in vivo PK profile and physicochemical property of KR-36996 will be discussed.

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Synthesis of Pulsatilla saponin D Derivatives as Anti-lung Cancer Agent

황혜민 김민규[1] 정만길*

연세대학교 화학과 [1]연세대학교 화학과

Pulsatilla saponin D, a main component of SB365?, is extracted from roots of Pulsatilla koreana and used as natural product anticancer agent. Total syntheis of Pulsatilla saponin D was carried out using L-arabinose as a starting material in our lab for large quantity production because the yield of Pulsatilla saponin D extraction is too low. Pulsatilla saponin D was produced in a thirteen steps and the yield was 21.4%. Besides, pulsatilla saponin derivatives were synthesized with changing sugar chain part is attached to hederagenin. The pulasatilla saponin derivative which has α-D-mannopyranosyl-(1?3)-α-L-arabinopyranoside in sugar part has more potent anticancer activity. From this outcome, the synthesis of hederagenin derivatives with disaccharide and sugar parts of Pulsatilla saponin D (hederagenin 3-O-α-L-rhamnopyranosyl-(1?2)-[β -D-glucopyranosyl-(1?4)]- α -L-arabinopyranoside) was designed.

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Organelle-dependent drug efficacy in camptothecin delivery

이호연 김은진 김환명[1,*] 김종승[2,*] 강철훈[*]

경희대학교 동서의학대학원 [1]아주대학교 에너지시스템학부 [2]고려대학교 화학과

Intracellular metabolisms are compartmentalized into various organelles so that an organelle may have an unique set of metabolic enzymes, which is a critical basis of intracellular location-controlled drug delivery. In this presentation, several camptothecin prodrugs, designed to be delivered into different organelles, were examined in terms of its cytotoxicity, revealing that camptothecin delivered into lysosomes are inactivated to show significant anticancer activity, probably due to lysosomal hydrolysis of their lactone ring converting them to an inactive carboxylate form.

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Synthesis and SAR of LDK378 analogs as ALK inhibitors

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A series of LDK378 derivatives were synthesized to discover novel preclinical candidates as Anaplastic lymphoma kinase (ALK) inhibitors. ALK is a receptor tyrosine kinase as one of the insulin receptor superfamily. Lately, ALK has obtained tremendous attention due to the presence of ALK fusion genes found in various cancers.

A few months ago, LDK378 was approved by the US FDA in 2014 for ALK-positive non-small cell lung cancer. LDK378 was developed from TAE684 by modifying the 2-position side chain of pyrimidine core structures to overcome toxicity issues related to metabolism. With a similar approach, a variety of LDK378 analogs were designed and synthesized. The synthesis and SAR of analogs prepared will be presented.

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Gold-Coated Liposomes enhance doxorubicin release by Near-Infrared irradiation

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Remote triggered drug release from liposomal carrier by near-infrared (NIR) laser irradiation have been vigorously studied to increase drug release at target disease site. Although these approachs are showing promise, new approachs for development of advanced liposomal system are needed to make additional gains. Here, we prepared gold coated thermosensitive liposomes (Gc-TSL) capable of controlled drug release by NIR laser irradiation. Gold coating on the liposomal surface was performed by reduction of Au(Ⅲ) chloride and the amount of gold coated on the liposomal surface was measured by inductively coupled plasma (ICP). Doxorubicin (DOX) as a model drug was encapsulated into liposomes by pH gradient method and then we measured concentration of DOX by UV-vis spectro-photometry at 490nm. The size of DOX-loaded Gc-TSL (DOX/Gc-TSL) was 171.5 ± 8.3 nm and encapsulation efficiency of DOX was up to 90 %, respectively. Additionally, the release of DOX from DOX/Gc-TSL was 70 % increased by NIR laser irradiation (1.00 W/cm2 for 1 min) compared to TSL without gold coating, which mean increasing surface permeability of liposome caused by gold coating through photothermal conversion. Moreover, DOX/Gc-TSL treated group with NIR laser resulted in high cell cytotoxicity compared to DOX/Gc-TSL without NIR, DOX/TSL, and DOX/TSL with NIR laser. Taken together, we demonstrate the effect of gold coating on the liposomal surface by NIR laser and the DOX/Gc-TSL support the potential for remote triggered drug release system, which could be used for broad range of applications for photothermal therapy for various disease.

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PharosPrimer: PCR Primer Design Tool

정우성 김한조 서영주 강경태 장병하 윤정혁[1,*]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

PCR(Polymerase Chain Reaction) technique is innovative method to amplify desired region of DNA or RNA. This technique is widely used in molecular biology field. Furthermore, the fields that can be used are expanding because it's principle is very simple and it can be easily applied other fields such as medical science, food science, environmental science and others. The starting point of these simply and useful technique is primer design. The primer design process has to be considered to many conditions which related amplification efficiency such as reaction temperature for DNA denaturation or annealing, kinds of DNA polymerase, concentration of salt and others. Moreover, the good primers have to satisfy following fundamental terms. i) A length of 18-30 nucleotides ii) Melting temperature(Tm) of the primers between 65˚C and 75˚C iii) GC content to be between 40% and 60% iv) Avoid region GC or AT-rich region v) Avoid runs of 4 or more of one nucleotide or dinucleotide repeats v) Avoid intra and inter homology. Conventional methods should be considered a lot of details by the researchers. Here we present a simple tool, PharosPrimer, which can suggest PCR primer and calculate primer suitability using protein sequences. PharosPrimer needs only a few information such as vector sequence, insert position, Tm, primer length and so on and above-mentioned fundamental terms are calculated by tool automatically. The researchers do not have to think the above-mentioned fundamental terms anymore, just look and select. The primer design using PharosPrimer helps many the researchers who fulfill PCR with simple and easy operating method.

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QSAR Data Format: QF file

서영주 김한조 정우성 강경태 장병하 윤정혁[1,*]

(주)이큐스앤자루 신약개발연구소 [1](주)이큐스앤자루 -

The QSAR(Quantitative Structure-Activity Relationship) technique is for analyzing quantitative relationship between the structure of chemical and the efficacy or characteristic of the chemical. The QSAR is a difference in that it analyzes the quantitative relationship of mathematical expressions compared to the SAR which routinely performed by medicinal chemists. Since the research began in earnest, it has been developed in the direction of the development of new molecular descriptor and the application of statistical methods. In recent years, the increase in the number of computing resources and available data exponentially, and the technique has been further noted. Despite these important but there no standardized format is widely used. The standard format is very important. There was some effort for standardized format such as QSAR-ML, but there a limit that does not include the all QSAR data such as chemical information, molecular descriptor, prediction model, etc. and continuous development of the format did not proceed. For this reason, the development of standardized format of QSAR is necessary. Here we present a new QSAR data format, QF file, which include xml for data definition can and above-mentioned all QSAR-related data. The use of standardized format of QSAR guarantee the sameness of results and it is possible to ensure the convenience of the researchers. New standardized format for QSAR data helps many researchers in a variety of fields to perform the QSAR.

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Pyrimidine analogs with Bicyclic Amines as ALK inhibitors

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Anaplastic lymphoma kinase (ALK) is a potential target for non-small cell lung cancers. Crizotinib was first approved by the US FDA as a ALK inhibitor and a few more second generation ALK inhibitors are in clinical trials, including LDK378. Crizotinib has some adverse effects such as tumor regrowth. Thus, a new generation of ALK inhibitors is greatly required to overcome resistant issues.

Most of the ALK inhibitors have pyrimidine or pyridine core structures in addition to various side chains. As our ongoing search for ALK inhibitors, we recently designed and synthesized a series of structurally diverse pyrimidine analogs substituted with bicyclic amines, distinct from the existing ALK inhibitors. Some of them are as potent as LDK378. The synthesis and structure-activity relationship of analogs prepared will be discussed.

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Synthesis and evaluation of novel 2,4-diaminopyrimidines bearing substituted tetrahydrobenzoazepines for anaplastic lymphoma kinase (ALK) inhibitor as anticancer agents

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Anaplastic lymphoma kinase (ALK) belongs to the insulin receptor superfamily of tyrosine kinase. ALK-fused genes such as NPM-ALK, EML4-ALK, KIF5-ALK are putative oncogenes and responsible for many cancers including anaplastic large-cell lymphomas (ALCL), inflammatory myofibroblastic tumors (IMT), diffuse large B cell lymphoma (DLBCL) and a variety of solid tumor types. Crizotinib (Xalkori, Pfizer) is the first approved drug by FDA in 2011 for the treatment of ALK-positive lung cancer patients. Although crizotinib demonstrates initial impressive efficacy, patients eventually develop resistance with ALK mutations including L1196M, S1206Y, G1269A, G1202R, 1151Tins, etc. Recently, Ceritinib (LDK378, Zykadia, Novatis) was approved in 2014 for the treatment of ALK-positive cancer following treatment with crizotinib. LDK378 retains potency towards L1196M, G1269A, and S1206Y, but loses potency towards G1202R and 1151Tins. Here, we present synthesis and evaluation of novel 2,4-diaminopyrimidines bearing substituted tetrahydroisoquinoline moiety for ALK inhibitor.

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Pegylated 7-dehydrocholesterol derivatives an viatmin D_3 Precursor

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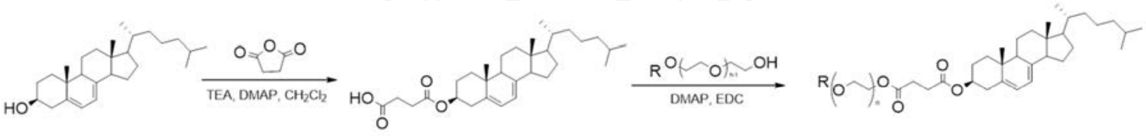
연세대학교 화학과 [1]연세대학교 화학및의화학과 [2](주)휴메딕스 경영, 중앙 연구소

7-Dehydrocholesterol (1) has been used as treatment of osteoporosis and antiaging and antioxidant reagent. Since the compound 1 is unstable and thus converted to several compounds by light, however, efficacy of 1 is quickly decreased. To improve the stability of 1, pegylation method was introduced. When 1 was reacted with succinic anhydride in the presence of TEA and DMAP in methylene chloride. 7-Dehydrocholesterol succinic acid 2 was obtained in good yield. The reaction of 2 with methoxy ethyleneglycol polymers in the presence of DMAP and EDC afforded the pegylated 7-dehydrocholesterol derivatives 3 in good yields. Thermal and light stability and solubility of 3 will be presented.



1 2 3

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Synthesis of Kojic acid derivatives and evaluation of their biological activity

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Kojic acid (KA) is produced by Aspergillus oryzae-sort of like mushrooms, which is commonly called as koji in Japan. KA is used as a chelation agent and a preservative preventing oxidative browning of fruits. KA also shows antibacterial and antifungal properties. Because KA stops the production of melanin by inhibiting tyrosinase in the biosynthetic pathway from tyrosine to melanin in skin, it has been applied as a skin lightening ingredient in cosmetics. Since some animal studies have shown that high amounts of KA had side effects such as in liver, kidney, reproductive, cardiovascular, gastrointestinal, respiratory, brain, and nervous system, more efficient KA derivatives are needed to be developed in order to safely apply as a skin lightening ingredient. A series of KA derivatives were synthesized and their in vitro tyrosinase inhibitory activities were evaluated. Specifically, the IC_{50} value of compound HBU-246 was 0.88±0.39 ?M against tyrosinase. It is about 50 times more effective tyrosinase inhibitor compared to KA itself (IC_{50} = 45.2±4.6 ?M).

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Identification of Antioxidative and Cholinesterase Inhibitory Compounds from Sargassum ringgoldianum

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In our continuing search for antioxidative and anti-cholinesterase compounds from marine alga, Sargassum ringgoldianum was examined and here we report the progress on the purification and structural determination of anti-cholinesterase compounds. From the 100 % methanol extract of S. ringgoldianum (300g), solvent partition fractions were prepared by using n-hexane(SRH), chloroform(SRC), butanol(SRB) and water(SRW). (SRH : 2.72g, SRC : 1.93g, SRB : 1.63g, SRW : 20.5g) Among them chloroform fraction (SRC) showed strong antioxidative and BuChE* inhibitory activities. The SRC of S. ringgoldianum showed about 56.0 % DPPH radical scavenging activity and 86.0 % BuChE inhibitory activity at 0.1mg/mL. Using various chromatographic methods and by the bioassay-guided fractionation, the SRC fraction was separated into six fractions, and each fraction showed antioxidative activity as 71.4, 88.8, 79.0, 79.7, 40.4, 34.1% at 0.1mg/mL, respectively. Especially, SRC-1 ~ SRC-4 showed strong antioxidative activities. The SRC-4 fraction (145mg) was further fractionated into 10 fractions(SRC-4-1~SRC-4-10) using preparative HPLC (Column : COSMOSIL packed 5C18, 20x250mm, 5um, Eluent : 90% MeOH, Flow rate : 5.0ml/min, UV : 220nm) and the SRC-4-6 (24.0mg) was further purified to give a single compound A (7.22mg). The structural analysis and biological activities of compound A will be reported.* BuChE : butyrylcholinesterase

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PET 진단용 방사성의약품을 위한 Sc,Ga-HBED-CC-Folate 합성 및 연구

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양전자 방출 핵종인 Sc-44 는, Ga-68 과 같이 방사성동위원소 발생장치 Generator 를 통해 쉽게 생산이 가능하고 Ga-68($t_{1/2}$:68 분) 보다 반감기가 약 3 배 길어 Ga-68 의 단점을 보완 할 수 있다. 양기능성 킬레이트제인 HBED-CC (N,N′-bis[2-hydroxy-5-(carboxyethyl)benzyl] ethylenediamine-N,N′-diacetic acid)는 Ga-68 과 표지 시 기존에 사용 되었던 DOTA (1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid), NOTA (1,4,7-triazacyclononane-1,4,7-triacetic acid) 킬레이트 보다 구조적 안정성과 반응성이 높고 암세포 섭취율과 혈류 내 제거속도가 더 뛰어난 것으로 보고된 바 있다. 따라서 Sc-44 를 HBED-CC 에 표지 하여 PET 진단용 방사성의약품으로 사용한다면 Ga-68 에 표지된 물질 보다 더 효율적일 것으로 사료된다. 타겟 물질인 Folate 는 난소암, 유방암, 간암, 폐암등과 같은 Folate-수용체를 발현하는 암세포에 잘 흡착되는 특성이 있기 때문에 Folate-수용체를 함유하고 있는 암세포에 대한 표적지향을 위해 Folate 를 HBED-CC 에 결합시켜 전구체인 HBED-CC-folate 를 합성하였다. 이에 기준물질로 안정동위원소인 Sc-45 와 Ga-69 로 ^{45}Sc-HBED-CC-Folate, ^{69}Ga-HBED-CC-Folate 착화합물을 온화한 조건에서 합성하였고 semi-prep HPLC 로 화합물을 분리하였다. 이후에 ^{1}H-NMR, LC/MS 를 이용하여 표지 여부 확인 및 표지수율을 측정 하였다. 그 다음 ^{45}Sc-HBED-CC-Folate 의 구조적 안정성을 확인하기 위해 2 시간 동안 37℃의 PBS(pH7)와 사람혈청 안에서 안정성을 측정하였고 차례로 ^{45}Sc-HBED-CC-Folate 의 신체 내 배설경로를 예측하기 위해 지용성 평가를 실시하였다. Ga-68 을 HBED-CC-Folate 에 표지시켜 CT-26, HeLa, HepG2 와 같은 Folate-수용체를 함유한 암세포와의 섭취도를 확인함으로서 Sc-44 와

Ga-68 표지 HBED-CC-Folate 착화합물의 방사성의약품으로서의 활용 가능성을 연구하였고, PET 이미징 시약으로서 사용가능 할 것으로 보여진다.

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Microwave Assisted Synthesis and Biological Activities of Novel Schiff Base Derivatives

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공주대학교 생명과학과

Recently, there has been significant interest in the design and synthesis of novel heterocyclic compounds with promising biological activities. Schiff base derivatives are an important group of organic compounds and its derivatives are significantly important because of their potential applications in medicinal chemistry. Herein, a series of eight imine derivatives have been synthesized through microwave assisted Schiff base formation by reacting 2-(4-methoxyphenyl)acetohydrazide (3) and 4-amino-3-(4-methoxybenzyl)-1H-1,2,4-triazole-5(4H)-thione (6) with different substituted aldehydes. The structures of the newly synthesized compounds were characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectral analysis. All the synthesized derivatives were screened for their in vivo anti-inflammatory as well as in vitro anti-oxidant activities using carrageenan induced rat paw edema test and DPPH free radical scavenging assay, respectively. The compounds 4a, 4c, 7a and 7c significantly lowers the volume of rat paw edema (P

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Synthesis and evaluation of 5-(3-(pyrazin-2-yl)benzylidene)thiazolidine-2,4-dione derivatives as pan-Pim kinases inhibitors

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Pim kinases are frequently overexpressed in leukemia, lymphoma and some solid tumors. Pim kinases are involved in many cellular phenomena such as transcription, translation, growth, survival and apoptosis resistance of cancer cell. Thus, Pim kinases are considered as a potential target for cancer therapy. A novel series of 5-benzylidenethiazolidine-2,4-diones were synthesized as Pim kinases inhibitors. The structure-activity relationships (SAR) studies were performed. Hydroxyl group at 2-position of the benzene ring in 5-benzylidenethiazolidine-2,4-dione was found to be important for inhibitory activity against Pim kinases. Introduction of a pyrazinyl group at 5-position of the benzene ring of 5-benzylidenethiazolidine-2,4-dione improved activity significantly. Potency of the synthesized compound were improved against Pim-1 and Pim-3 kinase up to the detection limit, IC50< 0.0005 uM. Compound 5i showed dose-dependent anti-proliferative activity with 0.8 uM EC50 value in MV4-11 leukemia cell line.

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Novel series of Meridianin C derivatives as potent inhibitors of Pim kinases with antiproliferative activity against cancer cells

MORE KUNAL HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

The proto-oncogene proviral integration site for moloney murine leukemia virus kinases i.e. Pim kinases are serine/threonine kinases which are involved in many cell processes such as survival, apoptosis, differentiation and proliferation of normal as well as cancerous cell lines.Overexpression or dysfunction of these kinases may leads malignancies such as colon, prostate cancer and hematologic malignancies including lymphomas, chronic lymphocytic leukemia and acute leukemias. Meridianins (marine indole alkaloids) are previously reported to have protein kinase inhibition activity. 3,5-Disubsitituted indole also known to possess potent Pim kinase inhibition activity. A novel series of Meridianin C derivatives was synthesized and evaluated for Pim kinase inhibition as well as antiproliferative activity against cancer cell lines. Introduction of substituted pyrazine-2-yl at 5-position of indole ring improve potency from micromolar to nanomolar level. Compound 7f showed potent pim-1 and 3 inhibitions with single digit nanomolar IC50. It also found highly selective towards Pim kinase when evaluated against panel of 14 protein kinases. In antiproliferative study 7f showed dose-dependent growth inhibition of leukemia cell lines.

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Synthesis of Quinolinyl Substituted Triazolothiadiazole Derivatives and their Bioassay

MUHAMMAD RAFIQ 서승염*

공주대학교 생명과학과

A series of aralkanoic acid Ia-h was converted into aralkanoic acid hydrazides IIIa-h through their esters formation. The aralkanoic acid hydrazides IIIa-h upon treatment with carbon disulfide and methanolic potassium hydroxide yielded potassium dithiocarbazinate salts IVa-h which on refluxing with aqueous hydrazine hydrate yielded 5-aralkyl-4-amino-3-mercapto-1,2,4-triazoles Va-h. The target compounds, 3-aralkyl-6-(substitutedquinolinyl) [1,2,4]triazolo[3,4-b][1,3,4] thiadiazoles VIa?v were synthesized by condensing various quinolinyl substituted carboxylic acids with 5-aralkyl-4-amino-3-mercapto-1,2,4-triazoles Va-h in phosphorus oxychloride. The structures of the newly synthesized compounds VIa-v were characterized by IR, ^{1}H NMR, ^{13}C NMR and elemental analysis studies. The structure of one of the compound Vf was unambiguously deduced by single crystal X-ray diffraction analysis. All the synthesized compounds VIa-v was screened for their acetylcholinesterase inhibition activities. Compounds VIi, VIk, VIn and VIs exhibited excellent acetylcholinesterase inhibition activities as compared to the reference inhibitor.

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Synthesis and Evaluation of Antioxidative activity of 2,4-disubstituted Phenol derivatives

이서정 HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

Interest in antioxidants has been increased with the accumulation of evidences that reactive oxygen species (ROS) in the body are the main causes of diverse diseases such as cancer, diabetes, inflammation, neurological disorders and cardiovascular disease. Phenolic compounds have been reported to have antioxidative activity. BHA and BHT (butylated phenolic compound) have known to deplete reactive oxygen species (ROS) and have been used as antioxidants and preservatives in food, cosmetics, rubber and medicine. However, intake of synthetic antioxidants such as BHT and BHA are restricted due to the risk of lipid transformation, odor and cancer. A novel derivatization of phenol was performed to improve antioxidant activity and overcome the adverse effects caused by antioxidants which are widely used. As an initial step, 2,4-disubstituted phenol analogues were synthesized and evaluated for their antioxidative properties using DPPH radical scavenging study.

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α-Glucosidase and Acetylcholinesterase Inhibition Activities of Novel Sulfonamide Derivatives

MUHAMMAD RAFIQ 서승염*

공주대학교 생명과학학과

Recently, there has been increasing interest in the design and synthesis of novel heterocyclic compounds with auspicious biological profile due to their fundamental medical and biological applications. Herein, a series of four substituted sulfonamide derivatives have been synthesized by refluxing 4-amino-3-(4-methoxybenzyl)-1H-1,2,4-triazole-5(4H)-thione (5) with several substituted sulfonyl chloride in methanol. The structures of the newly synthesized compounds were characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectral analysis. All the synthesized derivatives were evaluated for their in vitro acetylcholinesterase as well as α-glucosidase inhibition activities. Almost all of the synthesized compounds are excellent inhibitors of acetylcholinesterase and α-glucosidase as compare to the standard inhibitors tacrine in former case and acarbose in later case. The high product yield, short reaction time and convenient handling are the advantageous features of newly synthesized compounds 6a-d which might have practical applicability.

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Synthesis and antiproliferative activity of 3,5-Disubstituted indole

MORE KUNAL HONG VICTOR SUKBONG 이진호*

계명대학교 화학과

Pim kinase is a family of kinase comprising of highly homologus members as Pim-1,2 and 3, encoding for serine/threonine specific kinases. This enzyme is linked to many cell functions as cell growth, differentiation, proliferation and apoptosis. Deregulated Pim kinase expression or over expression may lead to many cancers as colon, pancreatic, and prostate cancer. Thus Pim kinases are very promising targets for the treatment of cancers.3,5-Disubstituted indole alkaloids have been reported to have inhibitory activity against protein kinases including Pim kinases. Based on the previous results, we synthesized a novel series of compounds bearing 2-aminopyrimidine at 3- and 5-position of indole. Structure activity relationship was studied by modifying the substituent at 6-position of 2-aminopyrimidine attached at 5-position of indole. Compound 6c found to be potent to all three isoformes of Pim kinase. It selectively inhibits Pim kinase among panel of 14 protein kinase. Also compound 6c showed dose-dependent inhibition in leukemic cell lines.

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Synthesis and Antitubercular Activity of Extended Carbon C-7 substituted Nitroimidazole analogues of PA-824

강영구 박찬용 Garima Arora[1] Ramandeep Singh[1] 유찬모[*] 이일영[2,*]

성균관대학교 화학과 [1]Translational Health Science and Technology Institute, India [2]한국화학연구원 신물질연구단 난치성질환치료제연구센터

Recently the re-emergence of tuberculosis (TB) in the world wide, accompanied by the rise of multidrug-resistant (MDR) strains, emphasizes the need for the discovery of new therapeutic drugs with greater efficacy, safety and novel mechanism of action against this disease. In the course of continuing efforts to sturdy for development new TB drug candidates like salicylanilides, recently we selected PA-824 as a promising new class. The PA-824 ((6S)-2-nitro-6-{[4-(trifluoromethoxy)benzyl]oxy}-6,7-dihydro-5H-imidazo[2,1-b][1,3] oxazine) containing nitroimiazole has entered phase II clinical trials as novel TB therapeutics. OPC-67683 has already done clinical trials. The mechanism of action of PA-824 and OPC-67683 involved as mycolic acid synthesis inhibitors and intracellular nitric oxide (NO) release for respiratory poisoning under aerobic and anaerobic conditions. Although many side chain analogue at C-6 position of PA-824, we try to extend carbon at C-7 position nitroimidazole derivate to improve inhibitory effect for antituberculosis than conventional monocyclic nitro imidazole compound.

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Novel Pyrrolo-Pyrimidine Derivativesas as FGFR4, Tie2/TEK and TrkA Kinase Inhibitors; Design, Synthesis and Biological Evaluation for Anticancer agents

이주현 서선희[1] 강순방[1] 정낙철 금교창[2,*]

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

Development of kinase inhibitors has been extensively progressed as a target of cancer therapy. Among kinase inhibitors, we are interested in the pyrrolo-pyrimidine based inhibitors such as PKI166 (EGFR), CP-690 (JAK3), MPS-1-IN-1 (Mps1) and Meriolins (CDK2).Herein, a series of pyrrolo-pyrimidine derivatives were synthesized, and assessed against cancer cell lines and kinases. Several compounds, in the preliminary screening, displayed high EC50 values less than 4.5 μM against SK-BR-3, MCF-7 and HCT116 in in vitro assay. Among them, KKK5097 and 50101 showed high growth inhibitory effects against 60 cancer cell lines in the NCI-60 DTP screening program. The two compounds displayed high selectivity of FGFR4, Ti2/TEK and TrkA kinases against 59 kinds of kinase by Reaction Biology Corp. In particular, KKK5101 showed high IC50 values of those kinases, 6.71, 6.84 and 2.25 μM, respectively.

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Highly Stable and Sensitive Iodine-125 embedded Au-NNPs for Sensitive SPECT Imaging Probe

임동권* 이상봉 국현[1] 김수민

전북대학교 BIN 융합공학과 [1]전북대학교 BIN융합공학과

Radio-labelled gold nanoparticles (AuNPs) have been investigated for sensitive CT, SPECT imaging probe because of excellent biocompatibility, facile synthesis, and easy surface chemistry of AuNPs. Due to the lack of robust modification chemistry of iodine on the AuNP, the sensitivity and biological stability of labelled Iodine (125) was not enough to be used as practical SPECT-based imaging modality. Here, we propose robust iodine modification chemistry achieved simply by use of adenine-rich oligonucleotide-modified AuNPs and additional chemistry with SHPP, which is similar functional group with tyrosine. Therefore, lots of radio-active iodine can be modified per single gold nanoparticle through the reaction with Na125I, chloramine-T, and sodium bissulfite. To generate stable imaging probe, additional gold shell was formed on iodine labelled AuNP core and then the resulting particle (Au-NNP) was protected with mPEG thiol. The efficiency of radio-labelling reaction on gold and radio-activities of resulting Au-NNPs depends on the core particle size were investigated by use of three different DNA-AuNP size (5 nm, 15 nm, 20 nm). The Au-NNPs showed greatly improved stability of 125I-labelling by preventing possible hydrolysis or enzymatic attacks in in-vitro performed with human serum at 37 °C and in-vivo studied with nude mice.

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3D-QSAR(quantitative structure-activity relationship) studies of selective thyroid hormone receptor β

김보혜 변나연 이성광*

한남대학교 화학과

Thyroid hormone is a type of hormone that is secreted by the thyroid gland of vertebrates, controlling metabolism by catabolic, involved in the development and growth of mammalian. Thyroid hormone receptor beta(TRβ) is particularly important for the growth of the liver or tissue. Especially, TRβ is a hormone-activated transcription factors known to be important in fetal and neonatal brain development. In this study, quantitative structure acitivity relationship were applied to construct a predictive model for the treatment of non-thyroid disease. Three-dimensional quantitative structure-activity relationship (3D-QSAR) models of 124 selective ligands for the thyroid hormone receptor β1(TRβ1) were developed using multiple linear regression (MLR) and support vector machine (SVM). The built model was fully assessed by various validation methods, including internal and external validation and Y-randomization test.

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Predicting human intestinal absorption and skin permeability of organic compounds using QSAR analysis

송현주 이성광* 변나연

한남대학교 화학과

Human intestinal absorption(HIA) for oral drugs, and skin permeability for transdermal patch are one of most important properties in the modeling in the development of new drugs. As such data are not available for new candidate drug, and therefore must be estimated. In this study, we were tried to predict HIA and skin permeability by using quantitative structure-activity relationships(QSAR). Using the collected data for HIA and skin permeability, the molecular descriptors were calculated from PreADMET program and dataset was divided into traning and test set by using the sphere exclusion method. Multiple linear regression(MLR) and support vector machine(SVM) were used to develop the QSAR models. After several validating the model with bootstrap and y-scrambling method, the reliable prediction range will be set from applicability domain(AD) in the model. The performance of each model were compared with R2 , RMSE(root mean square error), and MAE(mean absolute error) for training and test set.

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Quantitative Structure-Activity Relationship(QSAR) modelling for odor thresholds of odorous molecules

서민 이종혁 이성광*

한남대학교 화학과

The odor thresholds are detection thresholds for odor substances. The detection of odors in humans occurs at the nasal cavity through the olfactory nerve. These odors cause negative consequences, such as discomfort or annoyance or sick house syndrome. Therefore, we can prevent that warning signals of gas leakage or similar accidents by prediction of odor thresholds. In this study, QSAR models for predicting odor thresholds of odorous molecules with 2D molecular descriptors have been developed. Odor thresholds value for 223 compounds were obtained Nagata data set. Then, the data set was splitted into a training set for 111 compounds and a test set for 112 compounds by sphere exclusion method(SEM). Effective subset of descriptors was selected on forward selection method with multiple linear regression (MLR) and support vector machine(SVM). All models were evaluated by bootstrap method and y-scrambling. The results indicate that new QSAR models aids in designing a library a new odorous compounds with better predicted response.

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The analysis of water network for kinase inhibitor potency and selectivity prediction: A case study of kinase binding to staurosporine

장우대 강남숙*

충남대학교 신약전문대학원

Protein kinases are of important drug target within the pharmaceutical industry. However, the design of potent and selective inhibitors can be challenging, because almost all protein kinases share the same fold and similar ATP binding sites. Here, in order to understand the kinase inhibitor potency and selectivity, we studied complexes of protein kinases with staurosporine. By molecular dynamics simulations, we investigated the structural role of water molecules. The hydrogen-bonded cyclic water rings within the ATP binding sites especially revealed significant features about the flexibility and the potential interactions of the protein kinases. Displacing water rings with frequent formation on the specific regions by kinase inhibitors has a propensity to enhance binding affinity. These results were compared to most current theoretical models that only consider steric and electrostatic factors. We found that desolvation effect is a critical role in protein-ligand binding mechanisms. This information can guide rational drug design by suggesting regions of the binding hot-spots that will be beneficial to displace by adding new chemical fragments to the ligand.

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Cu-Catalyzed Domino Reactions for Indole- to All Regio-isomeric Azaindole-2-carboxylates

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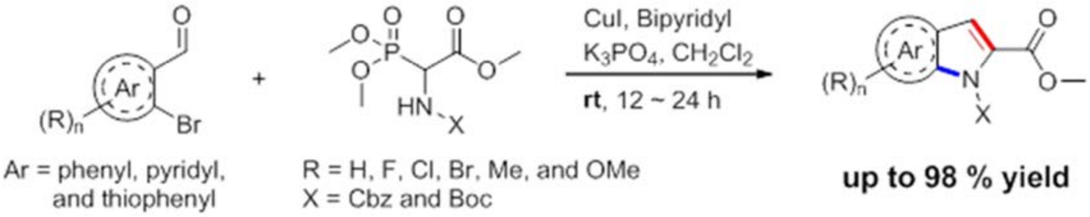
한국화학연구원 의약화학연구센터 [1]한양대학교 화학과 [2]충남대학교 신약전문대학원

The syntheses of various N-protected aromatic-ring fused pyrrole-2-carboxylate derivatives have been accomplished using mild one-pot Cu-catalyzed domino reactions. Cu-catalyzed domino reactions of various 2-bromo arylcarboxaldehyde with commercially available N-protected phosphonoglycine trimethylester gave the desired aromatic-ring fused pyrrole-2-carboxylates in good to excellent yields. The optimized conditions showed broad substrate compatibility, without the loss of the protecting group.



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Development of Fluorescent Chalcone-mimicking Probes for the Detection of β-amyloid Plaques in the Brain from Alzheimer's Diesease

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Alzheimer’s disease (AD) is a progressive neurodegenerative disease characterized by cognitive decline, irreversible memory loss, disorientation, and language impairment. The formation and deposition of β-amyloid (Aβ) plaques consisting mainly of Aβ peptides in the brain is now considered one of the most significant factors in AD. Currently, the definitive diagnosis of AD is dependent on only the histopathological examination of Aβ plaques in the postmortem brain. Therefore, in vivo imaging of Aβ plaques in the living brain may lead to the early detection of AD or monitoring the progression and effectiveness of novel treatments that are currently being investigated. In this study, we synthesized two chalcone-mimicking probes (9 and 10) and evaluated their fluorescent characterization and biological activities with Aβ aggregates. Two probes exhibited a approximately 50-fold increase of emission spectra after mixing with Aβ aggregates. The binding affinities for Aβ aggregates were shown as the KD value (1.59 for 9 and 2.30 for 10). We also investigated their neuropathological staining of Aβ plaques in transgenic mouse (APP/PS1) brain sections. The results suggest that chalcone derivatives have high binding affinities for amyloid plaques in transgenic mice brain, as reflected by an in vitro binding assay using Aβ aggregates may be more useful for presymptomatic and the early detection of AD pathology.

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Development of the fluorescent probe for the imaging of β-amyloid plaques : Catechol derivative

정승진 이준영[1] 김보람[2] 이상윤[1] 박정훈[2] 허민구[2] 양승대[2] 박용대[2,*]

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Alzheimer’s disease (AD) is a progressive neurodegenerative disorder pathologically characterized by deposition of mis-folded β-amyloid (Aβ) peptides as senile plaques in the brain. Because the deposition of Aβ plaques is an early event in the development of AD, a validated biomarker of Aβ deposition in the brain might prove useful to identify and to assist in the evaluation of new anti-amyloid therapies currently under development. Fluorescent probes that can stain Aβ plaques have gained increasing interest as potential tools for monitoring the progression of AD. In this study, fluorescent probe contained catechol ring for the Aβ plaques was developed and evaluated the optical properties for Aβ peptides. The developed catechol probe exhibited an approximately 34-fold increase in emission intensity after mixing with Aβ peptide, a high affinity for Aβ peptide (KD = 0.35 ?M),and the reasonable hydrophobic property (logP = 2.94) to penetrate the blood barrier brain. We also confirmed our catechol probe specifically stained Aβ plaques in the histological costaining using transgenic mice (APP/PS1) brain sections. Our catechol probe showed a possibility to be fluorescent probe for detecting Aβ plaques in the brain from AD.

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Development of a fluorescent probe for the in vivo staining of the Aβ plaques

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Alzheimer’s disease (AD) is a progressive neurodegenerative disease characterized by cognitive decline, irreversible memory loss, disorientation, and language impairment. The formation and deposition of β-amyloid (Aβ) plaques consisting mainly of Aβ peptides in the brain is now considered one of the most significant factors in AD. Fluorescent probes that can detect Aβ plaques have gained increasing interest as potential tools for monitoring the progression of AD in vitro and in vivo. In this study, three chalcone-mimicking fluorescent probes were designed and prepared. Of the developed probes, 14c had the emission spectra of 640 nm suitable for in vivo fluorescence imaging. 14c exhibited the highest fold increase (93.6-fold) in fluorescence intensity upon binding to Aβ aggregates and the highest binding affinity (KD = 0.85 uM) for Aβ1-42 peptides. 14c showed the suitable lipophilicity (Log P value = 3.15) to penetrate the BBB. Probe 14c also selectively stained Aβ plaques in brain sections from transgenic AD model mice that corresponded with the in vitro results. Finally, we confirmed that probe 14c could stain the Aβ plaques through the BBB in the in vivo imaging using double transgenic mice (APP/PS1). Chalcone-mimicking probe 14c fulfilled the most of the requirements for a fluorescent probe for the detection of Aβ plaques, which suggested that probe 14c could be a good probe for the diagnosis of AD.

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Design, Synthesis of Novel Heterocyclic-substituted pyrazolo-pyridine derivatives as inhibitors of NF-kB Transcription Regulation

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Pyrazolopyridine and related fused heterocycles are of interest as potential bioactive molecules. Novel heterocyclic ring-substituted pyrazolo-pyridine derivatives have been designed as inhibitors of NF-kB transcription regulation from the modification of previous studies. These inhibitors are expected to be useful candidates for treatment of inflammation-related diseases.

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In silico approach toward discovery of histone deacteylase III inhibitors: identification of substrate-binding site inhibitors based on structure-based drug design

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Histone deacetylases(HDAC) are enzymes that deacetylate ε-N-acetyl lysine amino acid on a histone, which play an important role to regulate DNA expression.They are categorized into four classes depending on sequence homology to the yeast original enzymes and domain organization. Among them, class III of mammalian HDACs includes seven members of enzymes, so called sirtuins (SIRT1-7) that share a conserved catalytic core domain with varying N-terminus and C-terminus. In humans, these enzymes possess either NAD+ dependent deacetylase activity or protein ADP-ribosyltransferase activity. Sirtuins have been implicated in influencing various cellular processes like aging, transcription, apoptosis, inflammation and stress resistance. Sirtuins can also control circadian clocks and mitochondrial biogenesis. Therefore, identification of selective SIRT inhibitors allows us to explore a wide range of epigenetic regulation involving human diseases.Up to date, only several pan-HDAC inhibitors have been developed. Thus, many researchers are searching for a more potent and selective inhibitors than the benchmark compounds. In general, substrate-mimic compounds provides a fresh starting point for the development of novel SIRT inhibitors rather than inhibitors binding putatively to NAD+ binding site. In addition, it is expected that compounds which could mimic the binding of the acetylated peptide substrate might be potent and selective inhibitors of Sir2 deacetylases over other NAD+-metabolizing enzymes.Herein, we report our efforts towards discovery of novel small molecule SIRT inhibitors targeting substrate binding site employing structure based drug design.

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Synthesis and biological evaluation of thienopyrimidine derivativesas GPR119 agonists

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Diabetes is a metabolic disorder that occurs when the pancreas does not produce enough insulin, or the body cannot effectively use existing insulin. Hyperglycemia (high blood glucose) can lead to various health consequences such as kidney damage, heart disease, stroke, nerve damage and blindness. Type 2 diabetes mellitus (T2DM, or noninsulin dependent), is the most common form of diabetes caused by insulin resistance, and loss of pancreatic b-cell function and approximately 95% diabetic patients are suffering from type 2 diabetes. This health burden is growing at an alarming rate, and it is estimated that there are approximately 350 million diabetic people globally. The prevalence of the disease is expected to escalate to 439 million by 2030. We identified a series of thienopyrimidine derivatives as GPR119 agonist and will present the synthesis and biological data.

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Unlocking the pH-Responsive Degradability of Fumaramic Acid Derivatives Using Photoisomerization

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본연구진은 fumaric acid derivatives 가 photosensitivity 와 pH-sensitivity 의 dual sensitivity 를 갖는다는 성질을 이용하여 효과적인 약물전달체로서의 역할을 기대하고 있음. fumaric acid derivatives 는 효과적인 dual signal sensitivity 를 갖는 moiety 로써 light sensitivity 는 wavelength, intensity 등을 효과적으로 조절할 수 있는 장점이 있으며,pH sensitivity 는 염증부위의 낮은 pH 에서 degradation 되는 성질을 갖는 장점을 갖음. 본연구진은 또한 fumaric acid 의 여러가지 derivatives 를 합성해 더 효과적인 약물전달체로서의 성질을 비교해 봄.

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The Synthesis and Biological Evaluation of 2-Amino-4-Arylthiazole Derivatives as 3D Polymerase Inhibitor against Foot-and-Mouth Disease

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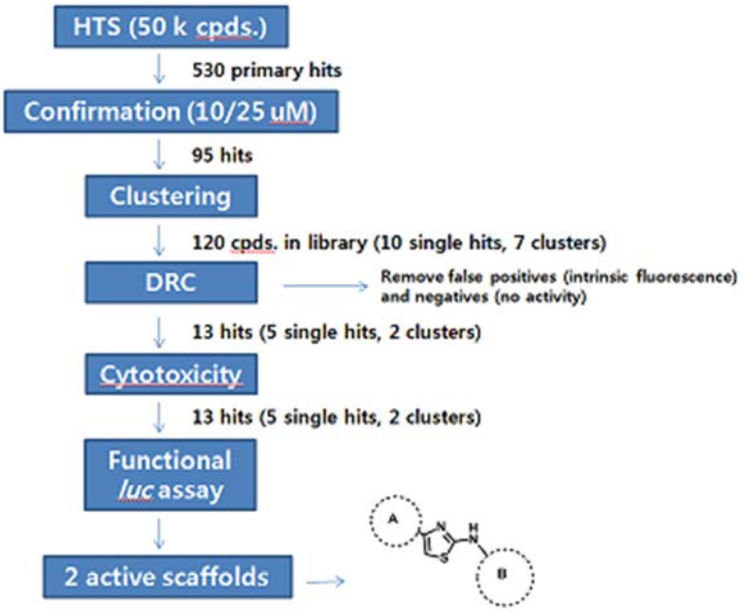
경기과학기술진흥원 연구개발팀 [1]경기바이오센터

Foot-and mouth disease(FMD) has been described as the most contagious disease of livestock, e.g. cattle, sheep, goats and other cloven-hoofed animals. Foot-and-Mouth Disease is caused by Foot-and-Mouth Disease Virus (FMDV) which is a member of the Aphthovirus in the Picornaviridae family. The FMDV genome is single-stranded RNA able to translate a single polyprotein including structural and non-structural proteins. The non-structural proteins are comprised of 3C protease to cleave single polyprotein into functional proteins and 3D polymerase to carry out RNA synthesis during transcription and replication. Unlikely structural proteins, non-structural proteins, especially 3D polymerase is the primary drug target because of the pivotal role in the viral life cycle.Initially, in order to find hit compounds to inhibit 3D polymerase of FMDV, 50,000 compounds stored in Gyeonggi-biocenter's chemical library were screened by High throughput screening (HTS) applied fluorescence polarization(FP) assay. 13 compounds showed enzyme inhibitory activity at concentration of in low uM range. For hit validation of these compounds, enzyme inhibitory activities were evaluated with functional luciferase assay. Cytotoxic molecules were also removed by CCK-8 using BHK cells. As well, false positive compounds showing non-specific binding and chemically unstable compounds were ruled out final hit validation.Subsequently, the derivatives of validated compound 1 were synthesized and evaluated for the inhibitory activity of 3Dpol via Structure-activity relationship. The derivatives were relatively stable against metabolic degradation or modification and showed antiviral activity at IBRS-2 cells infected by FMDV O/SKR/2010 strain which formerly provoked nationwide disaster in 2010.

[3D polymerase inhibitor screening]



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Chemical-thermal-electrical Energy Conversion via Thermopower Wave in ZnO Nanostructures/Fuel Composites

이강열

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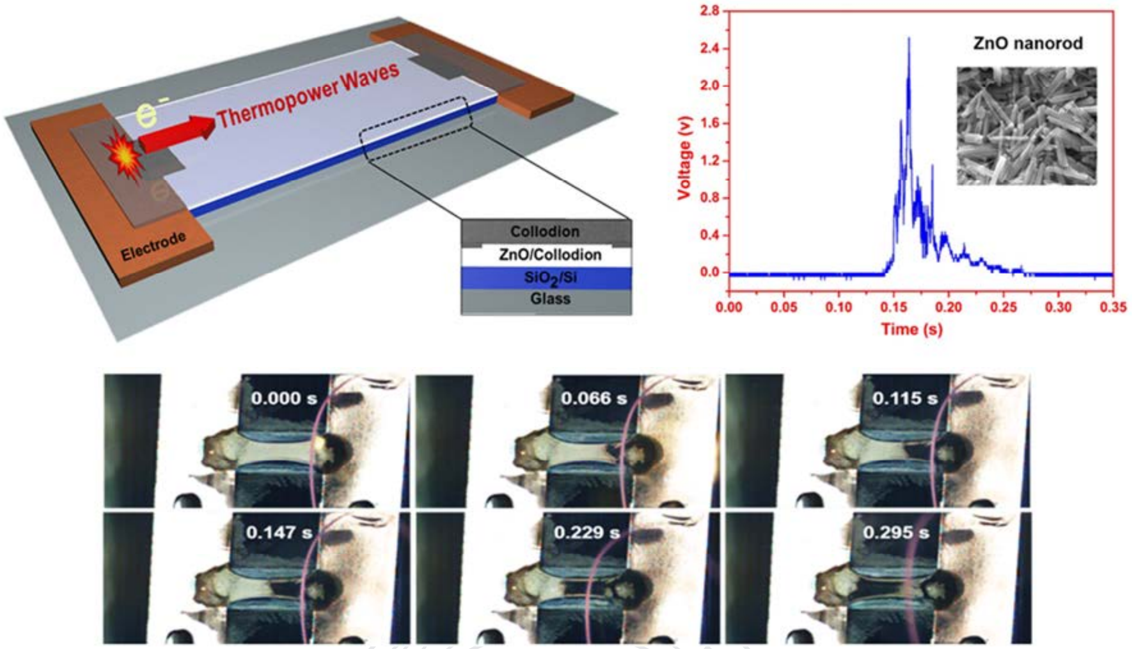
Thermopower wave is a new concept of energy conversion from chemical to thermal to electrical energy, produced from the chemical reaction in well-designed hybrid structures between nanomaterials and combustible fuels. The enhancement and optimization of energy generation is essential to make it useful for future applications. In this study, we demonstrate that simple solution-based synthesized zinc oxide (ZnO) nanostructures, such as nanorods and nanoparticles are capable of generating high output voltage from thermopower waves. In particular, an astonishing improvement in the output voltage (up to 3 V; average 2.3 V) was achieved in a ZnO nanorods-based composite film with a solid fuel (collodion, 5% nitrocellulose), which generated an exothermic chemical reaction. Detailed analyses of thermopower waves in ZnO nanorods- and cube-like nanoparticles-based hybrid composites have been reported in which nanostructures, output voltage profile, wave propagation velocities, and surface temperature have been characterized. The average combustion velocities for a ZnO nanorods/fuel and a ZnO cube-like nanoparticles/fuel composites were 40.3 mm/s and 30.0 mm/s, while the average output voltages for these composites were 2.3 V and 1.73 V. The high output voltage was attributed to the amplified temperature in intermixed composite of ZnO nanostructures and fuel due to the confined diffusive heat transfer in nanostructures. Moreover, the extended interfacial areas between ZnO nanorods and fuel induced large amplification in the dynamic change of the chemical potential, and it resulted in the enhanced output voltage. The differences of reaction velocity and the output voltage between ZnO nanorods- and ZnO cube-like nanoparticles-based composites were attributed to variations in electron mobility and grain boundary, as well as thermal conductivities of ZnO nanorods and particles. Understanding this astonishing increase and the variation of the output voltage and reaction velocity, precise ZnO

nanostructures, will help in formulating specific strategies for obtaining enhanced energy generation from thermopower waves.



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High Performance Flexible Supercapacitor Electrodes Composed of Ultralarge Graphene Sheets and Vanadium Dioxide

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Ultralarge graphene oxide sheets (ULGO) is highly desirable as a material for a variety of electronic devices because of outstanding electrical conductivity attributed to large surface area. Here, ULGO sheets were produced using Hummers method modified by a thermal expansion and centrifugation step. The largest lateral size of the obtained ULGO sheets was larger than 150 um, corresponding to ~ 22,500 um^2 in area. In addition, we report not only a facile approach to fabricate electrodes with vanadium dioxide (VO_2) /reduced graphene oxide (rGO) thin film using a vacuum filtration method, but also the effects on the electrochemical performances of the VO_2/rGO composite films according to lateral size of GO sheets. The electrochemical performances of VO_2/rGO film electrodes were investigated using a three-electrode system in 0.5 M K_2SO_4 electrolyte. The VO_2/ULrGO film electrode shows an improved capacitive performance compared to the VO_2/SrGO (small reduced graphene oxide) film electrode, yielding a specific capacitance of 769 F/g at a current density of 1 A/g. It was found that the size of 2D GO sheets have substantial influence on the electrical conductivity and electrochemical properties of the composite VO_2/rGO film, because large scale sheet area tends to contribute to the improvement of the electron transfer rates. Therefore, the VO_2/ULrGO film will be a promising electrode material for a high performance supercapacitor, because of their excellent flexibility and capacitive characteristics.

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Self-organization Process of Achiral Tetrathiafulvalene Molecule Induced by Face-to-face Interaction

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To control molecular arrangement and morphology from the nano to micro length scale , the achiral asymmetric molecule (abbreviated as AT1M) containing the tetrathiafulvalene (TTF) was synthesized and characterized. On the basis of the 2D WAXD techniques, a highly ordered monoclinic crystal of AT1M is clearly identified. Furthermore, the combination of SAED, TEM, AFM techniques observed formation of the scrolled and helical ribbons as well as flat ribbons from achiral AT1M compounds. The scrolled and helical structures are originated by imbalanced surface stresses resulting from the molecular packing in the monoclinic cell of the crystalline phase. The outstanding optical and electrochemical properties of AT1M is investigated using UV-Vis. and CV. This work was mainly supported by the Basic Science Research Program, and BK21 PLUS Program, Korea.

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Preparation of various twinned morphologies of ZnO crystals and their antibacterial activities

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Morphology-controlled synthesis of twinned structural ZnO crystals was prepared by using a hydrothermal reaction. The sodium 1-heptanesulfonate was used as a morphology modifier. The concentration of sodium 1-heptanesulfonate plays an important role in the formation of twinned structural ZnO crystals with various aspect ratios. The twinned ZnO crystals evolve from thin hexagonal rod with bipyramidal ends to thick hexagonal plates with the concentration of sodium 1-heptanesulfonate. The XRD intensity ratio of the (001) polar plane to the (110) nonpolar plane of ZnO crystals was also increases with the concentration of sodium 1-heptanesulfonate. The morphology-dependent antibacterial activity of the twinned structural ZnO crystals was also investigated. We found that the antibacterial activity of the twinned structural ZnO crystals was strongly dependent on a polar properties of the (001) plane of ZnO crystals.

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Size Dependent Photodynamic Anticancer Activity of Fe3O4@HP Nanoparticles

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강릉원주대학교 화학과

Until recently, photodynamic therapy(PDT) is quite promising approach for killing various cancer cells. The reason of this rapid growth was that PDT was a convenient and non-invasive treatment for several types of cancer. Herein, photofunctional magnetic Fe3O4@HP particles with controlled size were fabricated successfully via a simple surface modification process. Microstructure and magnetic properties of the Fe3O4@HP nanoparticles are investigated by FE-SEM, TEM and VSM. Biocompativility and photokilling activity are also evaluated using mammalian cells in vitro to confirm the potential as an agent for PDT application. From this work, our Fe3O4@HP nanoparticles can be useful for PDT, although further studies for evaluation the cell death mechanisms in vitro and in vivo will be needed to verify the potential for clinical PDT application.

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Nanocomposites of Au nanoparticles/Nanostructured Pt thin films and their SERS effect

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성균관대학교 자연과학부 화학과 [1]성균관대학교 화학과

We studied about the experimental and theoretical surface enhanced Raman spectroscopy (SERS) effect on Au nanoparticles (NPs) adsorbed on nanostructured Pt thin films. In order to find suitable SERS substrate, nanostructured Pt thin films was synthesized by electrochemical deposition into pores of cubic mesoporous silica thin films as a template and on these films, various sizes of Au nanoparticles are adsorbed. Using 4-aminobenzenethiol (4-ABT) as probe molecules, the substrate of Au NPs on nanostructured Pt thin films showed strong Raman intensity than that of Au NPs on Si wafer due to the coupling effect of Au NPs and mesoporous Pt thin films. So-called ‘hot spot’ in an interlayer of Au NPs and mesoporous Pt thin films makes strong electromagnetic fields and it can lead SERS effect. This SERS effect was confirmed through the computational results, which were applied by the finite difference time domain (FDTD). Through the simulation results, highly enhanced electromagnetic field was shown at the junction between two nanostructures. Based on experimental and theoretical results, we demonstrate that the electric field enhancement in the junction region of Au NPs and nanostructured Pt thin films leads SERS effect.

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Competitive Formation of the {111} and {110} facets of the Cu_2O microcrystals

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Various morphologies from octahedral through truncated octahedral and truncated rhombic dodecahedral and finally rhombic dodecahedral were obtained by using a simple solvothermal method. Only the {111} and {110} facets of the Cu_2O microcrystals are involved in this morphological variation. The effects of oleylamine and sodium oleate on the formation of these specific morphologies of Cu_2O were also examined. The understanding of crystal growth mechanism of Cu_2O microcrystals could provide a new strategy and control to design unique morphology-dependent optical, magnetic, and catalytic properties of Cu_2O, in near future.

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Synthesis of Platinum nanoparticles dispersed on Multi-walled carbon nanotubes via Proton Beam Irradiation

이윤지 송재희*

순천대학교 화학과

Carbon nanotubes (CNTs) have attracted considerable attention from many different research fields due to their unique chemical and physical properties. These exceptional properties make CNT an attractive support for metal nanoparticles. Carbon nanotube(CNT)-based nanohybrids have attracted significant research attention due to their potential applications in the fields of catalysis, biosensors, hydrogen storage, drug delivery, biomaterials, and nanoelectronics. Pt-based nanoparticles are widely used as a catalyst for application in fuel cells, where they are homogeneously dispersed on various types of carbon supports. In this study, a new synthetic route to decorate multi-walled carbon nanotube (MWCNT) with platinum nanoparticles (Pt-NPs) is presented via a simple proton beam irradiation process at room temperature. The characterization of the MWCNT-Pt composites has been done by using FE-TEM and EDS analysis.

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Room temperature preparation of Pt nanomaterials in aqueous solution using Proton Beam Irradiation

이윤지 송재희*

순천대학교 화학과

We present a facile one-pot synthetic route for the production of platinum nanomaterials via a simple proton beam irradiation process at room temperature. Hexadecyltrimethylammonium bromide (CTAB) was used as a stabilizing reagent for the preparation of pt nanomaterials. Size-and shape-controlled platinum nanostructures were prepared by simply varying the amount of added isopropyl alcohol to the reaction mixture. The morphology of Pt nanoparticels was controlled by the proton beam current and the duration of irradiation. The characterization was done by using UV-Vis absorption spectroscopy, TEM, and EDS analyses.

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Synthesis of Various Shapes of Silver Nanomaterials at Room Temperature

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Metal nanomaterials, especially noble metal nanomaterials, have fascinating optical, electronic, magnetic, thermal properties and widespread applications in catalysis, photography, information storage, medicine, and sensing. Ag nanostructures exhibit a strong ultraviolet-visible (UV-vis) absorption band arising from a localized surface plasmon resonance (LSPR) and have potential applications in surface enhanced Raman scattering (SERS), surface enhanced fluorescence (SEF), and chemical and biological sensors. In our studies, polyvinylpyrrolidone(PVP) was used as a stabilizing reagent for the preparation of Ag nanomaterials. Ascorbic acid was used as a reducing agent to synthesize silver wires, rods and prisms. Size-and shape-controlled Ag nanomaterial were prepared by varying the reaction conditions. The characterization was done by using UV-Visble absorption spectroscopy and transmission electron microscopy(TEM).

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

Fabrication of Superhydrophobic Silica Nanoparticles and Nanocomposite Coating on Glass Surfaces

황지수 김영아 안용현*

단국대학교 화학과

Superhydrophobicity(WCA >150°) is very interesting property. The self-cleaning property of the lotus leaf has been studying over recent decades. The self-cleaning effect is a wonderful natural phenomenon resulting from the low surface energy of the material coated on the nano-/micro-rough surface. Impurities are easily washed away by water droplets owing to their weak interaction in the superhydrophobic surface; therefore, the surface of the lotus leaf is always clean. It is composed of nano/ microscale protrusions and its surface covered with wax. A water droplet on the superhydrophobic surface does not penetrate the cavities of the nano-/micro-rough surface because of the air inside the cavities. In this work, we report the fabrication of a superhydrophobic surface using hydrophobic silica nanoparticles. The initial step is the chemical reaction of the hydroxyl groups on the silica surface with APTES, followed by the condensation of palmitoyl chloride with the modified nanoparticles. Superhydrophobic 3-palmitoylamido-propylsilylated silica nanoparticles (PASNPs) were successfully prepared. PASNPs formed stable liquid marbles with water. A nanocomposite coating solution is prepared by combining modified silica nanoparticles and PS in tetrahydrofuran (THF) and used to fabricate the superhydrophobic glass. The chemical composition of PASNPs was determined by XPS and FT-IR analyses. The composite solution of PASNPs/PS was used to fabricate a stable superhydrophobic surface on a glass plate. This solution endowed in the surface of the dip-coated glass with nano/microscale roughness which resulted in superhydrophobicity (WCA = 159.5°). PASNPs can be used in academic or industrial applications such as catalysis and design of sensors.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of SiO_2@Au nanoparticles and its optical property

이성희 김상욱[1,*]

아주대학교 분자과학기술학과 [1]아주대학교 응용생명화학공학부

We synthesized SiO_2@Au nanoparticles using colloidal methods. To confirm the effect of various structual changes such as the size of SiO_2 core and thickness of gold shell, we tested the reduction of 4-NP to 4-AP by photocatalysis.

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Synthesis of (E)-5,5'-(diazene-1,2-diyl)bis(1H-tetrazol-1-ol) and its energetic salts

배세원* 임영권[1]

국방과학연구소 4본부 2부 [1]국방과학연구소 4-2

Nitrogen- rich materials play an important role in the design of new energetic compounds and their use as explosives. The most promising heterocyclic backbone for the preparation of high performance energetics is considered to be the tetrazole ring. Tetrazole ring has allowed the preparation of a wide spectrum of energetic compounds from secondary explosives to highly sensitive primary explosives depending on its functional substituents and ion pairing. In this presentation, we report synthetic methods of N-oxide functionalized bisazotetrazole with its energetic salts and discuss their physical properties for the potential use as explosives.

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

Finely tuning oxygen functional groups of graphene nano-plateles and optimizing capacitor behaviors

박규태 이승준 오정훈 김승연[1] 최광록[2] 심연준 박성진*

인하대학교 화학과 [1]인하대학교 화학-화학공학 융합학과 [2]인하대학교 화학화학공학융합학과

Chemically modified graphene (CMG) systems have been intensively investigated for various applications. The development of methods that allow the fine control of oxygen functionalities would aid our understanding of mechanisms associated with CMGs, facilitate the optimization of materials properties, and provide standards for chemical characterization purposes. Here, the authors report a new method of finely controlling the levels of oxygen in CMG nano-platelets based on the refluxing of aqueous colloidal suspensions of graphene oxide for specific reflux times, which does not require reducing agents.

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Preparation of thin lanthanum foil

최정희 정용희*

한림대학교 화학과

Lanthanum foils were deposited on titanium with molecular electrodeposition in organic solutions at two voltages. The organic solutions were used by dissolving lanthanum nitrates in a small amount of ethanol and further in isobutanol. The applied voltages were 20 and 30 V. The deposition layers appeared to be uniform and showed good adhesion on titanium.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of MoS_2 on various substrates

홍광택 김성진[1,*]

이화여자대학교 나노과학부 [1]이화여자대학교 화학과

For post silicon device technology, the layered chalcogenides (MX_2, M = Mo, W and X = S, Se, Te) materials are potential alternatives for Si. However limited information is known for growth conditions and effect of substrate. We grew MoS_2 under various conditions and characterized by structural and device performances

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Amino-Functionalized Conductive Polythiophene Scaffolds

정의덕 이주운[1,*]

한국기초과학지원연구원 하이테크소재연구부 [1]한국교통대학교 교양학부 - 화학

Electroactive biomaterials such as polythiophene (PT) are highly attractive scaffolds for tissue engineering applications. The introduction of reactive functionalities into the PT backbone structure is desired to enhance the biomaterial-tissue interface for desired tissue responses. Here, we present amino-functionalized conductive polyterthiophene, poly(3´-aminomethyl-2,2´:5´,2´´-terthiophene) (PTTh-NH2), which successfully demonstrates the potential to influence cellular activity. The chemical structure of monomeric 3´-aminomethyl-2,2´:5´,2´´-terthiophene was confirmed by MS and the polymer characteristics of PTTh-NH2 were determined by AFM, XPS, profilometer and four-point probe. In vitro cell viability study with human umbilical vascular endothelial cells (HUVECs) indicates that the primary amine functionality grafted into polythiophene (PT) backbone improve the cell adhesion and proliferation compared to negative (-) control conventional PT. Thus, PTTh-NH2 could be useful in developing PT composites for various biomedical applications.This research was supported by a grant from the Academic Research Program of Korea National University of Transportation in 2014.

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발표코드: **MAT.P-1000**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of mesoporous $Li_{1.6}Mn_{1.6}O_4$ using KIT-6 as the template

채창완 박윤봉*

충남대학교 화학과

Mesoporous silica is useful in a variety of applications, including catalysis, adsorption, photonics, and electronics. The interest in such ordered mesoporous systems results from their interesting framework topologies, high surface area, and controllable pore size and pore volume. The ordered mesoporous Li-Mn spinels are of great interest as the cathode material of Li-ion batteries due to the decrease in the current density per unit surface area. Thin wall can also reduce the length of the diffusion path. Moreover, the well-ordered mesoporous materials can facilitate ionic motion more easily. $Li_{1.6}Mn_{1.6}O_4$ has been known to be the most suitable material for recovery of lithium from seawater, because it has a high chemical stability, high selectivity for lithium ions and large adsorptive capacity. In this work mesoporous $Li_{1.6}Mn_{1.6}O_4$ is directly prepared by a sol-gel method using mesoporous silica KIT-6 as a template. The Li^+ extraction experiments were performed in an acidic solution and then the Li^+ uptake experiments were achieved in Li-enriched solution. The physicochemical properties of the $Li_{1.6}Mn_{1.6}O_4$ and $H_{1.6}Mn_{1.6}O_4$ were characterized by X-ray powder diffraction (XRD), brunauer-emmett-teller(BET), inductively couple plasma-atomic emission spectroscopy (ICP-AES) and thermogravimetric analysis (TGA)/differential thermal analysis (DTA).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of hematite (α-Fe_2O_3) cubes and its growth mechanism

전현철 박윤봉*

충남대학교 화학과

Recently, magnetic nanoparticles have been under intensive study due to their interesting properties. The physical and chemical properties of magnetic nanoparticles largely depend on the particle size, shape, composition, and structure. Especially, Iron oxide exhibits excellent magnetic properties. Hematite (α-Fe_2O_3) of iron oxides has been of great interest towards the possible applications such as drug delivery, transplantation of cell, enzyme, gene therapy systems. We have successfully prepared hematite cubes by hydrothermal methods using ferric chloride and sodium acetate. Sodium acetate plays a role of shape controller in the formation of cube hematite structure. X-ray powder diffraction (XRD) was used to identify hematite formation and particle. Scanning electron microscopy (SEM) show that particle has cube shape with about 100 nm particle size.

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발표코드: **MAT.P-1002**
발표분야: 재료화학
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Extension of Shape-Retaining Reduction into Various Shapes of Silver Particles

조지희 임종국*

조선대학교 화학과

Herein, we introduce an unprecedented approach named as “shape-retaining reduction” to prepare hollow silver (Ag) particles. As an example, we demonstrate the synthesis of Ag hexapods that are reduced from silver oxide (Ag_2O) hexapods without changing their shapes. For the synthesis of Ag hexapods, Ag_2O hexapods are firstly synthesized, and secondly use them as templates to make hollow Ag hexapods. The Ag_2O hexapods are easily reduced to Ag hexapods especially in the vicinity of the outward surfaces of Ag_2O hexapods, and finally transform into hollow Ag hexapods. This new approach is extended to make many different shapes of Ag particles such as cubes, octapods, and octahedra.

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발표코드: **MAT.P-1003**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Controllable Dissolving of Silver Nanoparticles and Aggregation of Silver Ions

장형주 임종국*

조선대학교 화학과

Recently, we discovered that silver (Ag) nanoparticles are spontaneously dissolved into their ions, and dissolved ions are re-aggregated to form nanoparticles by light irradiance. This process is occurred only at a specific concentration of Ag nanoparticles, and reversible for several tens of periods. To reveal its mechanism for spontaneously dissolving of Ag nanoparticles and photomediated aggregation of Ag ions, systematic study is in progress. In this presentation, experimentally obtained several results are presented with a plausible mechanism.

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

Sonochemical Synthesis of Silver Nanoparticles in Polyol Solvent

임종국* 정형진 이동현 김한슬 조지희

조선대학교 화학과

It has been reported that silver (Ag) nanoparticles can be sonochemically synthesized in aqueous solvent under hydrogen gas environment. For the role of hydrogen gas, authors explained that hydrogen gas prevent Ag nanoparticles to be oxidized by hydrogen peroxide which is generated from hydroxide radicals. Ethylene glycol, like water, is polar solvent, however, in molecular structure aspect, ethylene glycol cannot generate hydroxide radicals, and therefore Ag nanoparticles are not oxidized even if they are exposed to atmosphere. If ethylene glycol is used as a solvent instead of water, it will be possible that Ag nanoparticles are sonochemically synthesized under atmospheric condition without hydrogen gas. Herein, we show successful synthesis of Ag nanoparticles in ethylene glycol, and suggest its mechanism with experimental evidences.

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Fabrication of Au nanoframes with Pt framework via chemical etching and regrowth

장희정 홍순창 함송이 송유경 박성호*

성균관대학교 화학과

In my presentation, I will introduce an effective synthetic strategy to produce Au-coated Pt (Pt@Au) nanoframes. The Pt nanoring at the inner core acts as a framework, and Au coated on the Pt nanoring allows the nanostructure to behave optically active as pure Au nanoframes because of the surface plasmon coupling between Au and Pt. This research provides fundamental basis in order to understand the optical property of Au nanoframes. The experimental process consists of two regimes, etching and regrowth process. We adopt site-selective grown Au@Pt nanoplates as a seed, in which Pt selectively grow along the edge of Au nanoplates. We took advantage of rim-preferential growth synthetic method to finally synthesize Au nanorigs, through etching and regrowth processes. Au^{3+} ions in growth solution play a critical role as both of an etchant and a metal precursor. In the etching process, as Au plates at the central part is selectively etched out by Au^{3+} ions in absence of reductant, leaving only Pt rims. Pt-dominant nanorings are remained at the end of reaction. By adding ascorbic acid, a reducing agent, it initiates the regrowth of Au on Pt nanoring by reducing Au^{3+} ions present in the growth solution. The resultant product is in the form of Au-coated Pt nanoframes, which take advantage of the empty space among the nanoparticle, providing relatively high light transparency and reactant permeability in nano-optics and catalysis.

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발표분야: 재료화학
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Double-Shelled Platinum Nanotube Arrays for Fuel Cells

김상민 김대진[1] 조상현 장호영 박성호[1,*]

성균관대학교 에너지과학과 [1]성균관대학교 화학과

Pt double-shelled nanotubes (Pt DNTs) with slender shell thickness were synthesized through the homogenous coating of Pd thin-wall nanotube array by the electrochemical deposition. The produced Pt DNTs obtained by the chemical etching of Pd templates have advantageous morphological characteristics namely; the coated Pt layers tag along with the Pd crystallinity, the inner nanotube has high porosity, non-carbon supported substrate, and the Pt DNTs are vertically oriented towards three-dimensional (3D) catalysts connecting with conducting electrode directly. In addition, The tube lengths can be controlled by monitoring the total amount of injected charge using electrochemical method. The electrochemical measurement of the resulting Pt DNTs significantly improved larger electrochemically active surface area (ECSA) and higher electrocatalytic activity towards methanol oxidation and CO oxidation behaviors than those of Pt single nanotube and Pt nanorod structures as well as other reported Pt-based catalysts under similar testing conditions. These results suggest that the Pt DNTS are excellent nanocatalytic systems for low-temperature catalytic reactions or surface-chemical processes.

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Optical Properties of Hybrid Nanostructure: Assembly of Au Nanoparticles and Au Nanorods

이경은 한송희 정인섭[1] **ACAPULCO JESUS ANTONIO JR** 박성호[*]

성균관대학교 화학과 [1]성균관대학교 에너지과학과

The assembly of metal nano materials is an appealing way to fine tuning of surface plasmon resonance (SPR). We prepared gold nanorods and gold nanoparticles using electrochemical deposition and wet-chemical method, respectively. The use of an octanedithiol, a linker molecule, enables to successfully synthesize hybrid nanostructures. In previous assembly study could not exploit the whole surface of nanoparticles because the bottom side of spherical nanoparticles is always attached onto the substrate which hinders it to be analyzed. However, nanorods synthesized by electrochemical method can be utilized with relatively high surface area and show the better stability than those of nanoparticles synthesized from wet-chemical method when it is dispersed in aqueous medium. Furthermore, gold nanorods with different aspect ratios can be easily fabricated via controlling the amount of current and exhibit higher-order modes of surface plasmon resonances. The resulting assemblies are consisted of gold nanoparticles (30 nm) attached onto the gold nanorods (300-600 nm). FE-SEM and HR-TEM images further proved that hybrid structures were successfully synthesized. Optical properties of hybrid structure were investigated by using UV-Vis spectroscopy. In the transverse mode, we could observe plasmon coupling between nanorods and nanoparticles. Longitudinal modes are red-shifted which is attributed to longer electron pathway after the attachment of nanoparticle on the nanorods. The plasmon coupling phenomenon depending on the number of gold nanoparticles is systematically investigated by varying the concentration of linker molecule.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Antimicrobial activity of nano-bio hybrid consisting of natural extract and engineered nanoclays

김형준 곽경현 오제민*

연세대학교 화학및의화학과

We prepared nano-bio hybrid materials consisting of natural extract with antimicrobial activity and engineered nanoclays such as illite (IL), holrait (H) and scoria (SC). Natural extract obtained from *Paeonia suffruticosa Andrews* (PSA) and *Agrimonia pilosa Ledeb* (APL) were determined to show strong antimicrobial activity on both Gram positive *Bacillus subtilis* and Gram negative *Escherichia coli* bacteria. In order to effectively incorporate those natural extract to clay nanomaterials, clays were ground and treated with 6 M HCl, resulting in enhanced specific surface area and pore volume. The nano-bio hybrid obtained by simply mixing nanoclay powders and extract solutions showed preservation of crystal structure and decrease in zeta potential, which were characterized by X-ray diffraction patterns and light scattered electrophoresis. According to the quantitative assay, the nano-bio hybrids were determined to contain natural extract in 10-18wt% range, depending on type of clays and extracts. All the hybrids were incubated with each bacterium in aqueous media for 3 h, and then the suspension was smeared on agar plate. We observed that the formation of bacterial colony was strongly inhibited with administration of nano-bio hybrids, of which activity was similar or better compared with the same quantity of natural extract itself.

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$CaCO_3$ Microcarriers Loaded with Numerous Hierarchical Nanomaterials and Catalytic Properties Thereof

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Since hierarchical nanomaterials show high performances in catalysis or adsorption due to their high specific surface area, tremendous efforts have been devoted to synthesis and application of hierarchical nanomaterials with a high specific surface area. Paradoxically, however, several problems have occurred due to extremely small size and light weight of hierarchical nanomaterials upon applications. For reuse, it is difficult to collect hierarchical nanomaterials without loss owing to difficulty in separation, leading the decrease in performance and second-hand contamination of environment. These problems led us to synthesize large and massive microstructures containing numerous hierarchical nanomaterials that play the roles of catalysts and adsorbents.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Polydopamine Nanocomposites Full of Novel Metal Nanoparticles

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A novel approach for synthesizing polydopamine (PDA)-based nanocomposites with a multifunction is demonstrated. Due to the special interactions between metal precursors and the PDA, individual nanoparticles (NPs) were selectively synthesized or positioned within the PDA from core to shell. By varying the reaction cycles, it was able to control the loading amount of metal NPs up to almost 100 % of the PDA particles. Thanks to highly loaded metal NPs within the PDA particles, we expect that the PDA nanocomposites described here can be used for an efficient catalyst for reduction of organics as well as a drug carrier for controlled release.

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발표분야: 재료화학
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Magnetic Mesoporous $CaCO_3$ Nanocomposites for Removal of Heavy Metal Ions

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With the growing demand for the removal of industrial pollutants such as heavy metals, synthetic dyes, and aromatic pollutants from water, tremendous efforts have been devoted to searching for effective water-purification methods. Calcium carbonate ($CaCO_3$) nanocomposites with highly porous structures were synthesized in the presence of polymers and magnetic nanoparticles (MNPs). Porosity and structure of $CaCO_3$ nanocomposites were controlled by varying the amount of polymers and MNPs, respectively. We expect that the porosity and the structure-tunable $CaCO_3$ nanocomposites can be used as a magnetic remover with high removal capacity for heavy metal ions or organic dyes.

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발표코드: **MAT.P-1012**
발표분야: 재료화학
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Facile Fabrication of Metal Oxide/Carbonate Films on Substrates irrespective of Hydrophilic or Hydrophobic Nature

배지영 이하진[1] 최원산[*]

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Metal oxide or metal carbonate films were prepared on hydrophilic or hydrophobic substrate by means of a simple solution method. Metal oxide or metal carbonate films were grown on the surface of the glass, tetrafluoroethylene (Teflon), and Au substrates by the addition of a metal precursor solution to the solution involving substrates and oxidants under controlled conditions. The substrates were very uniformly covered with metal nanoparticles or carbonates. The growth of metal nanoparticles or carbonates could be controlled by varying the reaction conditions. Our novel method described here is very useful for coating metal oxides on substrates irrespective of hydrophilic or hydrophobic nature.

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Single-Layered White OLED Based on Multi-Host, Dopant System with Interlayer

김승호 이재현 박종욱*

가톨릭대학교 화학과

Two color white EML is proposed by using blending and spin-coating method through a co-host/dopant system. Device performances were systematically compared based on the optical property of with/without interlayer PVK. When 1-[1,1';3',1"]Terphenyl-5'-yl-6-(10-[1,1';3',1"] terphenyl-5'-yl-anthracen-9-yl)-pyrene (TP-AP-TP) is a blue emitter with high luminance and external quantum efficiency, NPB is used as a co-host material which has HTL property and wide band gap like a blue emitter. DPAVBi and Rubrene were each used as blue dopant and yellow dopant. Luminance efficiency of the device used interlayer was 4.31cd/A, a value 30% higher than without interlayer (3.31 cd/A) at 10 mA/cm2.

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체계적인 Core Group 변화에 대한 새로운 Bipolar형 유기 발광체의 합성과 광학적 특성

정효철 신환규 안병관 김중한 강현미 양가람 박종욱*

가톨릭대학교 화학과

Core group 을 체계적으로 변화시켜가며, 새로운 bipolar 형 유기 발광체를 디자인하였다. Boronylation, bromination, suzuki aryl-aryl coupling 과 Buchwald-Hartwig amination 을 통해 3 종의 DPAT-Ph, DPAT-Na 와 DPAT-An 을 합성하였다. 각 물질들은 core group 의 conjugation 변화에 따라 solution 과 film state 에서 다른 최대 파장을 보였다. 또한 모든 물질은 bipolar 형 물질이므로 분자 내 dipole 을 형성한다. 다른 solvent polarity 를 가진 solvent 에서 UV-visible spectra 는 큰 변화가 없지만, PL spectra 는 solvent polarity 가 증가할수록 최대 파장도 장파장으로 이동한다. 특히, DPAT-An 은 solution state 에서는 약한 emission 을 나타내다가, solid 와 film state 에서는 강한 emission 을 나타내는 aggregation induced emission(AIE) 현상을 나타내고, 이를 THF/water volume% fraction test 를 통한 PL intensity 변화로 확인하였다.

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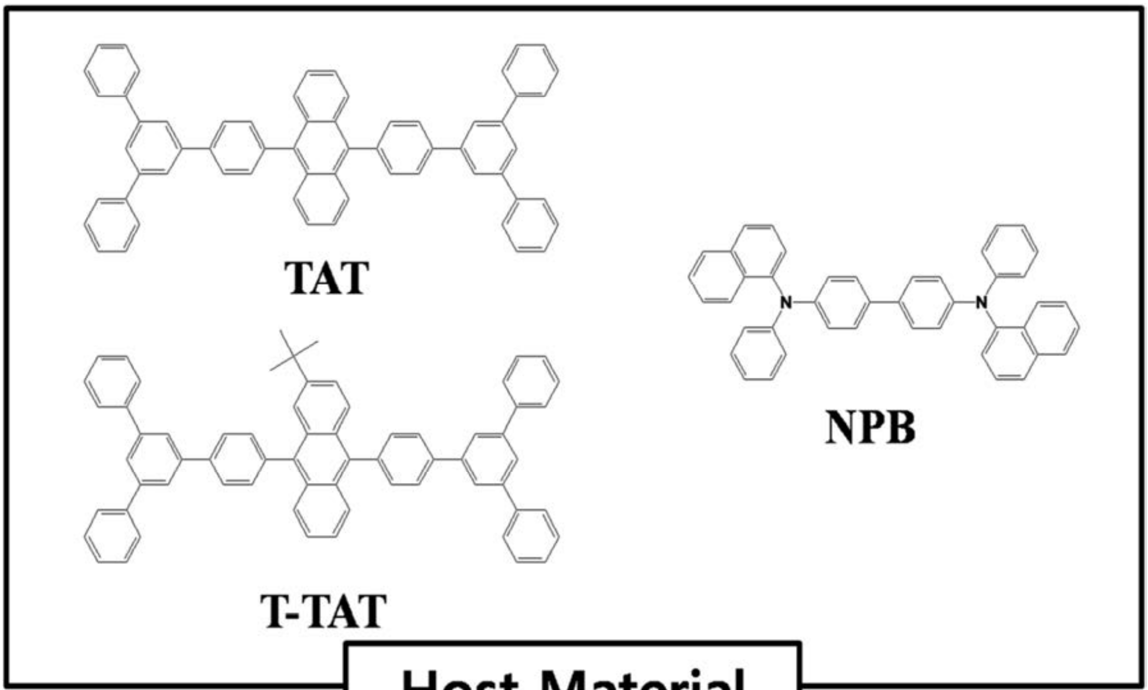
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

WOLED Using New Host Materials Including Substituent Group Based on Solution and Vacuum Methods

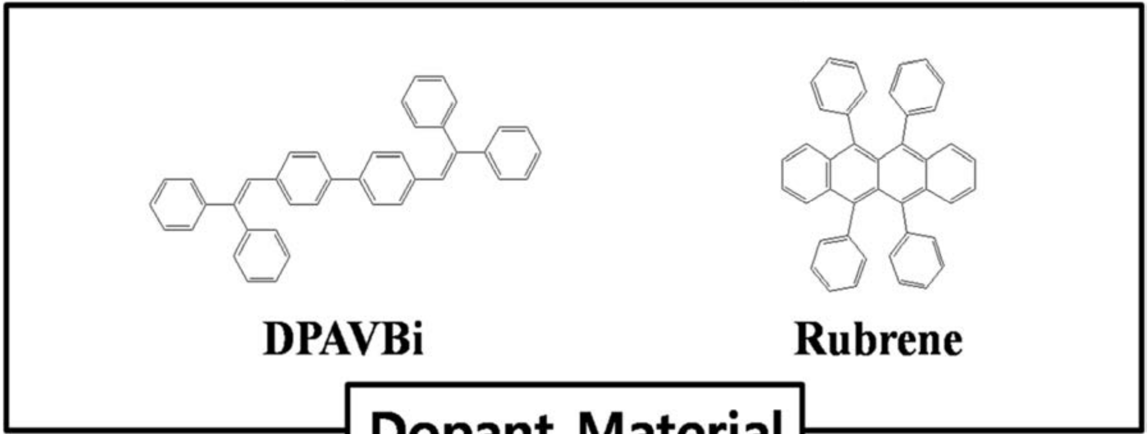
이재현 김승호 박종욱*

가톨릭대학교 화학과

The interest in organic light-emitting diodes (OLEDs) based on white OLEDs (WOLEDs) has been rapidly growing in the fields of OLEDs TV and lighting application. Until now, WOLEDs have been produced using a vacuum evaporation method, but this method involves drawbacks such as high cost, difficulty of large scaling, and difficulty of adjusting the doping concentration. Therefore, there is a lot of on-going research methods of producing solution processed WOLEDs such as spin-coating, screen-printing, and ink-jet printing that show advantages in large scaling and are relatively inexpensive production. In this study, we propose new approach method to prevent packing of chromophore by introducing alkyl into main chromophore. In our previous paper, 9,10-bis (3'',5''-diphenylbiphenyl-4'-yl) anthracene (TAT), a blue fluorescent emitter showed high efficiency through the deposition process. In here, we changed main core part with tertiary butyl group as shown in Fig. 1 and characterized new compound of T-TAT (2-tert-butyl-9,10-bis(3'',5''-diphenylbiphenyl-4'-yl)anthracene). A two-color WOLED of a co-host system using solution process method was demonstrated. The device configuration was ITO / PEDOT:PSS (40 nm) / emitting layer (50 nm) / TPBi (20 nm) / LiF (1 nm) / Al. The emitting layer consisted of TAT, NPB, DPAVBi (blue dopant), and Rubrene (yellow dopant). NPB was used to help hole carrier transport as well as blue host role. The device using the T-TAT compound as a co-host showed a luminance efficiency of 2.73 cd/A, which is 77% higher than TAT device of 1.54 cd/A at 20 mA/cm2.



Host Material



Dopant Material

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발표코드: **MAT.P-1016**
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Template free facile in situ syntheses of highly water-stable acidic sulfonated mesoporous silica

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A new simple method to prepare acidic mesoporous sulfonated silica in situ without any surfactant is reported. The prepared catalysts were characterized by XRD, nitrogen adsorption, thermogravimetric analysis (TGA), and elemental analysis. The concentration of ?SO3H groups was measured by titration, and FTIR was applied to confirm the successful incorporation of the strong acid sites. The in situ sulfonated silica (ISS) has a large surface area with a narrow range of mesoporosity and good thermal stability. Moreover, the preparation method has the advantage of easy control of the acid concentration and versatile synthesis. The ISS was used in catalytic hydrolysis and showed remarkable reusability even under very harsh conditions. The butylation of phenol was conducted over ISS to utilize the mesoporosity of the catalysts. Finally, the ISS catalysts might be used in various acid catalyses owing to the advantages of their simple/inexpensive preparation, reusability, and mesoporosity.

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발표코드: **MAT.P-1017**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characteristics of W-doped and W/Ti-codoped VO_2 nanoparticles

박희선 정영희[1] 김영일*

부경대학교 화학과 [1](주)마프로 기술연구소

Monoclinic VO_2(M) undergoes a reversible phase transition to rutile VO_2(R) at 68℃ from IR-reflective metal to IR-transparent semiconductor. By introducing dopants, VO_2(M) can be controlled some parameter, such as the transition temperature, morphology and optical properties and so on. Transition temperature of VO_2(M) can be reduced by adding W, Mo, Sn, etc. and the optical properties improved by Ti, Mg, F doping. In this study, we have synthesized W doped and W/Ti co-doped VO_2(B) via hydrothermal methods and then the doped VO_2(B) can be transformed to VO_2(M) by heat treatment under inert condition. Also we have investigated the relative properties of W doped VO_2(M) and W/Ti co-doped VO_2(M) that were prepared by these methods.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Thermoelectric Properties of Superionic Copper Selenide

JINYINGSHI 김성진[1,*] 한미경[2] 김하영[1] 유병규[3]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과 [2]이화여자대학교 화학나노과학부 [3]이화여자대학교 화학나노과학

High efficient thermoelectric material should behave as a “phonon-glass-electron-crystal” with a high charge carrier mobility and a low lattice thermal conductivity. The liquid-like behaviour of superionic conductors can be considered an extension of the phonon-glass electron-crystal concept and phonon-liquid electron-crystal (PLEC) thermoelectrics. Copper selenide $Cu_{2-x}Se$ is representative material as the liquid-like behaviour of superionic conductors. The Se atoms provide a crystalline pathway for semiconducting electrons and the copper ions are superionic with liquid-like mobility, resulting in a low lattice thermal conductivity κ_L which enables ZT improvement. We prepared $Cu_{2-x}Se$ bulk pellet from hand-grinded bulk ingot using spark plasma sintering (SPS) and evaluated their thermoelectric properties. The results indicate that competing with other conventional commercial materials $Cu_{2-x}Se$ could be potentially a new direction and interesting for high-efficiency thermoelectric material.

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발표코드: **MAT.P-1019**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Design of a Dopamine Derivative for Antibacterial Coatings on Various Substrates

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충남대학교 화학과 [1]충남대학교 생화학과

Microorganisms have a strong tendency to adhere and to grow on solid substrates under biological environments. Once bacteria attach to a surface, they quickly proliferate and form three-dimensional communities named as biofilm. Biofilms on surfaces can cost billions of dollars over the world due to equipment damage, product contamination, energy losses, and medical infections. Non-biofouling coatings have been realized as an environment-friendly and efficient method for preventing biofilm formation by resisting bacterial adhesion onto surfaces. Ethylene glycol/zwitterion-based materials have been used for the purpose, however; there is still unmet need to develop a facile and universal coating material for preventing bacterial adhesion on any kind of surface.Herein, we have synthesized a dopamine derivative with oligo(ethylene glycol) for non-biofouling coatings on various substrates. It is designed to have both catechol and amine moieties for facile coatings on various substrates without any additives. The dopamine derivative-coated substrates were characterized by ellipsometry, contact angle goniometry, and X-ray photoelectron spectroscopy. The bacterial adhesion on the coated substrates has been examined with E.coli.

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발표코드: **MAT.P-1020**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation of Ultra-Large Pore Mesoporous Silica Nanoparticles and Their Application to the Encapsulation of Large Guest Molecules

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한국외국어대학교 화학과

Pore-enlarged mesoporous silica nanoparticles (MSNs) were prepared directly from as-prepared MSNs through a new, simple method using divalent Ca or Mg salts as both efficient silica etching reagents and as ion exchangers in methanolic solution under mild conditions. The resultant MSNs became almost template-free simultaneously during this etching process. The pore-enlarged MSNs, referred to as Ca-MSN or Mg-MSN, maintained their original hexagonal pore symmetry and particle sizes, but several ultra-large mesopores were generated inside and outside the MSNs together with regular mesopores having expanded pore dimension of around 4?5 nm. The average pore diameters for ultra-large pores were 47.5 nm for Ca-MSN and 52.4 nm for Mg-MSN. The generation of ultra-large pores can be regarded as the collapse of several mesopores into an ultra-large pore. Both Ca-MSN and Mg-MSN were good sorbents for positively charged porphyrin molecules. Additionally, these ultra-large pore MSNs exhibited better adsorption ability than calcined MSN for large proteins and antibodies, such as bovine serum albumin (BSA) and immunoglobulin G (IgG).

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발표코드: **MAT.P-1021**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Biosynthesis of Au and Ag nanoparticles using Perilla frutescens leaf extract

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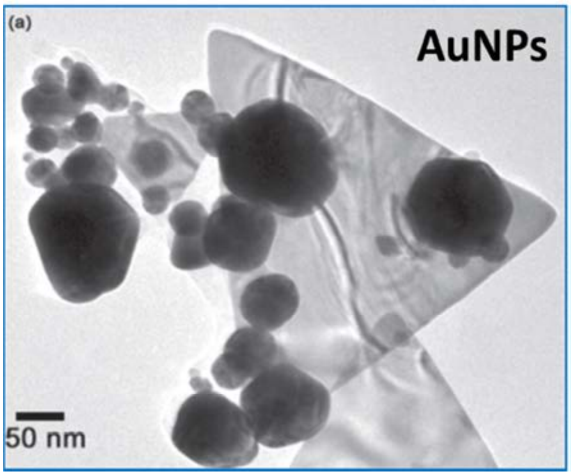
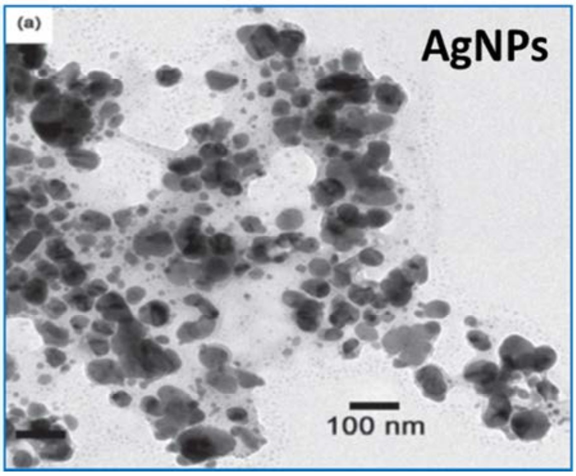
영남대학교 화학공학부

We describe a rapid synthesis of gold and silver nanoparticles using biologically important Perilla frutescens leaf extract as a reducing and stabilizing agent under ambient conditions. The nanoparticles obtained were characterized by UV-Vis spectroscopy, transmission electron microscopy, X-ray diffraction, and Fourier transform infrared spectroscopy. Surface plasmon resonance spectra confirmed the formation of of gold and silver nanoparticles. TEM studies showed that the particle sizes of gold and silver nanoparticles. X-ray diffraction studies confirm that the biosynthesized nanoparticles were crystalline gold and silver. Fourier transform infra-red spectroscopy revealed that biomolecules were involved in the synthesis and capping of the nanoparticles produced. XRD and EDX confirmed the elemental make up of gold and silver nanoparticles. This is a simple, efficient and rapid method to synthesize gold and silver nanoparticles at room temperature without use of toxic chemicals.





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발표코드: **MAT.P-1022**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A novel and green approach for the synthesis of palladium nanoparticles and their catalytic activity towards the construction of biologically interesting di(indolyl)indolin-2-ones

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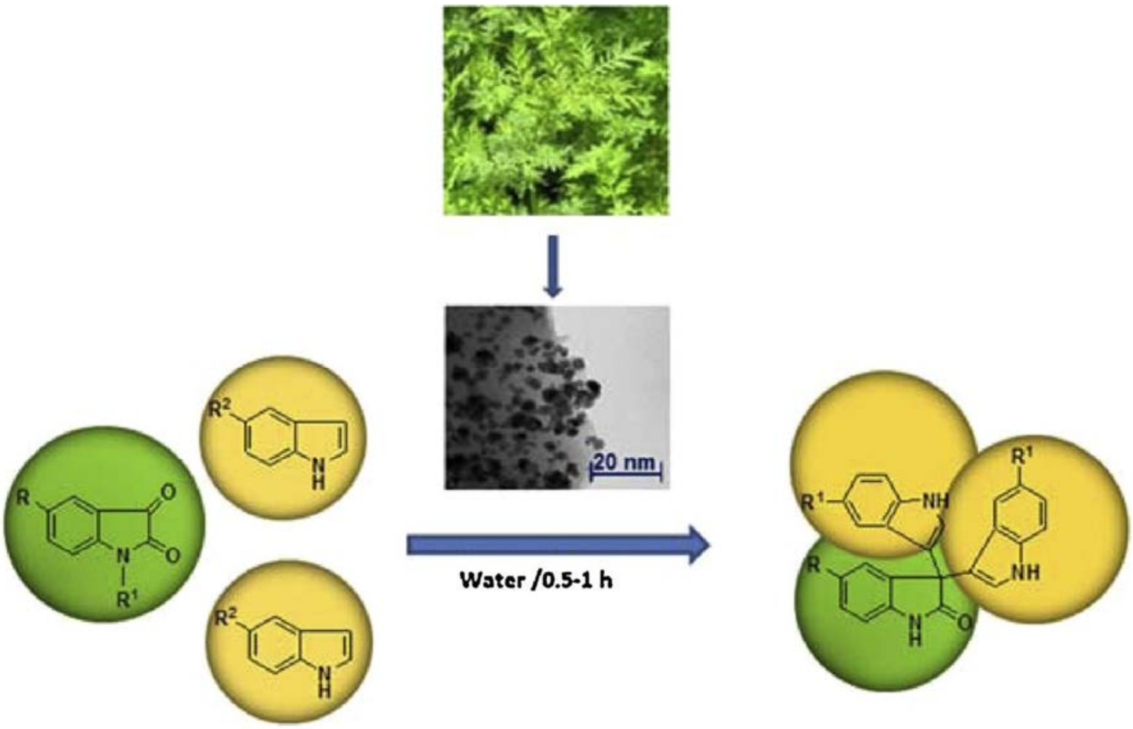
영남대학교 화학공학부

We describe a green method for biosynthesis of palladium nanoparticles (PdNPs) using Artemisia annua leaf extracts. This synthetic strategy used is straightforward, robust, green, and cost-effective, and exhibits great potential of practical applications for biosynthesizing biologically interesting materials. The synthesized PdNPs were characterized by using UV?visible spectroscopy. The crystalline structure of PdNPs was confirmed by transmission electron microscope with energy dispersive spectra (TEM-EDX) and X-ray diffraction (XRD) analysis. Thermogravimetric analysis (TGA) showed that bioactive molecules were capped on the PdNPs and were completely degraded under high temperature. Fourier transform infrared spectroscopy (FTIR) implicated the role of polyols and carbonyl groups in the synthetic process. The synthesized PdNPs capped by bioactive molecules showed potent catalytic application for the synthesis of several di(indolyl) indolin-2-ones in high yield in aqueous medium.


20 nm
R
O
O
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R¹
R²
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H
Water /0.5-1 h
R¹
NH
R
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H
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일시: 2014년 10월 15~17일(수~금) 3일간
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발표코드: **MAT.P-1023**
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Preparation of layered double hydroxides nanomaterials incorporated with antibacterial organic moieties

김태현 오제민*

연세대학교 화학및의화학과

We have incorporated organic molecules having antibacterial activity, such as citric acid (CA), eugenol (EU) and lactic acid (LA), into layered double hydroxide (LDH) nanomaterials. Pristine LDHs with chemical formula $Mg_2Al(OH)_6(NO_3)$ was prepared by co-precipitation and interlayer nitrate was exchanged with organic moieties through ion exchange reaction. X-ray diffraction patterns showed interlayer space expansion of LDH from ~0.37 nm for pristine LDH to ~0.56 nm, ~0.66 nm, and ~0.96 nm upon CA, EU and LA incorporation, suggesting the successful intercalation of those molecules having 0.77 (CA), 0.87 (EU) and 0.53 nm (LA) of molecular dimension. The Fourier transform infrared (FT-IR) spectroscopic results showed characteristic stretching vibrations of symmetric and asymmetric COO^- at ~1350 cm^{-1} and ~1610 cm^{-1} in both CA and LA incorporated LDH. Also the -C-O- stretching in $-OCH_3$ was clearly observed at ~1670 cm^{-1} for EU incorporated LDH hybrid, suggesting the intact structure of organic moieties in LDH structure. The size of pristine MgAl-NO_3 LDHs were determined to be ~20 nm by scanning electron microscopy (SEM) and size and morphology of CA, EU and LA incorporated LDH hybrids were determined to be well preserved after incorporation of organic acid molecules. High performance liquid chromatography was utilized to determine the amount of incorporated organic acids, showing approximately 10-20 wt% of organic moiety loading in LDH structure.

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발표코드: **MAT.P-1024**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Colloidal stability of food-grade TiO_2 and SiO_2 nanomaterials under protein and sugar dispersant conditions

송재호 김경민[1] 오제민[2,*]

연세대학교 화학 및 의화학 [1]연세대학교 화학과 [2]연세대학교 화학및의화학과

Metal oxide nanomaterials, such as TiO_2 and SiO_2 have been widely utilized in food industries as food additives; TiO_2 as whitening agent in sugar powder and SiO_2 as anti-caking agent in chocolates or salts. Upon increasing demand on those nanomaterials, there emerged concerns of their biological behaviors and potential toxicity. In order to evaluate biological behaviors of nanomaterials, it is important to prepare stable colloidal suspension for oral administration experiments. In this study, we evaluated colloidal stability of food-grade TiO_2 and SiO_2 nanomaterials under the presence of protein and sugar dispersants. We dispersed those nanomaterials in deionized water, phosphate buffered saline and solutions containing albumin or D-(+)-glucose with various concentrations (0.005 and 0.2 wt/v% of TiO_2 and SiO_2 in DI water and PBS, 0.2 wt/wt% of TiO_2 and SiO_2 in solutions). We monitored hydrodynamic size and zeta potential of colloids utilizing dynamic light scattering (DLS) and light scattering electrophoresis (LSE), respectively. TiO_2 and SiO_2 nanomaterials exhibited colloidal stability in albumin and D-(+)-glucose solution, respectively, showing the preservation of hydrodynamic size until 48h, while those nanomaterials in deionized water and phosphate buffered saline showed significant agglomerations.Acknowledgement This research was supported byu a grant (14182MFDS459) from Ministry of Food and Drug Safety in 2014

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발표코드: **MAT.P-1025**
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Size-Dependent Phase Transformation in Co Nanoparticles, and Its Impact on the Electrocatalytic Activity for Oxygen Reduction Reaction

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Cobalt nanoparticles (Co NPs) with controlled particle sizes (3.8, 6.4, and 9.0 nm) were synthesized. The Co NPs were supported on highly porous nitrogen-doped mesocellular foam carbon (MCF-C), and were mildly annealed at 185 °C to remove residual surfactant, affording Co/MCF-C. High-resolution transmission electron microscopy as well as linear combination fittings of X-ray absorption near edge structure (XANES) spectra over Co/MCF-C revealed that crystal phase of 6.4 and 9.0 nm Co NPs is predominantly $Co(OH)_2$ with a small portion of Co_3O_4 (less than 10%) whereas the smallest 3.8 nm Co NPs consists of ~50% of $Co(OH)_2$ and ~50% of Co_3O_4. This result is a strong evidence of particle size-dependent phase transformation and the propensity of smaller Co NPs toward the surface oxidation. Electrocatalytic activity measurements of the Co/MCF-C toward oxygen reduction reaction (ORR) in alkaline solution revealed that 9.0 nm Co NPs have the highest ORR activity per surface Co atom, followed by 6.4 and 3.8 nm Co NPs. This activity trend indicates that the ORR activity can be correlated with the composition of Co nanoparticles.

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Nanoscale Size Effects in Molybdenum Sulfides-Catalyzed Hydrogen Evolution Reaction

서보라 사영진 천재영 주상훈[1,*]

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The understanding of nanoscale size-dependent catalytic activities is central to designing advanced catalysts, which have yet been established limitedly with metallic catalysts. We demonstrate the first single monolayer precision preparation of molybdenum sulfide (MoS_2) nanoparticles from one to four layers with similar basal plane size of 5 nm, and their size-dependent catalytic activity for hydrogen evolution reaction (HER). We identified, with density functional theory calculations, the most favorable one, two, and three layer MoS_2 structures, and dissected elementary step energetics during the HER on these structures. We establish that the turnover frequency of MoS_2 nanoparticles for the HER increases in a quasi-linear manner with decreased layer number, with the single layer MoS_2 showing the highest activity. Cobalt-promoted MoS_2 nanoparticles also exhibit similar activity trend with enhanced HER activity. This insight into size-dependent HER activity trend would help design advanced HER catalysts as well as other hydrotreating catalysts.

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Scalable synthesis of yolk-shell structured silicon@carbon composition as high-performance anodes materials for LIB

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Lithium ion batteries(LIB) are widely used for consumer electronics, and have increasing application for electric-vehicles and stationary energy storage. The commercially available LIB requires low cost, high energy density cathode and anode materials. Silicon is regarded as one of the attractive candidates for anode materials because of high theoretical capacity (~4200mAh/g) which is 10-fold higher than that of graphite, as well as its abundance (about 28% in the earth's crust calculated by mass). In the well-designed yolk-shell Si/C composites, Si nanoparticles, which is easily synthesized by a two-step coating process, can expand into the void space without problems, such as crack of nanoparticles and growth of solid-electrolyte interphase(SEI) on the outer surface, originated from volume expansion. Despite its high potential in future Li-ion batteries, the large-scale and uniform synthesis of Si based anodes is still a great challenge. We report on investigation of production parameter for gram based scale-up process of yolk-shell Si/C composite and relation between scale-up product and its cycling performance as well as optimized synthetic method for well-designed yolk-shell structured nanocomposites.

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Highly Selective Hydrogen Production from Hydrous Hydrazine by Rhodium-doped Nickel Catalysts

유정보 김한솔 이자운 전도연 **HongYounghoonAndrew** 허남회*

서강대학교 화학과

We herein report the synthesis of microspheres (Ni-Rh@SiO_2) composed of rhodium-doped nickel and silica, which was accomplished via thermal hydrolysis of urea using core/shell silica microspheres as templates. The Ni-Rh@SiO_2 microspheres possess the hollow structure resulted from the repeated dissolution-and-deposition steps. The product was completely characterized by X-ray diffraction, transmission and scanning electron microscopy, X-ray photoelectron spectroscopy, Brunauer-Emmett-Teller surface area, and inductively coupled plasma atomic emission spectroscopy. Although the Ni-Rh@SiO_2 microsphere has a low Rh content, it shows an excellent catalytic activity towards the dissociation of liquid hydrazine into hydrogen and nitrogen. Complete release of hydrogen from liquid hydrazine was accomplished at room temperature with an exceptionally high selectivity (>99 %). Moreover, the used Ni-Rh@SiO_2 microsphere showed the virtually identical activities in subsequent reactions.

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Surface Modification of Halloysite Nanotubes by Octadecylphosphonic acids and Otadecyltrimethoxysilanes

노시은 강훈구 노재근*

한양대학교 화학과

Inner and outer surfaces of halloysite nanotube can be modified by the adsorption of octadecylphosphonic acid (ODTMS) and octadecyltrimethoxysilane (ODPA), which can be applied for hydrogen storage. The modification of halloysite by ODTMS and ODPA was investigated by Fourier transform infrared spectroscopy (FT-IR), Transmission electron microscopy (TEM), and Brunauer Emmett Teller (BET) surface area analysis. FT-IR measurements for halloysitse modified with ODPA and ODTMS show that CH2 vibration peaks were observed at 2918 and 2850 cm-1, which means that the surfaces of halloysites were modified by ODPA and ODTMS. We also confirm the surface modification of holloysites by electron mapping using TEM. Surface area of normal halloysite is measured to be 27 m2/g, whereas ODPA-modified halloysite is measured to be 31.3 m2/g, suggesting that the surface areas of halloysites can be increased by surface modification with ODPA molecules. From these results, we demonstrated that halloysite was successfully modified by ODPA and ODTMS molecules.

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근적외선 차단 재료로써의 TiO_2@Sb-SnO_2 복합재료 합성 및 특성 규명

고하니 이석우*

공주대학교 화학과

본 연구에서 우리는 TiO_2 와 ATO(Antimony doped tin oxide)의 반응을 통하여 복합재료를 합성하였으며, 근적외선 차단 재료의 응용성에 대하여 조사하였다. 마이크로 크기의 TiO_2 구는 titanium(IV) butoxide 를 전구체로 사용하여 가수분해 반응으로 합성하였다. TiO_2@ATO 코어-쉘 복합재료는 도핑된 Sb 의 원자 비율을 다양하게 조절하여 Pechini 방법으로 합성하였다. 이는 citric acid(CA)와 ethylene glycol(EG)을 이용하여 TiO_2 표면에 Sb 가 도핑된 SnO_2 를 컨쥬게이션하였다. 합성된 복합 재료는 SEM, PXRD, XRF, 전도도 측정을 통하여 형태와 크기, 결정 구조, 성분 분석 그리고 전기적 특성을 규명하였다. 마지막으로 DRS UV/VIS/NIR 분광기를 통한 복합 재료의 반사율(R%) 측정으로 근적외선 영역(750-1300 cm-1)에서의 차단 능력을 규명하였다.

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Synthesis and Crystal Structure Refinement of New Oxyapatites, $Sr_8Re_2(PO_4)_6O_2$ (RE=La, Pr, Nd)

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A series of oxyapatites, $Sr_8Re_2(PO_4)_6O_2$ (RE=La, Pr, Nd) have been synthesized by conventional solid state reaction at various temperature(900-1200℃). The crystal structure of $Sr_8Re_2(PO_4)_6O_2$ (RE=La, Pr, Nd) were characterized by powder X-ray diffraction. Rietveld refinements were performed with the FULLPROF package. The oxyapatite compounds crystallize hexagonal crystal symmetry with space group $P6_3/m$ and show a three dimensional network consisting of PO_4 group bridged by Sr^{2+} and RE^{3+} ions. The crystal structure of $Sr_8Re_2(PO_4)_6O_2$ indicates that a cation located at the 4*f* site and its surrounding nine oxygen atoms are connected by tetrahedral PO_4 groups. However the cations located at the 6*h* site with surrounding seven oxygen atoms. As compositions progress through the lanthanide series from La to Nd, the cell parameters tend to decrease due to the difference of the ionic radii of RE^{3+} ions.

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금속 산화물 졸을 이용한 해상 강관용 세라믹 방식재의 개발

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전북대학교 화학과

해상 풍력의 경우 바닷물에 들어 있는 나트륨(Na)이나 바닷물에 각각의 이온과 접촉이 용이하여, 강철로 되어있는 강관이 산화되어 녹스는 경우가 많다. 에폭시 도료의 경우, 기본적으로 원 재료의 비용이 비싸, 원가 절감 취지에 맞지 않으며, 내후, 내광성이 나쁘고, 재질에 대한 전처리 작업이 까다로워서, 작업 비용 역시 많이 들게 된다. 또한, 비스페놀 A(bis phenol A)와 같은 유해 물질을 포함하고 있어 환경 친화적이지 않으며, 입자의 크기가 일정하지 않아, 방식재로 적합하지 않다. 이러한 단점들을 보완하기 위해서는 강구조물에 사용되는 여러 가지 종류의 도장재료와 호환성을 높여야 한다. 본 연구실에서는 최근 폴리 실록산을 개발하여 나노사이즈의 금속산화물졸을 만들어 강구조물 구도막의 종류에 상관없이 보수도장이 가능하고, 도막간의 박리에 따른 문제 발생이 없고 균질한 시공이 가능하다. 연구하고 있는 제품에 대해서는 세라믹 성분으로서 인체에 무해하며, 기존 중방식 도료와 다르게 불연성 재료이다. 또한 황변이 발생되지 않고, 내산성, 내알칼리성, 내염수성이 우수한 것으로 나타났다. 그리고 기존 방식에서는 이끼 및 이물질 부착이 심각한데에 반해 방오성능이 탁월하여 본 연구물질의 유효기간이 더 늘어나는 것을 밝혀냈다. 본 발표에서는 연구되고 있는 무기나노소재에 대해 소개하고 향후 개발 방향에 대하여 논의한다.

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Electrical DNA sensor using self-assembled magnetoplasmonic nanochains

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We report an electrical biosensor based on magnetoplasmonic nanochains (MPNCs) of gold-coated iron oxide core-shell nanoparticles (Fe3O4@Au NPs) for rapid and label-free detection of DNA. Superparamagnetic Fe3O4@Au NPs were synthesized in aqueous solution by a simple one-step reaction. Subsequently, MPNCs with dimension controlled by varying an external magnetic field were formed on a microelectrode through magnetic-field-induced alignment of Fe3O4@Au NPs. Electrical properties of the as-prepared MPNCs were found to be poor due to quantum effect and cavities inside MPNCs. Accordingly, an annealing at a proper condition was performed to improve the electrical properties the MPNCs. Furthermore, the annealed MPNCs prepared on the microelectrodes were used as transducers for electrical DNA detection. Probe DNA was immobilized on to the MPNCs following by hybridization of complementary target DNA. A significant resistance increase was detected due to hybridization at reasonably low concentration of target DNA. The results show the potential of these sensors in for detection of pathogens, human genetic disorders, environmental monitoring.

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Position Effect of Anthracene Derivatives for OLED Emitters

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가톨릭대학교 화학과

Green-orange emitters based on anthracene core have successfully been synthesized by substitution with triphenylamine side group in the 9,10 or 2,6 positions. There are larger blue shifts in the UV-visible absorption and PL spectra of the synthesized 2,6-substituted derivative compared to 9,10-substituted derivative. When the synthesized compounds were used as emitting layers in non-doped OLED devices, a related trend was observed in their optical properties. In particular, OLED device containing 2,6-substituted derivative was found to exhibit excellent characteristics, with maximum EL emission at 518nm, pure green emission with CIE coordinates (0.334, 0.604), and an external quantum efficiency of 2.83%.

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Synthesis and Electroluminescent Properties New Emitting Materials Based on HTL Moiety with High Hole Mobility for OLEDs

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가톨릭대학교 화학과

New green emitting compounds based on tris(N-methylindolo)benzene1, anthracene, and pyrene were synthesized for the first time. NMT-An and NMT-Py as shown in Fig. 1 were used as an emitting layer in OLED device to examine emitting property. OLED device containing NMT-An emitting layer and conventional hole transporting layer (HTL) of NPB was found to exhibit better characteristics compared to NMT-Py, with maximum EL emission at 502nm and 550nm, CIE coordinates (0.38, 0.48), and an luminance efficiency of 2.06cd/A. Also when NMT and NMT-An were used as a HTL instead of NPB with NMT-An emitter, the device showed 2.67cd/A and 2.29cd/A in luminance efficiency. NMT-An compound can be used as an emitter without separate hole transporting layer in OLED device.

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Synthesis and electroluminescent properties blue emitting materials based onindenopyrazine derivatives

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가톨릭대학교 화학과 [1]한국교통대학교 나노고분자공학과

Two indenopyrazine compounds for organic light emitting diodes were synthesized with phenanthrene or pyrene side groups that have high photoluminescence (PL) quantum efficiency (QE); 6,6,12,12-Tetraethyl-2,8-di-phenanthren-9-yl-6,12-dihydro-diindeno[1,2-b;1',2'-e]pyrazine (PA-EIP) and 2-(10b,10c-Dihydro-pyren-1-yl)-6,6,12,12-tetraethyl-8-pyren-1-yl-6,12-dihydro-diindeno[1,2-b;1',2'-e]pyrazine (PYEIP). The PL spectra of PA-EIP and PY-EIP in film state were 440 nm and 468nm in the blue region, respectively. PA-EIP and PY-EIP showed luminance efficiencies of 1.35 and 5.15 cd/A, power efficiencies of 0.69 and 2.81 lm/W, and CIEs of (0.17, 0.15) and (0.19, 0.30), respectively. This result shows that efficiency of final emitter increases with increasing efficiency of side group.

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Phase-pure FeCr2Se4 and FeCr2S4 nanocrystals synthesis via wet chemistry method with high conductivity

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A novel facile synthetic route for iron-based ternary NCs, i.e., FeCr2Se4 and FeCr2S4 was introduced using a wet chemistry method. Narrow bandgap Fe ? based ternary semiconducting nanocrystals (NCs) offer a promising conductivity for electronic structure with different doping. Importantly, their higher potential to be industrialized in solar cells differs from Cd and Pb ? based compounds due to non-toxicity of inherited materials. General synthetic route of the ternary compounds passes through mixing and reacting different elemental powders in evacuated silica ampoules to consume long time under high temperature (700 - 1000 °C) but resulting in uncontrolled size and morphology of colloidal NCs. In the suggested method, the morphology of NCs was simply controlled using solvent and heating temperature where oleylamine was multi-utilized as surfactant, solvent, and reducing agent. The synthesized NCs possess excellent monodispersity of size and shape without any aggregation and the conductivity of the deposited layer of FeCr2Se4 and FeCr2S4 NCs shows 3.25µA and 2.33µA, respectively. Therefore, our iron-based NCs may substitute current chalcogenides that are environmentally toxic and low efficiency of energy transfer.

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Mass Transport inside Mesoporous Silica Thin Films

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Mesoporous silica thin films (MSTFs), which were three-dimensional structure, have been prepared by the evaporation-induced self-assembly (EISA) method using a block copolymer F-127. Low angle X-ray diffraction (XRD) and scanning electron microscope (SEM) were performed on films to characterize films' structure. We equipped these films on Teflon cell and investigated how mass transport inside MSTFs by cyclic voltammetry (redox probe : Ru(NH3)63+ and supporting electrolyte : KCl). The shape of redox curves were influenced by the concentration of electroactive species. At low concentration of redox probe, adsorption of Ru(NH3)63+ on silica wall was much predominant than diffusion of Ru(NH3)63+. At high concentration, these results were switched. In this case, adsorption Ru(NH3)63+ on silica wall was caused by attraction between negative-charged silica (in neutral condition) and Ru(NH3)63+. By adding HCl or KOH, we varied the surface charge of MSTFs, which affects interaction between silica wall and Ru(NH3)63+ ion. These changed interaction make an effect on redox peak of probe. At acidic condition, the redox peak was decreased, and at basic condition, the redox peak was increased. Also, we investigated how the inner-potential of pore affects mass transport inside MSTFs by altering the thickness of electrical double layer inside pore.When the concentration of nonelectroactive species were high, electrical double layer became thin, the intensity of redox peak was decreased. When the concentration of nonelectroactive species were low, electrical double layer became thick, that of redox peak was increased.

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Photo-induced Synthetic Strategy of Highly Uniform and Homogeneous Noble Metal Nanoparticles

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A photo-stimulation strategy was applied to synthesize colloidal noble-metal nanoparticles (NPs) with a highly uniform morphology and homogenous sizes with high yield at room temperature. In this controlled synthesis, photoreduction of a mixture of the noble metal precursor and a chemical reducing agent under ultraviolet (UV) illumination was used to produce electrons that reduce metal ions ($Au^{3+}$and Ag^{+}) in toluene. Prolonged UV irradiation at 365 nm at a power of 0.14 umol $S^{-1}m^{-2}$ induced ripening wherein the irradiation power, exposure time, and chemical interaction of the reducing and stabilizing agents were key factors in determining the nanoscale structure of the NPs. Current NPs generally have size and shape deviations of 10~30%. But, under optimal irradiation and chemical conditions, size and shape deviations of 4~6% of the Au and Ag NPs were obtained.

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Deep Oxidative Desulfurization of Dibenzothiophene Catalyzed by Mesoporous metal Oxides

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성균관대학교 화학과 [1]성균관대학교 화학과

In this work, various kinds of mesoporous metal oxides (Co3O4, Fe2O3, TiO2, MoO2, WO3, CuO) were synthesized by using nano-replication method via mesoporous silica KIT-6 as a hard template. The mesoporous metal oxides were well-characterized by X-ray diffraction (XRD), N2?adsorption and Scanning electron microscope (SEM). The catalytic activities of those mesoporous metal oxides for the oxidative desulfurization of dibenzothiophene (DBT) with H2O2 as the oxidant in model oil were also investigated under atmospheric pressure at 50oC. The results showed that the catalytic activity was decreased in the order: WO3> MoO2 > TiO2> Co3O4 > CuO > Fe2O3. Further investigation also confirmed that WO3 can be considered as the best catalyst in this research. Mesoporous WO3 was also investigated to be used for catalytic oxidation of sulfur-containing molecules in model oil under different reaction conditions (including different desulfurization systems, H2O2/S molar ratio and temperature). The catalytic activity decreases in the order of DBT > 4, 6-DMDBT> BT for the various sulfur-containing compounds (benzothiophene (BT), dibenzothiophene (DBT), and 4,6-dimethyldibenzothiophene (4,6-DMDBT)).

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Removal of Aromatic Sulfur Compounds using the Oxidative Desulfurization process Catalyzed by various mesoporous silica Supported Tungsten Oxide

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In the research, various kinds of mesoporous silica supported WO3 catalysts were synthesized by incipient replication method and used as the catalysts for oxidative desulfurization of model oil. The WO3/meso-SiO2 materials were well-chracterized by X-ray diffraction(XRD), N2-adsorption, Scanning electron microscopy(SEM),H2-TPR and Raman spectroscopy. The catalytic activities of those for oxidative desulfurization of Dibenzothiophene (DBT) with hydrogen peroxide(H2O2) as the oxidant in model oil(S:2000ppmw) were investigated under atmospheric pressure at 50oC. The results show that the catalytic activity was decreased in the order: WO3/MCM-48>WO3/MCM-41>WO3/KIT-6>WO3/n-SBA-15>WO3/SMS. Further experiment was conducted with WO3/MCM-48 which can be considered as the best catalyst in our research. 10wt% WO3/MCM-48 was also investigated to be used for catalytic oxidation of sulfur-containing aromatic compounds in model oil under different reaction condition (including H2O2/S molar ratio and reaction temperature). The catalytic activity decreases in the order of DBT>4,6-DMDBT>BT for the three sulfur-containing aromatic compounds. And treatment of BT, DBT, 4,6-DMDBT with 10wt% WO3/MCM-48 showed 100% removal of sulfur-containing aromatic compound within 2hours.

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Fabrication of three-dimensionally ordered nickel cobalt sulfide electrodes for supercapacitor

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We have fabricated three-dimensionally ordered nickel cobalt sulfide electrode directly on stainless steel substrate as a current collector without binder or conducting agent. First, 400 nm silica nanoparticles dispersion is spin-coated on the stainless steel substrate to obtain three-dimensionally ordered silica template. And then SiO_2@nickel cobalt silicate core-shell structure was synthesized in aqueous solution of $Ni(NO_3)_2$?$6H_2O$, $Co(NO_3)_2$.?$6H_2O$ and urea. The nickel cobalt silicate shell was converted into nickel cobalt sulfide through a hydrothermal reaction in the presence of Na_2S, where silica core are etched at the same time. The thickness of nickel cobalt silicate shell was changed by the concentration of nickel and cobalt precursor. Also, three-dimensional structure nickel cobalt sulfide was synthesized by proper quantity of sodium sulfide. The obtained nickel cobalt sulfide was characterized by Scanning Electron Microscopy (SEM), X-ray diffraction (XRD) and Electron dispersive spectroscopy (EDS). We will discuss electrical performances in details.

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Optimization of Iron Oxide (Fe_3O_4) Nanoparticles for Magnetic Hyperthermia Application

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Magnetic hyperthermia is cancer therapy by using heat generated from magnetic nanoparticles; magnetic nanoparticles can generate heat in alternative magnetic field by converting magnetic energy to thermal energy and tumor cells are damaged or killed from this. Therefore, it is important to optimize the condition of heat generation such as influence of size, frequency of alternative magnetic field, current, and concentration for efficient magnetic hyperthermia treatment. Here, we have successfully synthesized iron oxide nanoparticles in a wide range of diameters from 20 nm to 140 nm by the synthetic method of solid-state phase transformation. Iron oxide nanoparticles, which were synthesized, were dispersible in agarose gel for viscous medium condition like cytoplasm of cell through the surface modification with polymer. Time-dependent temperature changes of the medium were monitored as functions of nanoparticle size, current level, and frequency of alternative magnetic field. Based on these data, various sized iron oxide nanoparticles were treated to several cancer cells, and the magnetic hyperthermia effect was investigated.

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Hierarchically Nanostructured N-Doped Carbon Electrode for Electrochemical Charge Storage

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Electrochemical double layer capacitor (EDLC) has received a great deal of attention as one of the most potential energy storage devices. Despite the successful utilization of EDLC in the energy storage market, its merits have been somewhat limited because of lower energy density than Li-ion batteries can provide. Tremendous effort has been devoted to boosting the energy density of carbon-based EDLC electrodes, and one of the promising approach is building a hierarchically nanostructured carbon electrode that can increase surface area and facilitate electrolyte diffusion. In this work, we demonstrated a novel synthesis route to the preparation of N-doped carbon nanocoils on carbon fiber paper (CFP). A common approach to prepare one-dimensional carbon on CFP is based on chemical vapor deposition, which requires expensive vacuum equipment and time-consuming processes. In our newly proposed synthesis, polypyrrole nanowire array that was electrochemically deposited on CFP was utilized as a precursor. After carbonization at 700 °C, the N-doped carbon nanocoils on CFP were obtained with a high specific surface area (567 m^2/g). Our in-depth electrochemical investigation revealed that the N-doped carbon nanocoils on CFP exhibited a superior performance, which is attributed to the high surface area, improved electrical conductivity due to N-doping, and three-dimensional carbon network that enables fast electron transport and electrolyte diffusion.

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A Novel Strategy for Maintenance of Catalytic Activity by Using Wrinkled Silica Nanoparticle (WSN) Support for FT-Synthesis

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서울대학교 화학부

Recently, Fischer-Tropsch (FT) synthesis has been receiving much attention again for the conversion of natural gas, coal, and biomass-derived synthesis gas into liquid, due to the increasing crude oil price and the demand for clean fuels. Cobalt catalysts immobilized on the porous solid support are preferred for the FT synthesis because of their high productivity, high selectivity for linear long chain hydrocarbons, and also low activity in the water-gas shift reaction. However, the sintering of the catalyst can be induced by the harsh temperature and pressure conditions of the FT synthesis and it can reduce catalytic properties such as activity and life time. The catalyst deactivation is a serious problem and continuing concern in industrials catalyst development and process. Herein, we synthesized cobalt catalysts supported on the hierarchical mesoporous silica nanoparticles with a wrinkle structure (WSNs), Co-WSN, for the FT synthesis. The wrinkle structure can isolate adjacent Co catalysts from each other and prevent them from sintering. Therefore, Co-WSN can maintain initial catalytic activity and increase life time of catalyst.

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Heteroatom doped ordered mesoporous carbon supported Pt nanocatalyst for the oxygen reduction reaction

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성균관대학교 화학과

Proton exchange membrane fuel cells (PEMFCs) have attracted widespread attention due to their high energy density and low pollution. In PEMFCs, the oxygen reduction reaction (ORR) at the cathode is the rate limiting reaction. Up to now, the most efficient catalysts for ORR is Pt nanoparticles (size of 2~3 nm) dispersion on carbon. But, Carbon corrosion becomes even more serious with increasing temperature, leading to electrical isolation, aggregation and loss of Pt nanoparticle. Due to the above problems with carbon supports, development of alternative support materials has been investigated (eg. Carbon, Metal Oxide and Metal Carbide etc)The focus of this work is to evaluate the dependence of heteroatom doped OMC used by support materials and loading 20 wt% Pt on OMC exhibited good electrocatalytic activity toward the ORR and increase of durability in acidic medium. The heteroatom-doped OMC was synthesized used by impregnation method and its structure was examined by SAXS, SEM, XRD, N2 sorption. And Pt nanoparticles supported on heteroatom-doped OMC were electrochemically characterized.

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New Blue Emitting Materials based on Anthracene derivatives for OLEDs

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가톨릭대학교 화학과

Two related emitting compounds as shown in next page, namely, 9,10-Bis-[1,1';3',1"]terphenyl-5'-yl-1,5-di-o-tolyl-anthracene [TP-DTA-TP] and 9,10-Bis-[1,1';3',1"]triphenylbenzene-5'-yl-1,5-di-o-tolyl-anthracene [TPB-DTA-TPB] were synthesized through typical boration, Suzuki and Sandmeyer reactions. In here, the EL performance was improved by varying the chemical structures of the side groups. Physical properties such as optical, electrochemical, and electroluminescent properties were investigated. Two compounds and DTA were used as an EML in OLED device: ITO / 2-TNATA (60nm) / NPB (15nm)/ TP-DTA-TP or TPB-DTA-TPB (35 nm) / Alq3 (20nm) / LiF (1nm) / Al (200nm). OLED device using TP-DTA-TP showed C.I.E. value of (0.36, 0.53) and luminance efficiency of 3.58 cd/A at 10mA/cm2. TPB-DTA-TPB device exhibited C.I.E. value of (0.17, 0.23) and high luminance efficiency 4.85 cd/A at 10mA/cm2. It was found that TPB-DTA-TPB showed better luminance efficiency and better C.I.E. value than TP-DTA-TP device because it had the increased size of side group.

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Synthesis and Property blue emitting materials based on Fused Chromophore

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Two related emitting compounds as shown in next page, namely, TP-AFF-TP, TP-ASF were synthesized through typical boration, Suzuki and Sandmeyer reactions. In here, the EL performance was improved by varying the chemical structures of the side groups. Physical properties such as optical, electrochemical, and electroluminescent properties were investigated. Two compounds were used as an EML in OLED device: ITO / 2-TNATA (60nm) / NPB (15nm)/ TP-AFF-TP, TP-ASF (35 nm) / Alq3 (20nm) / LiF (1nm) / Al (200nm). OLED device using TP-AFF-TP showed C.I.E. value of (0.25, 0.45) and luminance efficiency of 2.55 cd/A at 10mA/cm2. TP-ASF device exhibited C.I.E. value of (0.17, 0.31) and high luminance efficiency 5.17 cd/A at 10mA/cm2. It was found that TP-ASF showed better luminance efficiency and better C.I.E. value than TP-AFF-TP device.

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Highly selective Zn^{2+} colorimetric sensor using silver nanoparticles

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A variety of chemosensors have been developed to detect Zn^{2+} ions. However, their performance has been achieved at the expenses of sophisticated instruments, time-consuming and laborious experimental procedures to synthesize chemical sensors. However, colorimetric sensors based on nanoparticles have shown the immediate optical feedback, their simplicity, rapidity, and ease of measurement. In this study, we have developed a new potential colorimetric sensor for the selective and sensitive recognition and monitoring of Zn^{2+} ions through bare silver nanoparticles(AgNPs). The fresh synthesized silver nanoparticles are yellow in color due to the intense surface plasmon resonance(SPR) absorption band. In the presence of Zn^{2+}, the yellow AgNPs solution was turned to prussian blue, accompanying the red shifting of SPR band. To support this phenomenon, the synthesized silver nanoparticles were characterized with UV-vis, SEM, and TEM analysis. Additionally, we have searched to optimize the detection conditions such as pHs and proper surfactants.

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Artificial pheomelanin nanoparticles and their photo-sensitization properties

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Pheomelanin-type nanoparticles (PMNPs) were synthesized through a simple oxidative polymerization of 3,4-dihydroxyphenylalanine (DOPA) in the presence of cysteine by KMnO4. The synthesized PMNPs had a diameter of approximately 100 nm, exhibited high dispersion stability in neutral water and various culture media and possessed similar morphology to naturally occurring pheomelanins. The efficiency of photoinduced generation of hydroxyl radicals from PMNPs was determined and related in-vitro cell experiments were carried out, with data being compared to those from eumelanin-type nanoparticles (EMNPs) and natural sepia melanin nanoparticles. Endocytosed PMNPs showed the highest phototoxicity (~50% viability) to UV-irradiated HeLa cells, confirming the direct relationship between phototoxic efficiency and the generation of hydroxyl radicals.

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Thermal conductivity analysis of conductive epoxy adhesive containing Cu nano materials

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Thermal conducting epoxy adhesive(TCEA) is an important thermal interfacing material used between the heating element and heat proof plate.It generally consists of polymer resin, hardener and metal particles such as Au, Ag, Cu, Ni and Al. In order to improve thermal conducting properties of TCEA, we have applied copper nano wires and nano particles.Bisphenol-A-diglycidyl ether (DGEBA), triethylene tetraamine(TETA) and Copper nano particles and nano wires was used as polymer, hardener and metal, respectively.Thermal conductivity of TCEA containing Cu nano materials was studied of as a function of Cu nano particle size, Cu nano wire length and the concentration ratio between nano particles and nano wires.

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microfluidic 장치를 위한 여러가지 가스 플라즈마를 이용한 울의 젖음성 변화

황기환 주동우 부진효*

성균관대학교 화학과

microfluidic 장치는 비용이 저렴하고 제작이 용이하다는 등의 장점을 가지고 있기 때문에 최근 많은 분야에 적용되고 있다. 의료진단 분야나 환경 모니터링, 음식물 안정성 검사 등에 적용되지만 그 중에서도 특히 의료진단에 제일 많이 이용되고있다. 하지만 장비의 속도조절은 현재까지도 쉽지 않은 문제이다. 그래서 본 연구에서는 소수성 성질을 가진 울의 표면에 플라즈마 처리를 하여 친수성으로 만드는 방식으로 속도 조절을 시도하였다. 또한 플라즈마 발생시 이용하는 가스의 종류를 다양화하여 그 종류에 따른 젖음성 변화를 서로 비교하였다. 사용된 가스는 질소, 산소, 아르곤 그리고 공기이다. 이렇게 표면처리 된 울을 이용해 microfluidic 장비를 만들었을 때 우리는 micro mixing 이 충분히 가능하다는 것을 관찰하였다. 또한 플라즈마 처리 속도와 이용된 가스의 종류의 조절을 통해 wicking 속도를 조절 할 수 있다는 것을 관찰하였다.

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Silver Nanowire Based Transparent Heating Film

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Transparent Heating Film (THF) has many applications such as refrigerators, glasses and strollers, and also can be used in automobile window and building windows for defrosting purpose. Indium tin oxide (ITO) or fluorine doped tin oxide (FTO) has been used in a conventional heating film. However, the relatively high sheet resistance and the low flexibility of ITO or FTO films limit their applications in many areas. Carbon nanotubes (CNTs) based films have been studied intensively due to their excellent bending stability. Still high sheet resistance in CNT-based films cannot be overcomed and did not reach commercialization stage (~200 Ω/sq and >85% transmittance at 550 nm). As an alternative film, we have studied flexible silver nanowire heating film (SNWHF), which exhibits excellent bending stability as well as low sheet resistance. (~50 Ω/sq and >90% transmittance at 550 nm). SNWHF is fabricated by the simple coating of SNWs on PET films followed by additional over-coating of stabilizing layer. By varying applied voltages, we have measure temperature change of SNWHF. The SNWs diameter was varied from 25 nm~100 nm to study the thermal stability.

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Selective Detection of Copper (II) Ions Utilizing the Intercalated-Molecules in Layered Gadolinium Hydroxide Matrices

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Copper is an essential trace element in the human body and plays important roles in a variety of fundamental biological process in organism. However, free Cu^{2+} ions, potentially very toxic, can cause oxidative stress and disorders associated with neurodegenerative disease if being unregulated, such as Menkes disease, Wilson disease and Alzheimer's disease. In this study, we have developed a novel sensor based on Eu-doped layered gadolinium hydroxides (LGdH:Eu) with artificial receptors (dinitrostilbenedisulfonate, DNSBDS) for the detection of Cu^{2+} ions in aqueous solution containing various divalent metal ions such as Mg^{2+}, Ni^{2+} and Zn^{2+}. The uptake of Cu^{2+} ions into DNSBDS-intercalated LGdH:Eu matrices has occurred within a few minutes due to high binding affinity between Cu^{2+} and the sulfonate groups of DNSBDS. Interestingly, in X-ray diffraction patterns, the shift of *(00l)* reflections of LGdH:Eu-DNSBDS was only observed under the presence of Cu^{2+} ions. It indicate that the DNSBDS-intercalated layered matrices can be used as a sensor for selective detection and removal of Cu^{2+} ions. Also, we have demonstrated that LGdH:Eu-DNSBDS matrices have both sensitivity and selectivity for detection of Cu^{2+} ions through the study of the photoluminescence (PL) properties. The red emission of LGdH:Eu-DNSBDS was drastically quenched when Cu^{2+} ions were adsorbed. This organic/inorganic hybrid sensor will provide an analytical method for detection of heavy metal in pollutant.

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Detection and removal of Cr(VI) ions in aqueous solution by using terbium-doped layered yttrium hydroxychlorides

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Chromium is one of the major pollutants of ground and surface waters and is often find in contaminated industrial or urban waste waters. It is present in a number of oxidation states but mainly exist as trivalent chromium, Cr(III) and hexavalent chromium, Cr(VI). However, between the two chromium states, hexavalent chromium, Cr(VI) is considered as a major environmental and health threat. Too much intake of hexavalent Chromium can lead to serious illnesses such as cancer, ulcer, dermatitis, and extremely, death. World Health Organization (WHO) and most of environment protection agencies limit the Cr(VI) content of drinking water to 0.05ppm. Thus, detection and removal of such heavy metal is of great importance. In this study, Terbium-doped layered yttrium hydroxychlorides (LYH:Tb) was applied to detect Cr(VI) in aqueous solutions, where the inner filter effect (IFE) system is constructed by the excellent overlap between the excitation bands of LYH:Tb and the absorption band of Cr(VI) (both $HCrO_4^-$ and CrO_4^{2-} forms). The effective shielding of excitation light for LYH:Tb by the adsorbed Cr(VI) could achieve a feasible IFE-based detection sensitivity. Therefore, it would be possible to use our system for monitoring the chromium contamination at low concentration levels in natural surface water bodies or wastewater treatment plants.

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Luminescence Quenching of Tb-doped Layered Rare Earth Hydroxides by Nitrate Anions

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Layered rare earth hydroxides (LRHs), which are composed of rare earth hydroxocation layers and inorganic/organic anions layers, are similar to well-known layered double hydroxides (LDHs) and exhibit a ready anion-exchange reaction in the interlayer galleries. Moreover, because the presence of 4f electronic shells in rare earth ions leads to abundant luminescence characteristics, LRHs have been used for optical applications. Generally, quite low luminescence efficiency of Tb-doped layered rare earth hydroxynitrates (LRH:Tb-NO_3) has been explained to be mainly due to nonradiative energy transfer to O-H vibrations. However, when Tb^{3+} ions were doped into layered rare earth hydroxychloride (LRH-Cl) matrices, the efficiency of green emission is largely enhanced and broad excitation band at approximately 250 nm is assigned to the spin-allowed (low-spin, LS) or spin-forbidden (high-spin, HS) interconfigurational Tb^{3+} f-d transition. Here, we demonstrate that the shielding of excitation light by nitrate anions causes the luminescence quenching of LRH:Tb-NO_3 (RE = Gd, Y); When Cl- anions of LRH:Tb-Cl were replaced by NO_3^- anions, the bright green emission of LRH:Tb-Cl was significantly decreased. Considering that the absorption band of NO_3^- anions is observed at similar wavelength range to the excitation band of LRH:Tb, this phenomenon of luminescence quenching is conceptually similar to the inner filter effect (IFE). The quenched luminescence was recovered by deintercalation of NO_3^- anions from LRH:Tb matrices.

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Au/Ag NPs decoration on different lengths of MWCNTs and their optical properties

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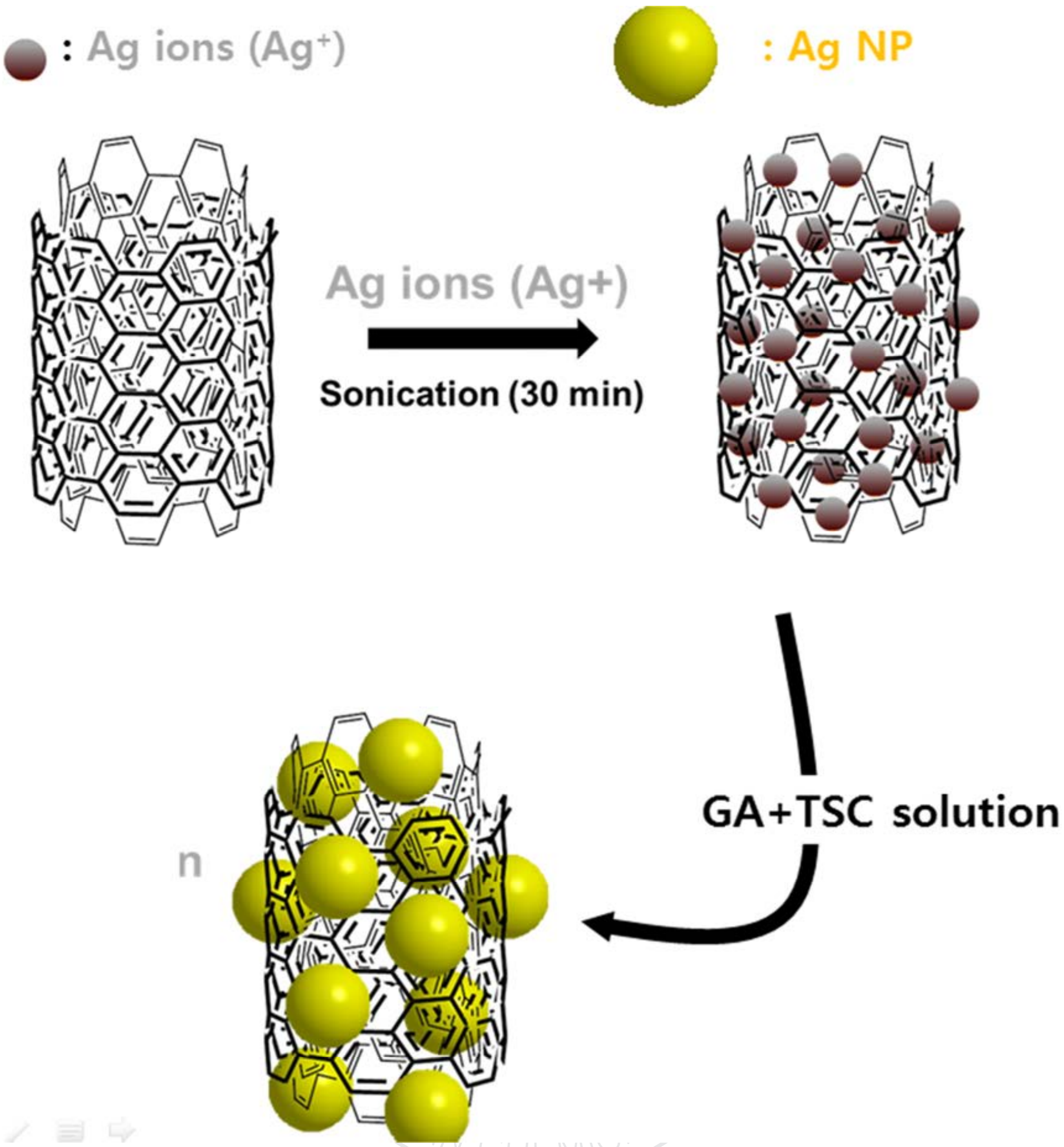
As a new and very promising class of functional materials, noble metal NPs/CNTs nanohybrids become one of the family of composite materials with extraordinary properties by combining the advantages of noble metal NPs and CNTs. Different lengths of Multi-walled carbon nanotubes (CNTs) functionalized with Au or Ag NPs were obtained using a single step system by using phytochemical as reducing agent. Au/Ag decorated MWCNT with different lengths were dispersed in water and characterized systematically by applying UV spectroscopy, TEM. In particular, the characteristic of absorption of the CNT depending on their lengths was analyzed by monitoring SPR spectra of Au NPs or Ag NPs. It may expect that the MWCNT with different length conjugated with Au or Ag NPs exhibit different interaction files to the cells proliferation and electronic properties.


● : Ag ions (Ag⁺)
● : Ag NP
Ag ions (Ag+)
Sonication (30 min)
GA+TSC solution
n

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Graphene QDs conjugated with Fe_3O_4 NPs for multifunctional nanocomposites

오상진 이재범[1,*]

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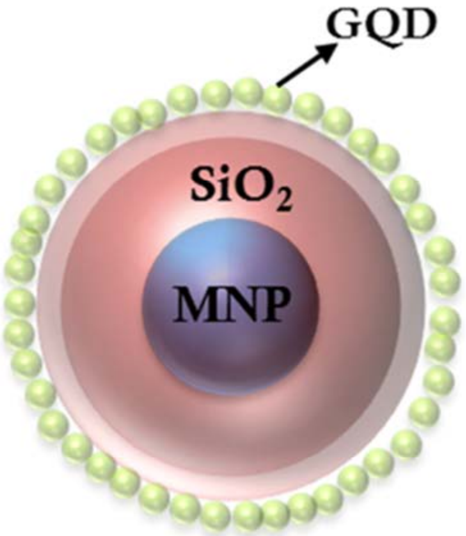
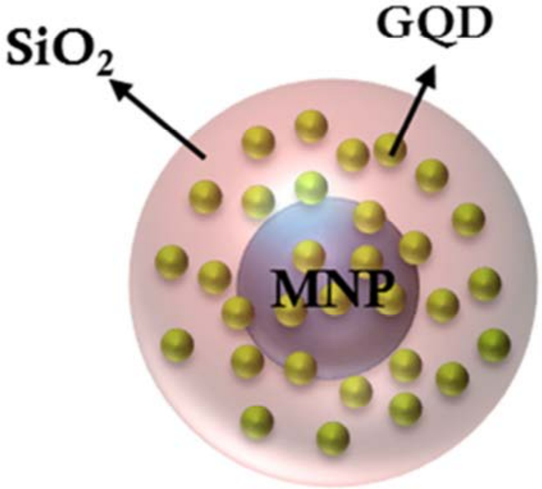
Multimodal imaging and imaging-guided therapies have become a new trend in the current development of medical theragnostics and drug-delivery system. It is expected that the combination of magnetic and fluorescent properties in one nanocomposite would enable the engineering of unique multifunctional nanoscale devices, which could be manipulated using external magnetic fields. The aim of this research is to present an "two in one" magnetic-fluorescent nanocomposite materials which combine both magnetic and fluorescent properties in one entity, in particular those with potential applications in biotechnology and nanomedicine. MNP@SiO_2@Graphene QD nanocomposites with superparamagnetism and luminescence have been prepared by a facile chemical method. Nontoxic fluorescent graphene QDs were assembled around the Fe_3O_4-silica core-shell nanocomposite via two kinds of method. The bifunctional nanocomposites exhibit superparamagnetic behavior and fluorescence. This demonstrates the potential of conjugated silica shell based dual-modal nanocomposites for bio-application in future.


GQD
SiO₂
MNP


SiO₂
GQD
MNP

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엽산을 이용한 실리카 나노입자의 물성변화 연구

박정훈 이상윤[1] 이준영[1] 허민구 양승대 김상욱[1,*]

한국원자력연구원 방사선기기연구부 [1]동국대학교 신소재화학과

나노 입자는 유기 또는 무기 소재의 기본물질로 생체의학적 약물전달을 목적으로 많이 사용되고 있으며, 실리카 나노입자는 독성이 낮아 다양한 작용기를 도입한 연구가 있으며, 특히 엽산은 세포 표적지향성으로써 약물전달체로 많이 연구가 되어지고 있다.본 연구에서는 전위차 변화에 따른 세포 섭취도 변화를 보기 위해 실리카 나노입자에 엽산을 일정한 비율로 증가시켜 표면개질한 후 전위차 변화에 대해 확인하였다.다양한 사이즈의 실리카 나노입자를 합성하기 위해 가수분해 대표 화합물인 TEOS (Tetraethly orthosilicate)를 출발물질로 Stoeber 방법으로 50nm 크기의 실리카 나노 입자를 합성한 후 다양한 작용기를 도입하기 위하여 아민기가 결합된 실란화합물인 APTS (3-Aminopropyl triethoxysilane)로 실리카 나노입자 표면을 개질 하였으며, 아민기의 합성여부를 FT-IR 로 구조분석 하였으며, 표면계질한 실리카 나노입자에 가교제를 이용하여 엽산을 합성하였으며 XRD, 13C-CP MAS Solid-NMR 로 화합물의 구조분석을 하였으며, SEM, TEM 을 이용해 나노입자의 표면 크기와 형태를 확인하였다. 또한, 엽산의 비율을 1~5 배로 증가시켜 실리카 나노입자와 합성 한 후 Zeta potential 과 size 그리고 UV-Vis 을 통해 전위차 와 흡광도가 증가되는 것 을 확인 하였다.

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Diketopyrrolopyrrole-based Highly Sensitive Optical Sensor Material for Fe^{3+} and Cu^{2+}: Synthesis and Spectral Investigation

홍한나 이대희 엄현아 신지철 조민주 **MATINDERKAUR** 최동훈*

고려대학교 화학과

Heavy and transition metal (HTM) ions have significant functions in many biological systems and environmental processes. The fluorescent probes for the recognition and the selective detection of HTM ions attract much interest in supramolecular chemistry because of the importance of these ions. Among the HTM ions, recognition of iron (Fe^{3+}) and copper (Cu^{2+}) is particularly interesting because of their toxicity and vital role in biological systems. We have synthesized a new π-expanded diketopyrrolopyrrole (DPP)-based fluorescent probe for selective recognition of Fe^{3+} and Cu^{2+}. UV/Vis absorption spectroscopy indicates that the probes behave as good chromogenic chemosensors for Fe^{3+} and Cu^{2+} over other metal ions. These probes exhibited pronounced Fe^{3+}/Cu^{2+} on-off type fluoroionophoric properties with significant color change. Both UV-Vis and fluorescence spectroscopic studies demonstrated that probe was highly sensitive and selective towards Fe^{3+}/Cu^{2+}.

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Exfoliation of Boron Nitride Nanosheets with Surface Functionalization of Oleylamines

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한국과학기술연구원(KIST) 소프트혁신소재연구센터 [1]한국과학기술연구원(KIST) 전북분원 복합소재기술연구소

Boron nitride nanosheets (BNNSs) are two dimensional crystals composed of boron and nitrogen atoms covalently bonded in a hexagonal manner having exceptional physiochemical properties. Similar to graphene, BNNSs have remarkable mechanical properties and thermal conductivity.In this study, we demonstrate a simple method to produce few layers of boron nitride nanosheets (BNNSs) based on a solvo-thermal method by functionalization of the BNNSs with oleyl amines. By this simple method, BNNS of 4~5 layers with lateral size of several hundreds of nanometers were produced. The BNNSs were characterized by transmission electron microscopy, atomic force microscopy and infrared spectroscopy, and X-ray photoelectron spectroscopy measurement. The concentration was verified by filtering the BNNSs dispersion as 40 mg/ml. We also confirmed improved dispersion stability of the functionalized BNNSs by oleyl amines within some organic solvent such as toluene. We confirmed potential of the surface modification of BN through this experiment. Accordingly, we have studied functionalized BNNSs by using different organic material. We have further researched a variety of applications of the prepared BNNSs as a nanofiller for a polymer matrix with desired properties.

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Geometrically precise nanoscale phase segregation within a facet-controlled binary alloy nanoparticle

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고려대학교 화학과

The synthesis of high energy-faceted alloy nanoparticles has been zealously pursued for the development of high performing nanocatalysts. While the facet-control of alloy nanoparticles, namely the organization of surface atoms, is attained by understanding the growth kinetics and surface-stabilizing effects of surfactants, little is known for the atomistic organization within the matrix of a nanoparticle. Herein we report that the atomistic organization within the alloy nanoparticle matrix is greatly affected by the surface energies which are governed by the geometrical parameters of the nanoparticle and the identities of surface bound moieties. With this understanding, we could prepare phase-segregated binary nanoparticles that exhibit excellent electrocatalytic activities relevant to the fuel cell applications.

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Electronic structure of quasi-one dimensional superconducting material, $Ta_4Pd_3Te_{16}$

남대현 조성우 정동운*

원광대학교 화학과

The electronic structure of $Ta_4Pd_3Te_{16}$ was analyzed by tight-binding band calculation based upon the given structure. DOS and Fermi surface calculated for this compound showed that $Ta_4Pd_3Te_{16}$ is a quasi one-dimensional metal. A strong Fermi surface nesting was found, which means that this compound may exhibit electronic instability. The nested Fermi surface was supposed to work as a driving force to show a metal-superconducting transition in this compound.

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Synthesis of Ag coated Cu particles using galvanic displacement and their sintering by intense pulsed light for printed electronics

정혜리 조미숙 이영관*

성균관대학교 화학공학과

Recently, as an alternative for silver and gold, the demand for low-cost copper-based conductive ink increases in printed electronics. But copper has relatively low conductivity and rapid oxidation properties. Here we designed Cu metal particle coated with Ag and sinter them by Intense pulsed light (IPL) for printed electronics. Ag was coated on Cu particles by a galvanic displacement, and the thickness of silver was controlled by the concentration of silver precursor. The Ag coated Cu particles were characterized by scanning electron microscopy (SEM), energy Dispersive Spectroscopy (EDS), and x-ray diffraction (XRD). The conductive ink based on Ag coated Cu particles was prepared and printed on PET film. We sintered Ag coated Cu film utilizing IPL system, which facilitates fast sintering without any damage on the flexible PET. Depending on the irradiated energy and pulse number, Ag coated Cu film was studied for morphology and resistivity.

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Janus behavior of melanin; antioxidant vs. oxidant

김지태 이진규*

서울대학교 화학부

Melanin is one of the well-known biomacromolecules and is found in most organisms, which is believed to play various roles such as photoprotection, photosensitization, radical quenching, and metal ion chelation. Based on not only their beneficial biological functions, but also on some implications in disease-related events such as skin cancer and neurodegenerative disorders like Parkinson's disease, melanins have attracted much attention as a challenging biomaterial in a wide range of disciplines. In this regard, a fundamental study about the establishment of exact structure-property-function relationships of melanin has been one of the key issues in understanding the various contradictory biological functions of melanin. There have been several researches which link the various biological properties to the structure of melanin. However, these researches cannot provide the clue to establish that two contradictory properties of melanin come from its structure. To understand exact structure-property-function relationships of melanin, we have studied the effect of redox-active metal to change the structure of melanins and ultimately its biological properties. Details on the correlation between both properties and structure will be discussed.

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Preparation and Derivatization of Keggin Lacunary Silicotungstates for Immobilization on Various Solid Supports

YUNHYUNSIK 문두식 이진규*

서울대학교 화학부

In recent decades, there have been remarkable growths in attention towards polyoxometalates (POMs) because these anionic inorganic clusters have interesting structural and chemical properties that have led to a wide variety of applications such as oxidation catalysts. One of the most intensely studied polyoxometalates is the Keggin-type silicotungstate, $[SiW_{12}O_{40}]^{4-}$, because of its superior stability in solution than any other POM species. Herein, we have prepared the Keggin-type, lacunary silicotungstate and subsequent silylation for immobilization on various support materials. In many cases, it is desirable to support the POM cluster on solid materials because the heterogeneous system enable easy recycling of the catalyst for reuse and allow convenient catalyst/product separation. Therefore, we made use of 3-chloropropyltrimethoxysilane and derivatized the chloropropylsilyl chain onto dilacunary silicotungstates and characterized them in order to immobilize them onto solid silica support that has been treated with aminopropyltriethoxysilane (APTES). Detailed experimental procedure for the derivatization and immobilization of dilacunary silicotungstates will be presented.

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Luminescence spectra of Ce^{3+}-doped blue phosphors prepared from the CeF_3-Al_2O_3 reaction system

최연희 이민호 정우식*

영남대학교 화학공학부

Ce^{3+}-doped blue phosphors were prepared by calcining a mixture of CeF_3 and Al_2O_3 powders under a flow of inert gas. The emission wavelength (330 to 450 nm) and intensity of the phosphors depended on calcination temperature, duration time and amount of CeF_3. The dependence was ascribed to the difference of host materials (Al_2O_3, CeF_3, $CeAlO_3$, and etc) formed by the calcination. XPS spectra of the phosphors were measured to identify the chemical state of Ce(III).

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The addition of alkaline earth ions for tuning color of $Eu^{3+/2+}$-doped $LaAlO_3$ phosphors

이민호 최연희 정우식*

영남대학교 화학공학부

Luminescence spectra of the $Eu^{3+/2+}$-doped $LaAlO_3$ powders prepared by calcination of a mixture of La_2O_3, Al_2O_3 and EuF_3 powders under a flow of inert gas showed two peaks at 593 (orange) and 460 nm (blue). The intensity and wavelength of the emission bands were tuned by varying the mole ratio of Al_2O_3 to La_2O_3 and adding alkaline earth ions such as Ba^{2+} and Sr^{2+}. The emission peaks at 490 (blue-green) and 520 nm (green) were assigned to Eu^{2+}-doped $BaAl_2O_4$ and $SrAl_2O_4$ in $LaAlO_3$ powder, respectively. The white emission phosphors with three colors can be obtained by the addition of alkaline earth ions.

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The Behavior of Hela Cells on Mesoporous Thin Films of various metal oxides

김근오 김강영 홍다영[1] 박현욱 곽진수 권영욱[*]

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In this work, we reported the behavior of Hela cells on mesoporous thin films of various metal oxides(SiO_2, TiO_2, ZrO_2 and Al_2O_3) with 10 nm pore size. Various mesoporous thin films were synthesized by sol-gel process with metal precursors and surfactant. In order to confirm the stability of thin films, each film was immerged in a cell culture media for 2 days. And then, we confirmed that all films except for SiO_2 are stable in a cell culture media. Finally, we observed the cytotoxicities of Hela cells on various films for 3 days in a cell culture condition. As a result, we found that the cytotoxicities order of films is followings; Al_2O_3(calcine: 400°C)> SiO_2> ZrO_2> Al_2O_3(calcine: 800°C)> TiO_2

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Synthesis and Characterization of New Copolymer for Organic thin film transistor

김형남 김윤희* 마재열 김란 전찬우[1] 천예림 황재영[2]

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A novel copolymer was synthesized by Still coupling reaction. The synthesized materials have moderate solubility in organic solvents such as chloroform, chlorobenzene, and dichlorobenzene. This copolymer contains electron donating thiophene, thienothiophene moiety, which is big fused aromatic unit having a high thermal stability and good air stabilit. We present electrochemical, thermal properties of the synthesized polymer and OTFT property

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Photocatalytic degradation of methylene blue solution in presence of graphene oxide-supported TiO_2 nanoparticles

오명은 최현철*

전남대학교 화학과

Graphene oxide (GO) have been one of the most extensively studied nanostructured materials over the last decade because of their unique chemical and physical properties, as well as their technological applications. Recently, significant interest has been devoted to developing a variety of GO-based materials to generate new functionalities. Some researchers have reported GO-supported catalysts that exhibit good photocatalytic behaviors for various organic pollutants. In this study, we report a simple and effective process for preparation of GO-supported TiO_2 (GO-TiO_2) using amidated GO. N,N'-dicyclohexylcarbodiimide (DCC) was used as a coupling agent for the formation of an amide linkage. The resultant GO-TiO_2 sample was characterized by transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) measurements. The photocatalytic properties of the prepared GO-TiO_2 catalysts were evaluated by measuring the photodegradation of methylene blue (MB, $C_{16}H_{18}N_3S$-Cl-3H_2O) in aqueous solution.

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CNT-SnO_2 as photocatalyst for degradation methylene blue

김성필 최현철*

전남대학교 화학과

Semiconductor supported photocatalysis has recently attracted as an efficient method for air purification, water disinfection and purification. Among the semiconducting catalysts, Tin Oxide (SnO_2) has been used as a photocatalysis for degradation of a wide variety of environmental pollutants due to its advantages like low cost, easy production, and compact size etc. The photocatalytic efficiency of SnO_2 mainly depends on high specific surface area of SnO_2 particles, crystal structure, particle size and porosity. One of the methods to improve the photocatalytic efficiency is to increase the surface area of the catalyst. In this study, tin oxide nanoparticles synthesized by sol?gel method were easily decorated on the thiolated carbon nanotubes (CNT?SnO_2). The CNT?SnO_2 nanocomposites were investigated with transmission electron microscopy (TEM), X-ray diffraction (XRD) and X?ray photoelectron spectroscopy (XPS) and its photocatalytic activities are studied for photodegradation of organic dyes like methylene blue.

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Preparation of Ag-decorated graphene oxide and investigation of its antibacterial activity

김지당 최현철*

전남대학교 화학과

Silver (Ag) compounds have high bactericidal activity and biocompatibility. However, their high surface energy makes them highly reactive and susceptible to aggregation into large particles, which results in the deterioration of their unique chemical properties and the loss of their antibacterial activities. In an effort to overcome these problems, nanocomposites composed of Ag nanoparticles dispersed on suitable substrates have been intensively studied. In this study, we report a simple and effective process to prepare Ag-decorated graphene oxide by depositing Ag nanoparticles on thiolated graphene surfaces. Thiol groups were utilized as linkers to secure the Ag nanoparticles without agglomeration. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The Ag-decorated graphene oxide exhibits high antibacterial activities against Gram-negative E. coli bacteria.

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Preparation of CNT-TiO_2 for the electrochemical sensor of hydrazine

김성필 최현철*

전남대학교 화학과

Hydrazine is widely used in industrial applications, such as a fuel in rocket propulsion system, also pesticides, blowing agents, pharmaceutical intermediates, photographic chemical materials, corrosion inhibitors, antioxidants, catalysts, emulsifiers, herbicides, dyestuffs and explosives. However, hydrazine is a toxic material. Exposure to hydrazine can also damage the liver, kidney and central nervous system in human, which must be treated with care. Due to the reasons above, sensitive detection of hydrazine is practically important. In this study, we synthesized titanium oxide decorated on thiolated carbon nanotubes (CNT-TiO_2). Morphology properties of the CNT-TiO_2> were investigated with transmission electron microscopy (TEM), X-ray diffraction (XRD) and X?ray photoelectron spectroscopy (XPS). Cyclic voltammetry (CV) and amperometry (at an applied potential of 0.39 V) were used to investigate electrochemical properties.

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Synthesis and Structures of New Strontium Chromium Phosphates

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The transition metal phosphates have been widely investigated due to their potential applications for secondary batteries. Among them, alkaline earths transition metal phosphates have not been widely investigated. As a result to find new phases in this system, single crystals of new quaternary compounds, $Sr_{1.5}Cr_3P_4O_{16}$, $Sr_{1.97}Cr_{2.82}P_4O_{16}$ and $Sr_2CrP_3O_{11}$ have been prepared with the use of $SrCl_2$ and their structures have been characterized through X-ray diffraction. The structures of the compounds share the common features. They consists of CrO_6 octahedra and PO_4 tetrahedra which are linked via sharing oxygen atoms. Depending on linking modes, these polyhedra form two or three-dimensional structures with large empty channels. The Sr ions stay in these empty channels and stabilized by oxygen atoms through electrostatic interactions. In this poster structural comparison will be discussed. We found that the compositions of Sr can be controlled by the amounts of Cr to satisfy charge neutralities. This lead us to search new materials by varying the amount of metals. We believe that these phases could play a crucial role for cathode materials of secondary batteries. The classical charge balance of the title compounds can be represented as $[Sr^{2+}]_{1.5}[Cr^{3+}]_3[P^{5+}]_4[O^{2-}]_{16}$, $[Sr^{2+}]_{1.97}[Cr^{3+}]_{2.82}[P^{5+}]_4[O^{2-}]_{16}$ and $[Sr^{2+}]_2[Cr^{3+}][P^{5+}]_3[O^{2-}]_{11}$.

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New Hexanary Compounds, ANbPO$_4$SCl. (A = Rb, Cs)

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The two new 2-dimensional compounds, ANbPO$_4$SCl (A = Rb, Cs) have been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. They are isostructural and they crystallize in the space group *P4/nmm* of the tetragonal system with two formula units in cell dimensions, a=6.4960 (5) ? c=8.0840(5) ?, and V=341.13(4) ?^{3} (RbNbPO$_4$SCl); a=6.5168(3) ?, c=8.1942(4) ?, and V=348.01(3) ?^{3} (CsNbPO$_4$SCl). Each niobium atom is surrounded by one sulphur, one chlorine, and four oxygen atoms in the octahedral fashion and phosphorus atoms are coordinated by four oxygen atoms in a tetrahedral geometry. These polyhedral are combined to form the two-dimensional infinite anionic layers, $^2_\infty$[NbPO$_4$SCl$^-$]. Alkali metal ions reside between the layers to complete the three-dimensional structures. The classical charge valence can be described as [A$^+$][Nb^{5+}][P^{5+}][O^{2-}]$_4$[S^{2-}][Cl$^-$].

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Synthesis and Structure of a New Mixed-metallic Phosphate, $Li_{3-4x}(Ti_{2-y}/Nb_y)_2(PO_4)_3$

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아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

Due to the ionic mobility of Li^+ ions, lithium trivalent metal phosphates, $Li_3M_2(PO_4)_3$(M = Fe, Ti, V, Sc) have been widely investigated as materials for rechargeable batteries. The positions and stoichiometries of Li ions in this phase play crucial roles to determine the efficiency of the system. In our group we have focused on the systematic approach toward the synthesis of new members of this family via partial substitution of metal sites with different oxidation states. Partial replacing of Ti with metals of different oxidation states have lead us to find new mixed-metallic phases with non-stoichiometric Li contents, $Li_{3-4x}(Ti_{2-y}/Nb_y)_2(PO_4)_3$. The framework is comprised of (Ti/Nb)-centered octahedra and P-centered tetrahedra. The metal sites are occupied by statistically disordered Ti and Nb atoms. These polyhedra are sharing O atoms to form a three-dimensional framework with huge empty space. , relationship between stoichiometry of Li and the sum of the oxidation states of each metal will be discussed as will the occupational behavior of Li+ ions over the three Li sites. The classical charge valence of the compound could be described as $[Li^+]_{3-4x}([Ti^{3+}]_{1-x}[Nb^{5+}]_x)_2[P^{5+}]_3[O^{2-}]_{12}$

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Intermetallic Distances Vs. Composition of Alkali Metals in The Mixed-metal Thiophosphate, $A_x(Nb_yTa_{1-y})PS_6$

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Mixed-metal thiophosphates, $A_x(Nb_yTa_{1-y})PS_6$ (A=K, Rb, Cs), have been prepared from reactive alkali metal halide fluxes and characterized with single-crystal X-ray diffraction techniques. The title compounds are closely related with the previously reported ternary phase, $TaPS_6$, which is composed of the three-dimensional open framework with empty tunnels. In the title compound, disordered alkali metal cations reside in this space and simultaneously partial electron densities are transferred to the low-lying acceptor levels, d orbitals of group 5 metals. Therefore substantial decrease of M---M interatomic distances are observed. We have found that the intermetallic bond lengths can be controlled gradually by the amount of the alkali metals. In this presentation, the relationship between composition of alkali metals and intermetallic bond lengths will be analyzed along with the effect of alkali metal size differences on the shape of the empty channels.

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Noble Copolymers Composed of Symmetric Dialkylated-Terthiophene and Thiophene Derivatives for OTFT and Organic Solar cell

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We designed new polymers composed of dialkylated terthiophene and thieno[3,2-b]thiophene,2,2`-bithiophene for the fabrication of organic thin film transistors and polymer solar cells.Poly[5-(thieno[3,2-b]thiophene-2-yl)3`,4`-dioctyl-2,2`:5` ,2``-terthiophene] (PTTOT), and poly[5-((2,2`-bithiophene)-5-yl)3`,4`-dioctyl-2,2`:5`,2``-terthiophene] (PBTOT) were synthesized via Stille coupling and Suzuki coupling reaction. Field-effect hole mobilities of PTTOT and PBTOT based solution-processed OTFTs were 3.54 × 10^{-3} cm^2 V^{-1} S^{-1} and 1.73 × 10^{-2} cm^2 V^{-1} S^{-1}, respectively. And, each of the polymers was investigated as an electron donor material with $PC_{71}BM$ as an electron acceptor in bulk hetero junction solar cells. The polymers of PTTOT and PBTOT showed the power conversion efficiency (PCE) of 0.096% (Jsc = 0.1 mA/cm^{-2}, FF = 83.49%) and 3.2% (JSC = 8.9 mA/cm^{-2}, FF = 51.9%), respectively.

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Synthesis of Magnetoplasmonic Bumpy-like Nanoparticle Using Layer-by-Layer Assembly

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Core-shell nanocomposite with large sized Fe3O4 core and Au shell has magnetic and plasmonic properties, which originated from the composite materials. With large sized Fe3O4 core we absorbed much strong magnetic property. We synthesized Au coated Fe3O4 bumpy-liked core-shell nanoparticle through seed growing method with layer-by-layer assembly. The bumpy surfaces of this nanoparticle have rough surface area with many hotspots on noble metal surface. Geometry of gold shell has been constructed by simple method coating second layer of PEI on gold seed during synthesis. This material can be used for detecting, imaging and treating disease because of their magnetoplasmonic property, and also used as catalyst, and substrates of optoelectronic devices.

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Enhanced Colloidal Stability of Functionalized Mesoporous Silica Nanoparticles with Reactive Groups

조은범* 김준석

서울과학기술대학교 정밀화학과

We present the preparation of functionalized mesoporous silica nanoparticles with reactive groups and the additional chemical modification for colloida stability of the silica nanoparticles. Recently, there have been so many publications for mesoporous silica nanoparticles because the non-toxic silica materials have been known as a strong candidate for drug carrier and various medical treatments. However, the performance is somewhat related with the maintenance of nanoparticles' shape without aggregation among silica nanoparticles. We have tried to modify the functionalized mesoporous silica nanoparticles using ethane- and phenylene-groups additionally. We found the colloidal stability of functionalized mesoporous silica nanoparticles is enhanced available to various biomedical applications.

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Formation of mesoporous hollow silica spheres using cationic surfactant as template

진현탁 배재영*

계명대학교 화학과

Hollow silica spheres containing ordered mesoporous were prepared from core-shell structured polystyrene (PS) core with mesoporous silica shell. The formation of the mesoporous hollow silica spheres (MHSS) were proposed to be due to the presence of electrostatic interactions between the supramolecular template and silica precursors, which were assumed to self-assemble around the cationic surfactant molecules. The morphological, structural, and textural properties of MHSS were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), N_2-sorption, and thermal gravity analyzer (TGA). TEM images indicated that well defined PS had a diameter range about 152-352 nm, and shell thickness range about 34-150 nm. XRD results showed uniformed mesoporous structure, TGA indicated removing temperature of polystyrene, and BET surface area was 1384 m^2/g high surface area.

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Synthesis of TiO_2 hollow spheres with size controllable polystyrene particles by core-shell structure

김재욱 배재영*

계명대학교 화학과

Synthesis of polystyrene (PS) particles with controllable size using relatively simple process and to demonstrate their application as the template in the production of TiO_2 hollow spheres (THS). THS is synthesized to titanium tetraisopropoxide (TTIP) with PS particles by core-shell structure. The size of the PS particles was proportional to the composition of styrene and the amount of initiator. Transmission electron microscopy (TEM) showed well-defined hollow sphere. Defined THS with diameter ranging from 280 - 380 nm and PS diameter ranging from 200 to 300 nm. Result of Thermogravimetric Analyzer (TGA) showed the removal temperature of PS. The X-ray diffraction (XRD) peaks showed Anatase structured and Brunauer-Emmett-Teller (BET) surface area was 61 m_2/g.

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Preparation and Characterization of Hexagonal and Cubic Structured Mesoporous Silica materials by Sol-gel method

서원호 배재영*

계명대학교 화학과

Mesoporous silica materials were prepared by sol-gel method using tetraethyl orthosilicate (TEOS) as a silica source and cetyltrimethylammonium chloride (CTACl) as a template. The resulting silica materials were characterized by fourier transform infrared spectrometer (FT-IR), X-ray diffraction (XRD), transmission electron microscope (TEM), and N_2 sorption isotherms. The FT-IR spectra confirmed the removal of surfactant after calcination and the occurrence of symmetric Si?O stretching. TEM images and XRD patterns confirmed well-ordered mesostructures in all of these silica materials. According to N_2 sorption isotherms, the surface areas of materials evaluated from the N_2 sorption isotherms are about 1270 m^2/g for hexagonal mesoporous silica and 1441 m^2/g for cubic mesoporous silica.

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Amino group Functionalized organosilanes of cubic mesoporous silica obtained at room temperature

구병진 배재영*

계명대학교 화학과

Functionalized ordered cubic mesoporous silica have been obtained by a post-grafting method using 3-aminopropyltriethoxysilane (S330,Osung) as modifying agent. The dependence of S330 concentration, and reaction time on average pore size, pore volume, superficial area, and morphology was studied. The modified silicas were characterized by powder X-ray diffraction (XRD), infrared spectroscopy (FT-IR), transmission electron microscope (TEM) and nitrogen adsorption?desorption experiments. According to the TEM results, no morphological changes were observed in the modified cubic mesoporous silicas by comparing with bare silicas. The gas absorption capability of the mesoporous silica absorbent show the highest performance of 4.08 mol co_2 / kg

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Characterization of Solid Acid Electrolyte CsH_2PO_4 and $CsH_5(PO_4)_2$ by solid-state NMR Spectroscopy

채신애 한옥희*

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Solid acids are both an acid and salt in a solid state, and can generally be described as $M_aH_b(XO)_c$, where M is Cs, Rb, K, Na, or NH_4 and X is P, S, As, or Se. Ever since $CsHSO_4$ (CHS) electrolyte was demonstrated for fuel fells (FCs) by Halie et al. various solid acid electrolytes for FCs have been reported. Even better performance than that with CHS was reported with CsH_2PO_4 (CDP) only, or with CDP/Si-oxide composites in humidified conditions. All of the CDP in the CDP/SiP_2O_7 composite electrolyte was observed by X-ray diffraction (XRD) to convert to $CsH_5(PO_4)_2$ (CPDP) at 220 °C and higher, indicating that the good conductivity of this composite electrolyte over 150~ 250 °C was mainly from CPDP, not CDP. Solid acid electrolytes have been characterized primarily by XRD. However, solid-state nuclear magnetic resonance spectroscopy (SS-NMR) can be more powerful. SS-NMR can be used to directly observe nuclei, detect light atoms and phases without a long-range order, and provide dynamics information such as ionic movement and molecular motion in more detail. We prepared CDP and CPDP compounds known to be promising solid acid electrolytes for FCs and characterized by SS-NMR techniques. The ^{133}Cs and ^{31}P MAS NMR spectra of CDP and the ^{1}H, ^{133}Cs, and ^{31}P MAS NMR spectra of CPDP were presented for the first. The NMR peaks were assigned to the corresponding sites of the atoms in the compounds. We also MAS MMR spectroscopy demonstrated to be more advantageous than XRD techniques to confirm the quality of the syntheses of solid acid electrolytes, especially when liquid impurities such as H_3PO_4 or H_2O are present

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Substrate-engineering of graphene by polymers for intrinsic doping control

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서울대학교 화학과 [1]서울대학교 화학부

Doping is a principal process to control the work function and conductivity of graphene for higher performance electronic devices including substitutional atomic doping by reactive gases, electrical/electrochemical doping by gate bias, and chemical doping by electron-donating or ?withdrawing agents. However, before the doping process, the intrinsic doping level of wet transferred graphene prepared by chemical vapor deposition (CVD) varies significantly and seems to depend strongly on processing details and the substrate. In this study, we report that it is possible to reliably obtain low intrinsic doping levels even wet transfer method by transferring graphene on top of a surface reformed substrates. We have demonstrated that the overlying a thin, hydrophobic, and transparent polymer layer of methylcyclohaxane (MCH) or ethylcyclohaxane (ECH) screen the influence of substrate. To reveal the polymer effects on the graphene, we studied through the wettability of substrates, atomic force microscopy (AFM), Raman, UV/vis spectroscopy and Hall effect measurement.We expect this method to be used for obtaining constant template, which will be widely used in graphene based transparent electronic devices by further doping.

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Synthesis of metal chalcogenide nanostructures and their electromagnetic properties

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Metal chalcogenide materials are possible candidate for the future electromagnetic devices due to their unique atomic properties. One of the metal chalcogenide, β-Ag2Se is possible candidate for the topological insulator which has surface conductive character with time reversal symmetry. We synthesized β-Ag2Se nanostructures to figure out topological ordering in via electrical transport properties. The synthesis mechanism was related with substrate roughness significantly. The rough surface can induce the aggregation of atomic vapor to make seed of nanostructures. Significant magneto-resistance (MR) features, including weak antilocalization, Aharanov-Bohm (AB) oscillation, and Schubnikov-de Haas (SdH) oscillation, visualize archetypal topological insulating properties within both β-Ag2Se nanowires and nanoribbons. We demonstrate β-Ag2Se, one of the silver chalcogenides to be topological insulators with anisotropic Dirac cone, could provide insight in both fundamental physics and device applications.

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Direct Chemical Vapor Deposition Growth of Graphene Layer on SiO_2/BN for Device Applications

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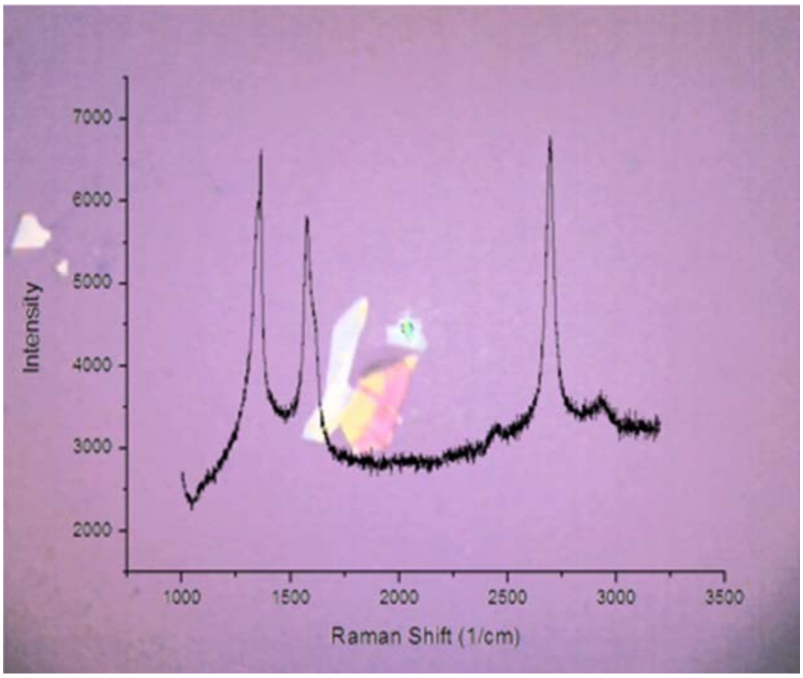
Graphene due to its characteristics of owning zero bandgap shows limitation in its applications as semiconductor devices. However with the help of dielectric layers such as BN, graphene too can be manipulated to meet the requirements to be used in semiconductor devices. Realizing the importance of arranging graphene and dielectric layers in device applications, many scientists have attempted to form graphene/BN and vice versa layers or their heterogeneous structures. Here we report a simple step of directly growing graphene on BN flakes which are transferred on SiO_2. This mechanism, unlike any other BN/graphene layer structures reported before, is free of chemical etching and transfer process induced defects.The proposed method is as follow. First, mechanically exfoliated BN flakes are transferred on the SiO_2 wafer. Then, only a few tens of nm of Cu metal layer is e-beam evaporated to uniformly cover the BN/SiO_2 substrate. Such prepared templates directly undergo high temperature (1000ºC) chemical vapor deposition(CVD) process at which graphene is synthesized as the thin metal catalysis layer is annealed and completely evaporated. As the result, the fully grown graphene layer on BN/SiO_2 substrate was characterized by Raman spectrum, where the sharp G and 2D peaks inform that monolayer graphene layer is well grown directly above the BN flakes and on SiO_2. In addition SEM and HRTEM images show that such grown graphene grains are fully developed and the layers are well arranged. This newly introduced growth mechanism of graphene layer on BN/SiO_2 substrate will allow developing graphene based semiconductor devices of enhanced performance.


Intensity
7000
6000
5000
4000
3000
2000
1000
1500
2000
2500
3000
3500
Raman Shift (1/cm)

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Continuous Patterning and Transfer of Large-Area Graphene by Roll-to-Roll Embossing

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Emerging electronics including bendable and rollable displays, and flexible sensors come closer to reality by showing the feasibility of industrial-level production of high quality graphene sheets by Chemical Vapor Deposition (CVD). However, transferring on the desired substrate and patterning for graphene device fabrication are still limited. The quality degradation is evitable during transferred on a desired flexible substrate, which is mainly incurred by the chemical damage and residues on removal of the support layer such as PMMA and the thermal damage by the use of a Thermal Release Tape (TRT). As for patterning, existing methods including lithographical methods and plasma etching are costly and hardly scalable as well as require complicated pre-defined masking and wet chemical etching processes. Here we present a roll-to-roll patterning and transfer of graphene sheets capable of residue-free, no chemical treatment, and fast patterning. The graphene sheet attached to a Pressure Sensitive Film (PSF) is continuously patterned by applying pressure selectively with the pre-defined embossed roll. The patterned graphene sheet is adhered to the PSF with very low strength and can be easily transferred to the curved surface or a variety of flexible substrate without the aid of any heating mechanism. Compared to the transfer by the TRT and the PMMA support, the reduction in the occurrence of debris and defects was verified through Raman spectroscopy. The patterned graphene electrodes fabricated by the proposed method was incorporated into a fully functional touch-screen panel device. The width of the patterned film was 220 mm with the smallest line width of 20μm and the production rate of 0.3 m/min for patterning and transfer was achieved.

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Preparation of Silicon Encapsulated in Mesoporous Carbonaceous Shell Nanostructure (Si@void@mC) via Nanocasting and Magnesiothermic Reduction for an Anode Material of the Li-ion Battery

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Si encapsulated in mesoporous carbonaceous shell nanostructure (Si@void@mC) was prepared via nanocasting and magnesiothermic reduction method. Structurally well-defined and tunable Si@void@mC could be prepared from the established method. The prepared material was examined as an anode material for the Li ion battery. The influence of material structure to the electrochemical performance could be systemically studied due to the well-defined and tunable structure. Especially in our study, the influence of carbonaceous shell thickness and pore size in the carbonaceous shell to the electrochemical performance was elucidated. Detailed preparation procedure, characteristics, and electrochemical properties of the materials will be presented and discussed.

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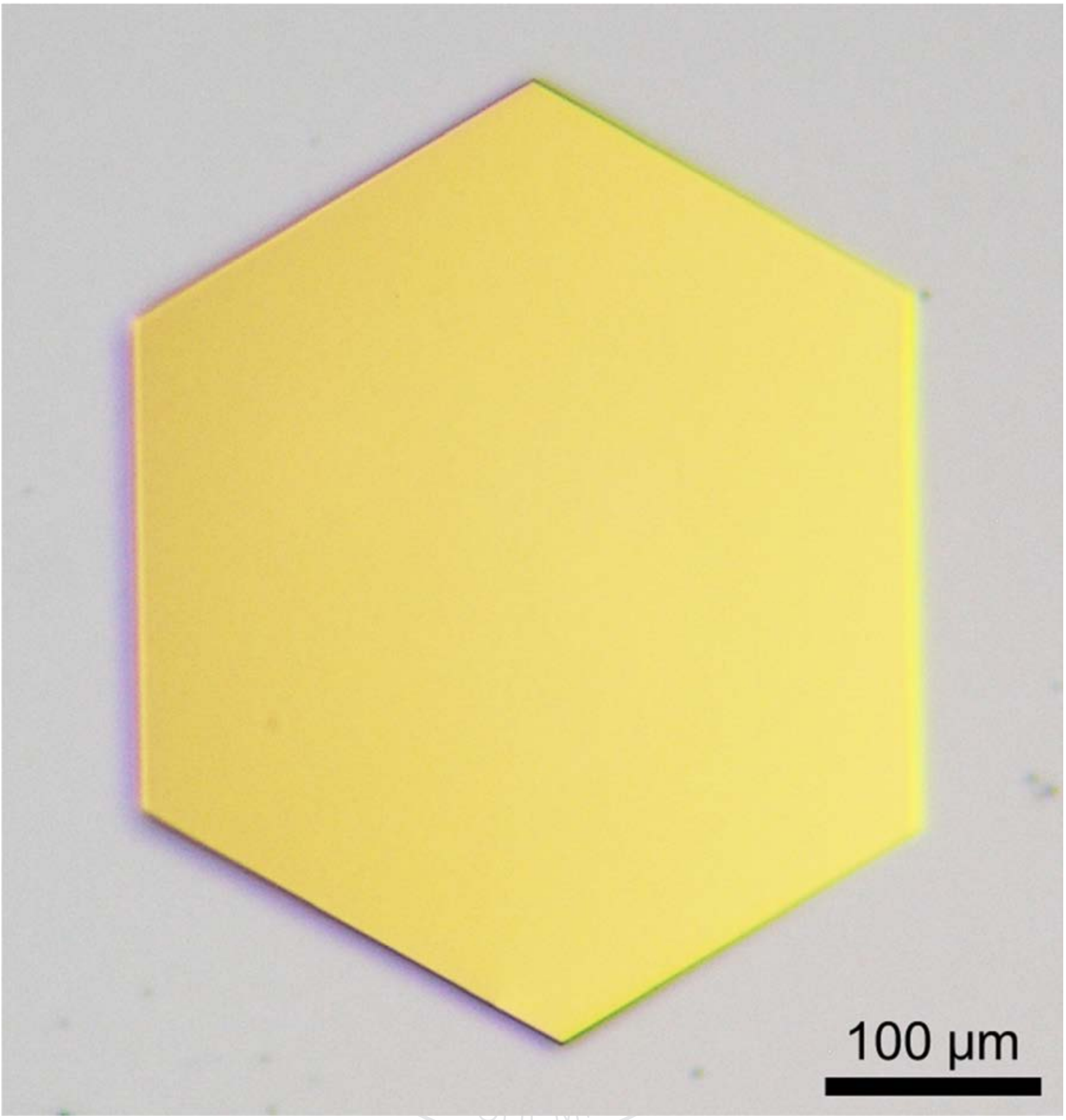
A Growth of Two-dimensional Single-Crystalline Gold Structure: a Material for a Highly Long Range Ordered Structure

양시영 김봉수*

한국과학기술원(KAIST) 화학과

Gold as a representative plasmonic material have been studied about not only a synthesis of various gold nano-structures, but also an application using their catalytic, optical properties. Gold have been usually used for a supported form on other materials. When gold was used for a supporting material, however, the experimental results could be different from when the gold was used for a supported material. So it is academically and practically important that a synthesis of 1D or 2D gold structure supporting another material. Our group already have synthesized the gold nanowire(1D) and gold nanoplate(2D) by Vapor transport method. Based on our experience, we have succeeded in synthesizing the sub-millimeter, twin-free and single-crystalline gold 2D structure. Since the structure was synthesized in highly high temperature (1100 ℃ ~ 1200 ℃), the structure had no defect. A material having an epitaxy relationship with Au (111) such as MoS2, Pt and so on needs Au (111) to continuously grow on the surface. Because the gold 2D structure had a well-ordered surface (exposed lattice plane was (111)), the gold 2D structure could be a promising tool for fabricating the highly ordered composite structure.


100 µm

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Synthesis and structure determination of new oxynitride perovskites compounds, $A_{0.7}Li_{0.3}Ta_{0.7}O_xN_y$ (A = Ca, Sr, La)

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영남대학교 화학과

New oxynitride perovskites compounds of $Ca_{0.7}Li_{0.3}Ta_{0.7}O_2N$, $Sr_{0.7}Li_{0.3}Ta_{0.7}O_2N$ and $La_{0.7}Li_{0.3}Ta_{0.7}ON_2$ have been synthesis and compared qualitatively, quantitatively. Amonolytic heating of the layered perovskies $Ca_2Ta_2O_7$, $Sr_2Ta_2O_7$ and $LaTaO_4$ with Li_2CO_3 produced defect perovskites oxynitrides containing lithium on the octahedral site. resulted in the perovskites with substantial amounts of vacancy defects both on the cation and anion sites. Above process can be induces cooperative Li^+ insertion into the precursor and the charge-balancing O^{2-}/N^{3-} exchange. The crystal structures of these compounds have been determined by Rietveld analysis through X-Ray powder diffraction patterns and combustion analysis.

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Preparation and characterization of Ag doped TiO_2 nanoparticles for photocatalytic applications

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전남대학교 화학과

TiO_2 is a wide band-gap semiconductor that can produce powerful oxidations and reductions by absorbing photons. Besides, due to its low cost and good chemical stability, it has been widely studied. TiO_2 has high recombination rate of electron-hole pairs formed in photocatalytic processes. In order to overcome this limitation, many studies have been devoted to the improvement of photocatalytic activity of TiO_2 by depositing noble metals. Ag is considered as the relatively cheap noble metal and Ag loaded TiO_2 can enhance the photocatalytic activity of TiO_2 effectively according to the previous reports. In this study, we fabricated Ag dopping TiO_2 powder. The obtained Ag doped TiO2 was characterized by using X-ray diffraction (XRD), Energy dispersive X-ray spectroscopy (EDX) and scanning electron microscopy (SEM). The photoactivity of the prepared materials was evaluated by the conversion of methylene blue in aqueous solution under UV irradiation.

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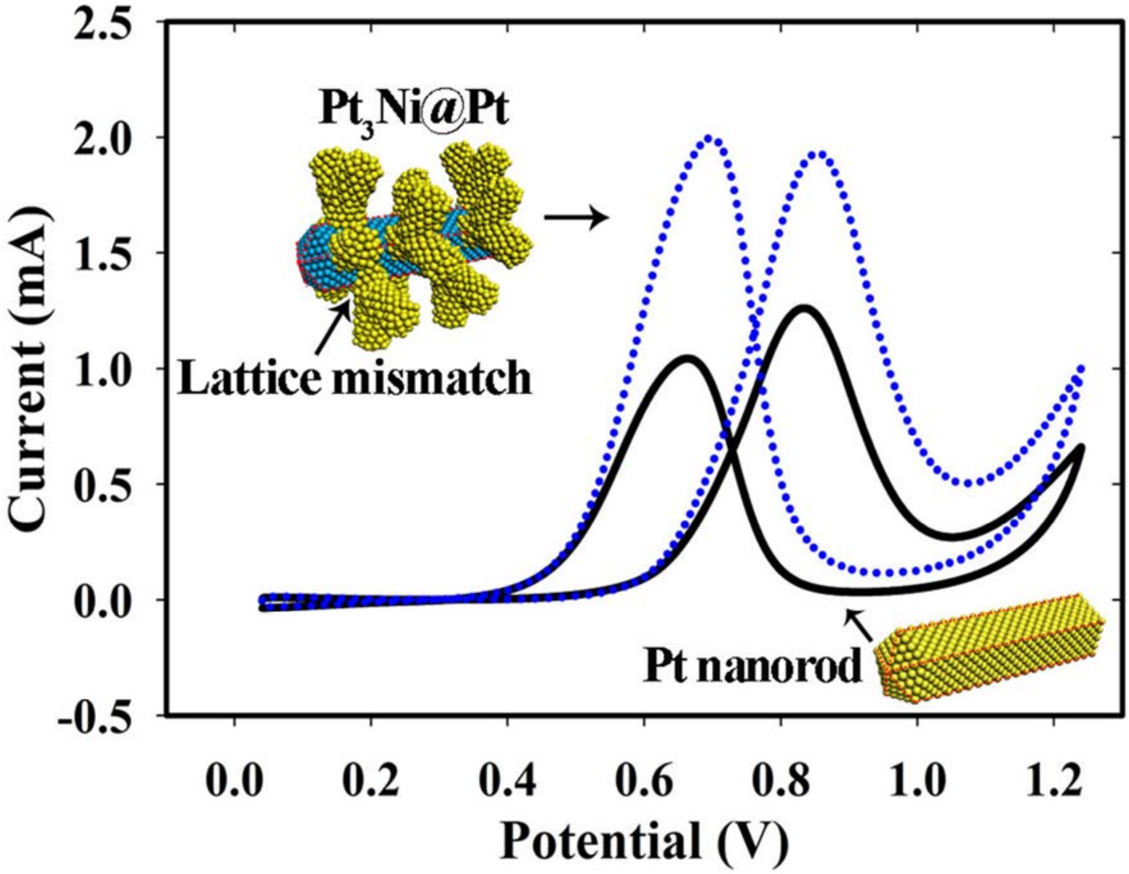
Hierarchically dendritic core-shell Pt nanorod and its excellent catalytic performance

진하늘 이광렬*

고려대학교 화학과

An outstanding electrocatalytic activity is achieved by using Pt dendritic nanostructures with axially elongated twinning boundary. Pt_3Ni nanorods served as a platform for the synthesis of exquisitely controlled hierarchical Pt dendrites. The excellent performance is due to combination of two critical properties for highly energetic structural features, namely, lattice mismatch between Pt_3Ni core and Pt shell and elongated twinning boundary. The worm-like Pt nanorod with elongated twinning boundary shows considerably enhanced current density over Pt nanorod.



Current (mA)
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Potential (V)
$Pt_3Ni@Pt$
Lattice mismatch
Pt nanorod

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The development of drug delivery system combined convergence technology for conducting diagnostic and therapeutic inner ear diseases simultaneously

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부산대학교 인지메카트로닉스공학과 [1]부산대학교 나노융합기술대학 [2]부산대학교 나노메디컬 공학과

Using general diagnostic criteria, the diagnosis of Meniere's disease have been hard to receive definite diagnosis. Assessing the symptoms of Meniere's disease is difficult due to similar other ear disease and lack of a gold standard. In order to improve diagnostic challenge, recent studies focus on the use of magnetic resonance imaging (MRI) after intratympanic gadolinium injection to monitor inner ear in vivo. And intratympanic gentamicin treatment (ITG) is effective to relieve severe episodic vertigo but optimal dose and period of administration have been ambiguous. For optimal protocol, we synthesize hollow silica nanoparticles (HSNPs) loaded gentamicin and gadolinium based contrast agent simultaneously. Utilizing HSNs, we can monitor gentamicin efficacy real time by aid of gadolinium based contrast agent. HSNPs were characterized by X-ray diffraction (XRD), transmission electron microscope (TEM), thermo gravimetric analyzer (TGA) and N_2 adsorption-desorption isotherms.

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Electrochemical Characteristics of N-P- Dual Heteroatom Doped Mesoporous Carbon

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성균관대학교 화학과

Porous polymeric materials especially have received an increased level of research interest due to their potential to merge the properties of both porous materials and functional group witch in polymers. For example, they have high specific surface area and well-defined porosity, uniform pore diameter, and easy processability. (e.g. Functional porous polymers can be designed), so porous polymeric materials have gained much attention for adsorption, gas separation, and as precursors of nanostructured carbon materials.

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Oligonucleotide-Catalyzed Formation of DNA-Silica Hybrid Material

정영환* **박지훈[1]**

한국폴리텍대학 바이오캠퍼스 바이오나노소재과 [1]한국과학기술원(KAIST) 화학과

Ever since artificial DNA synthesis techniques, such as chemical oligonucleotide synthesis and polymerase chain reaction (PCR), were developed, DNA was found to be a fundamental building block for nanomaterials in a precise control because double strand DNA is rigid and stable on the basis of phosphate back bone structure, which could endow enough negative charge with DNA. 2D or 3D nanostructures, such as various origami structures, nanotubes, and nanomeshs, were constructed by DNA self-assembly. With the self-assembled DNA structures, researchers made great achievements in the formation of DNA-inorganic hybrid material by DNA-templated mineralization (metal reduction). In contrast to the conventional reduction method, DNA has now been utilized as a template for catalytic polycondensation of silica, resulting in DNA-silica hybrid material, which displayed hierarchical or crystalline structure. In this study, we demonstrated the formation of DNA-silica hybrid material with DNA nanostructure consisting of three oligonucleotide branchs from trifunctional linkers. The results could open the possibility to increase the morphological diversity of nanometric silica hybrid material.

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Highly Efficient Nucleic Acid Drug Delivery by Graphene Quantum Dots (GQDs) - Mediated Hyperthermia

유제민 홍병희*

서울대학교 화학부

Over the last few decades, graphene has attracted enormous attention due to many of its remarkable properties. In recent years, researchers endeavor to broaden the area of graphene applications even to the fields of biology and medical science, namely as a delivery tool for various drugs and nucleic acids. When designing a system for drug delivery, high transfection efficiency is regarded as one of the most important factors to increase therapeutic efficacy which could also minimize effective dose of the drug and the accompanying toxicity and/or adverse side effects. In case of nucleic acid drugs, the poor cellular uptake and instability in biological fluids have complicated their universal applications. To solve the issues, various targeting molecules and peptides were utilized, which have still resulted in endosomal trapping and eventual degradation. Hence, devising a novel delivery system that increases stability in biological fluids and also disrupts the endosome to assist endosomal escape from the vesicles has been demanded. In this study, graphene quantum dots (GQDs) are employed as a novel siRNA delivery material for high transfection efficiency. Unlike previous studies, the formation of strong disulfide bonds between GQDs and siRNA enabled minimized siRNA loss in biological fluids. The disulfide bonds can only be selectively in the cytosol with the presence of glutathione (GSH). In addition, siRNA successfully escaped from endosome through near infrared (NIR) laser induced GQDs hyperthermia, yielding high gene silencing ratio compared to other delivery methods. This study provides novel approach to effectively deliver nucleic acid drugs and it is expected that the system could be applicable for other drug delivery experiments.

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3D nano structured $Co(OH)_2$/Graphene oxide hybrid composite by graphene oxide wrapping as pseudocapacitor electrodes

배상미 정덕영*

성균관대학교 화학과

We synthesized binder-free $Co(OH)_2$/graphene oxide(GO) hybrid electrode which has high-performance, e.q. high specific capacitance, cyclic stability at room temperature. Two factors were considered to enable capacitor to have high efficiency performance, the first is the feature of large surface area of nano structure and the second is the GO wrapping effect that are enhancing conductivity and protecting the surface of active materials. $Co(OH)_2$ plate has the larger surface area and larger contact area with GO, the higher capacitor performance developed. We synthesized $Co(OH)_2$by ammonia gas transfer method and then GO wrapped on $Co(OH)_2$ by electrostatic force. $Co(OH)_2$/GO hybrid electrode showed the specific capacitance increase of 158% during 1000 times charge-discharge and its maximum value was 2710 Fg^{-1} . The durability at high current density increased remarkably. The specific capacitance was maintained 83.4% when increasing the current density from 2 Ag^{-1} to 50 Ag^{-1} .

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Anion-exchange synthesis of $CuInS_2$ compounds in aqueous solution at room temperature

이상남 차지현 정덕영*

성균관대학교 화학과

Chalcopyrite $CuInS_2$(CIS_2) has been promising materials for highly efficient thin film solar cells. However, vacuum-based processes for these absorber layers raise cost and technical limitation on the fabrication of photovoltaic devices. We report the non-vacuum syntheses of precursor materials for CIS_2 absorber layer. Advantage of hydroxide-based precursors synthesis is stability of in atmosphere and facile synthetic routes. Metal hydroxide precursors for CIS_2 thin films were synthesized by using a co-precipitation method. We prepared mixed metal hydroxides containing Cu^{2+}, In^{3+} with various molar ratios and added an aqueous NaOH solution at room temperature. The pH value of precursors was changed to obtain stoichiometric ratio of the precursors of Cu : In = 1 : 1. After dispersion of solid metal hydroxide precursors in ethanol, the colloidal solution was mixed with the aqueous Na_2S. After heat treatments to obtain a crystalline powder. CIS_2 compounds were characterized by SEM, TGA, EPMA and Raman spectroscopy.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Colloidal Solutions of $CuInS_2$ Nanocrystals

김유중

성균관대학교 화학과

Surfactant-free synthesis of the $CuInS_2$(CIS) were prepared using facile sonochemical process under ambient conditions. The CIS nanoparticles were synthesized with CuCl, $In(NO_3)_3$ and thiourea in ethylene glycol. The synthesized CIS nanoparticles exhibited single phase zinc-blend XRD peaks. The heat treatment at 550°C in H_2S atmosphere of CIS led to chalcopyrite structure and the composition of Cu : In : S = 1.01 : 1.02 : 2.11. $CuInS_2$(CIS) thin film was produced by a precursor solution based coating method with a heat treatment precess. The CIS solution was prepared by dissolving appropriate amount of CuI, $In(OAc)_3$ and thiourea in propanol, followed by addition of propionic acid and butylamine. The CIS solution was spin-casted on the glass substrate and the film was dried on a hot plate at 150°C. After annealing process performed at 300°C for 10 min in air, the film showed chalcopyrite structure.

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

Oxygen-Induced Self-Polymerization of Polydopamine Thin Film

김명신

성균관대학교 화학과

Effective techniques for fabricating mussel-inspired polydopamine (PDA) thin films with dense and conformal surface were investigated. Polydopamine thin film on substrate was formed by self-polymerization of dopamine (DA) using dip-coating in Tris buffer solution at pH 8.5. Polymerization of DA using O_2 gas as an oxygen source showed the optimized synthetic conditions on film surface and thickness. The additional washing procedure of the PDA thin film by sonication in alcohol was effective to remove the nano-sized aggregates formed on the PDA thin film during dip-coating. PDA thin film from several tens to hundreds nm thickness was successfully fabricated by continuous deposition of the pristine PDA thin film in a freshly prepared DA solution, providing a synthetic strategy to fabricate a functional multilayer film by layer-by-layer deposition. Soaking in acid solution (pH2.1) is another fabrication strategy to provide PDA thin film to control the thickness. PDA thin film thickness is the thinner as soaking time is the longer.

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Layer-by-layer assembly of layered double hydroxide nanosheets/Graphene Oxide hybrid multilayer nanocomposite films

<u>박은비</u> 정덕영*

성균관대학교 화학과

Hybrid multilayer nanocomposite films of layered double hydroxide(LDH) nanosheets and graphene oxide(GO) were prepared through layer-by-layer(LBL) assembly. Crystallized LDH nanoplates were synthesized by hydrothermal method using hexamethylenetetramine as ammonia releasing reagent. As-prepared LDH nanoplates were exfoliated into LDH nanosheets(LDH-NS) by high power ultrasonic treatment in formamide solution. Through electrostatic interaction between exfoliated GO and LDH-NS, Hybrid multilayer nanocomposite films were successfully deposited alternately with GO and LDH-NS on ITO substrate. Thickness of films could be accurately controlled through LBL repeated assembling cycle. Hybrid multilayer nanocomposite films are potentially used as electrode materials to construct flexible supercapacitor devices. Hybrid multilayer nanocomposite films were characterized by UV-vis absorption spectroscopy, zeta-potential, AFM, SEM and cyclic voltammetry measurement.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Stable $CuInS_2$ Colloidal Solution

정선호 이상남 차지현 정덕영*

성균관대학교 화학과

We present synthesis of $CuInS_2$ colloidal nanoparticles via a facile solution-processed method; using $CuIn(OH)_5$ powder as the precursor, oleic acid (OA) as the solvent, and bis(trimethyldisilyl)sulfide (TMS) as the sulfur source. $CuIn(OH)_5$ powder was dissolved in OA and 1-octadecene (ODE). Then, TMS-ODE solution was injected into the mixture. The zinc blende-type $CuInS_2$ colloidal nanoparticles were obtained and well-dispersed in hexane. The particle size varied as a function of reaction time, temperature, and precursor concentration. The prepared $CuInS_2$ nanoparticles were analyzed by X-ray diffraction (XRD), UV-Vis-NIR spectrometer, and transmission electron microscope (TEM). TEM images showing $CuInS_2$ nanoparticles have an average size of 10 nm.

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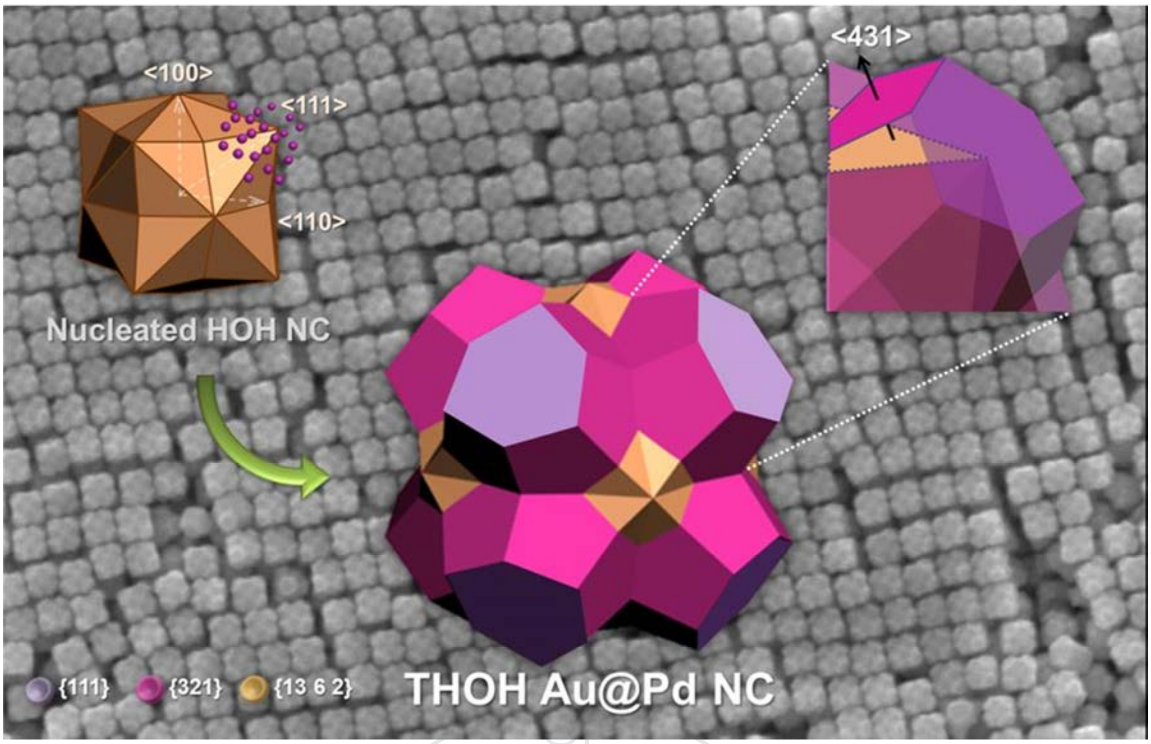
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Synthesis of Au@Pd Core-Shell Nanocrystals with Multiple High- and Low-Index Facets and Their High Electrocatalytic Performance

박양선 한상우*

한국과학기술원(KAIST) 화학과

Bimetallic nanocrystals (NCs) enclosed by high-surface energy facets have been of enormous interest due to their pronounced catalytic performance in numerous chemical and electrochemical reactions. However, it remains a significant challenge to develop a facile method to synthesizing bimetallic NCs with high-surface energy facets in the form of finely-tuned structures due to the difficulties in manipulating the nucleation and growth kinetics of NCs in the presence of multiple metal precursors. In the present work, a facile one-pot aqueous synthesis method is developed for the production of bimetallic Au@Pd core-shell NCs with an unusual truncated hexoctahedral (THOH) shape without pre-synthesized seeds. The THOH Au@Pd NCs are bound by multiple high- and low-index facets. The formation of this unique structure is realized through the co-reduction of Au and Pd precursors under precisely controlled kinetic conditions. The prepared THOH NCs exhibit a prominent electrocatalytic performance for ethanol oxidation, which is attributed to their characteristic structural features. This study significantly expands the understanding of NC growth and will lead to fabricating novel nanomaterials with desired morphologies and functions.


<100>
<111>
<110>
Nucleated HOH NC
<431>
THOH Au@Pd NC
● {111}
● {321}
● {13 6 2}

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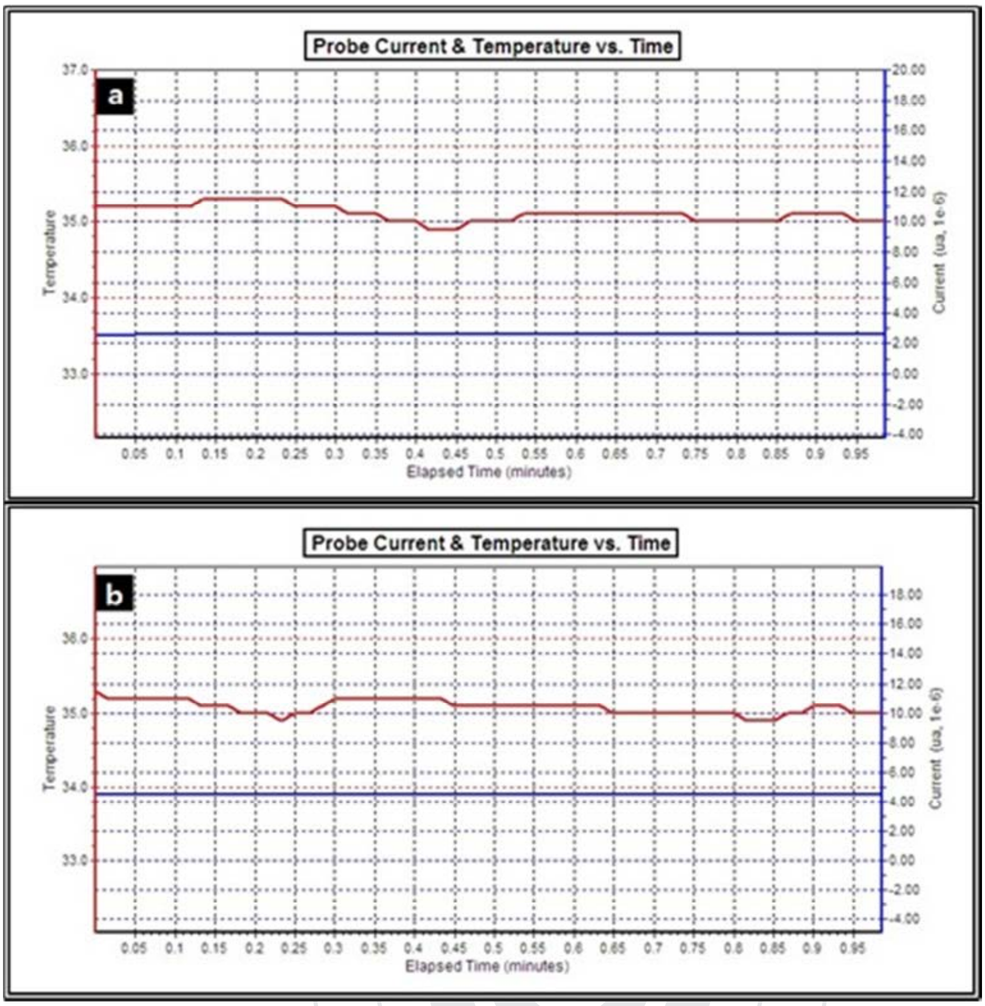
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on the ophthalmic materials of high oxygen permeability containing silicone acrylate

김동현 성아영*

세한대학교 안경광학과

The oxygen and carbon dioxide permeability is one of the most important physical of ophthalmic hydrogel lens. The decrease of oxygen can significantly alter the physiological equilibrium of the component cells and the tissue itself. The physical properties of the polymerized ophthalmic hydrogel lenses with silicone acrylate and initiator AIBN were measured and assessed. The oxygen permeability and water content of the produced polymerized was in the range of 29.80~54.09 x 10-11(cm x mlO2)/(sec x ml x mmHg) , 12.95~64.47% respectively.(Fig.1) The oxygen permeability(Dk) value of silicone containing polymer increased with increasing the addition ratio of silicone acrylate. The produced ophthalmic lenses have high oxygen permeability, indicating that the material can be used to fabricate high performance hydrogel ophthalmic lenses. Fig 1. Current and temperature VS. time of sample(a) addition of silicone acrylate10% b) addition of silicone acrylate50%)

Probe Current & Temperature vs. Time
a
Temperature
37.0
36.0
35.0
34.0
33.0
Current (ua, 1e-6)
20.00
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
-2.00
-4.00
0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95
Elapsed Time (minutes)
Probe Current & Temperature vs. Time
b
Temperature
36.0
35.0
34.0
33.0
Current (ua, 1e-6)
18.00
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
-2.00
-4.00
0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95
Elapsed Time (minutes)

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다양한 PDMS 기판위에서의 BALB/3T3 섬유아세포의 이동과 증식 확인

이유나 이소명 진예나[1] 이석우[*]

공주대학교 화학과 [1]공주대학교 화학

본 연구에서는 PDMS 를 이용한 다양한 pysical barrier 와 간격, 전하에 따른 BALB/3T3 섬유아세포의 이동과 증식, polarization 정도에 대한 연구를 수행하였다. 다양한 높이의 physical barrier, 간격을 가지는 기판을 만들기 위하여 lithography 과정을 이용하였고, 전하를 가지는 PDMS 기판을 제작하기위해 PLASMA 처리와 TESPSA 코팅을 이용하였다.시간에 따른 세포 이동과 증식을 광학현미경 Image pro plus 7.0 을 이용하여 조건별로 좌표를 지정 이미지를 촬영 후 분석하여 이동 세포의 polarization 정도를 분석하였다. Physical barrier 가 높아질수록 control 에 비해 이동과 증식이 느려짐을 확인하였고, 세포의 polarization 상태는 정지한 confluent 상태보다 이동하는 frontier 에서 그 정도가 크고 physical barrier 방향에 따라 세포 이동방향이 나타남을 확인하였다. 광학현미경을 이용하여 얻은 전하세포 사진의 세포 이동속도는 -OH > - NH_2 > -COOH 작용기를 갖는 기판 조건 순으로 나타났다. 세포부착은 -NH2 > -OH > -COOH 의 순으로 더 잘 이루어지고, 세포의 확장은 -OH > -NH_2 의 순으로 나타난다. 실험결과 -OH > -NH_2 를 갖는 기판순으로 빠른 이동을 나타내었으므로 부착보다 확장의 영향이 더 크게 작용한 것으로 판단된다.

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Calcium-Doped P2-type Sodium Cobalt Oxide Cathodes in Sodium Ion Batteries

한수철 임햇살 표명호*

순천대학교 인쇄전자공학과

The discovery of large thermopower (high Seebeck coefficient) for sodium cobalt oxides (P2-Na_xCoO_2) in late 20th centry has triggered extensive investigations on changes in the structure and the related phycal property with Na^+ contents. Soon after, the enhancement of thermopower in P2-Na_xCoO_2 for high Na^+-contents ($x \geq 0.75$) was reported, envisioning potential thermoelectric applications of this interesting material. Besides, P2-Na_xCoO_2 was found to possess the interesting magnetic properties and the unexpected superconductivity when hydrated. The layered P2-Na_xCoO_2 allows the high Na^+ ion diffusion between weakly attracting CoO_6 slabs, comparable to Li^+ diffusion in $LiCoO_2$ and possesses metallic conductivity at RT, due to direct overlap of Co 3d orbitals. Since these two characteristics of P2-Na_xCoO_2 fullfilled necessary conditions for an intercalation compound, the P2-Na_xCoO_2 as a cathode in sodium ion batteries (SIBs) was investigated by several authors. In this work, $Na_xCa_yCoO_2$ ($0.45 \leq x \leq 0.64$, $0.02 \leq y \leq 0.10$) was synthesized by a solid-state method and examined as a cathode material for improved cyclability in SIBs. The substitution of Ca^{2+} for Na^+ does not alter the crystal structure, maintaining P2-phase of pristine Na_xCoO_2. Only a slight change was observed in a cell dimension. The existence of Ca^{2+} in prismatic sites, however, caused the distinctive charge-discharge behaviors of $Na_xCa_yCoO_2$. While pristine Na_xCoO_2 showed well-known sharp voltage drops at several peculiar Na^+ compositions, the immobility of Ca^{2+} hindered Na^+-vacancy orderings, resulting in gradual changes of cell voltages. The mitigation of sudden phase transitions in $Na_xCa_yCoO_2$2 contributed to the improvement of cyclability of SIBs. For example, although initial discharge capacity of $Na_{0.5}Ca_{0.07}CoO_2$ was smaller than that of pristine $Na_{0.64}CoO_2$ (105.2 vs. 108.0 mAh/g), the capacity of the former was retained at 101.1 mAh/g after 60 C-D cycles, in contrast to 74.5 mAh/g of the latter. Moreover, the Na+ diffusion rate of

$Na_xCa_yCoO_2$, which was substantially decreased in phase transition regions, was counter-balanced by the faster diffusion in the other whole, leading to greater capacities at high C-rates.

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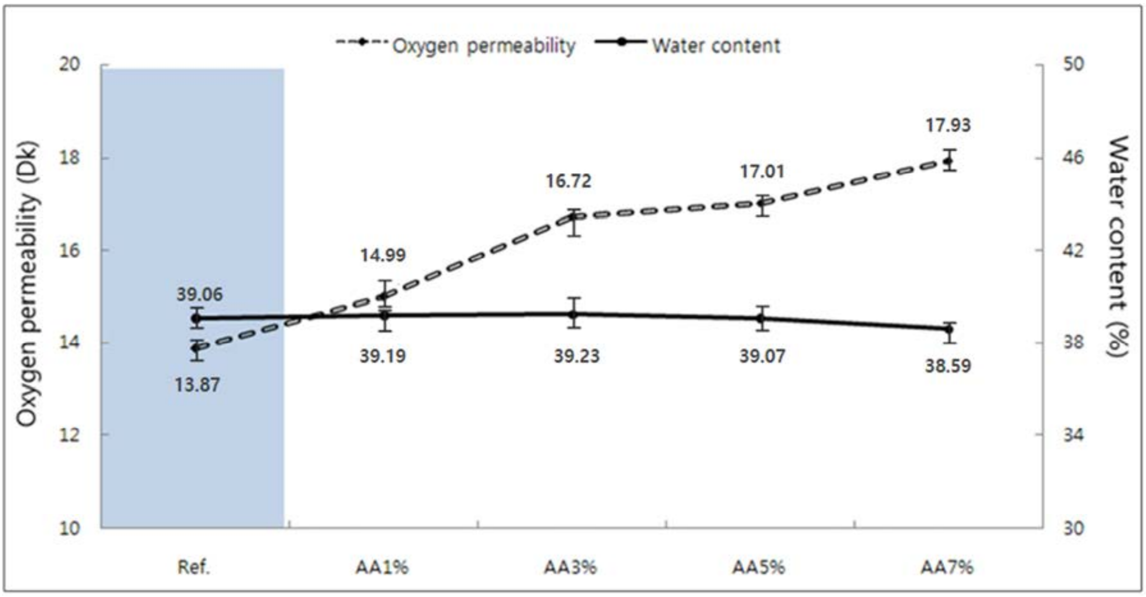
발표종류: 포스터, 발표일시: 수 16:00~19:00

Study on high performance hydrogel lens material for improvement of oxygen permeability

김동현 이민제 성아영*

세한대학교 안경광학과

The significant physical characteristics of hydrogel ophthalmic lenses include oxygen and carbon dioxide permeability, tensile strength, elasticity modulus, water content, physical and chemical stability, mechanical properties and biocompatibility. Oxygen permeability is one of the most important physical characteristics of hydrogel ophthalmic lens. Hydrogel ophthalmic lens was prepared by the copolymerization of 2-hydroxyethyl methacrylate(HEMA), acrylic acid(AA)and initiator AIBN. The ophthalmic hydrogel lenses of all combinations showed flexible and soft characteristics after being hydrated for 24 hrs in standard saline solution. The water content of polymerized ophthalmic lenses, was in the range 38.09~ 39.23%. The oxygen permeability value of the lenses ranges from 13.86 to 17.93 x 10-11(cm x mlO2)/(sec x ml x mmHg). (Fig.1) The ophthalmic hydrogel lens material produced using acrylic acid as an additive satisfied the major physical properties required for ophthalmic lenses and also showed an increase in oxygen permeability while having no significant changes in water content.Fig 1. Oxygen permeability and water content of samples including acrylic acid


Oxygen permeability
Water content
Oxygen permeability (Dk)
Water content (%)
20
18
16
14
12
10
50
46
42
38
34
30
Ref.
AA1%
AA3%
AA5%
AA7%
39.06
13.87
14.99
39.19
16.72
39.23
17.01
39.07
17.93
38.59

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One-Pot Synthesis and Electrocatalytic Properties of Pd@Pt Core-Shell Nanocrystals with Tailored Morphologies

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한국과학기술원(KAIST) 화학과

A direct one-pot synthesis method for the production of core-shell nanocrystals with tailored core and shell structures can offer a convenient and valuable approach to the development of promising nanocrystal-based catalysts for diverse applications. In the present work, we developed a new facile aqueous one-pot synthesis method for the generation of Pd@Pt core-shell nanocrystals consisting of well-defined Pd nanocube cores and dendritic Pt shells, which was realized by the temporal separation of the Pd core and Pt shell formation through the controlled reduction kinetics of metal precursors. The thickness of the Pt shell in the Pd@Pt nanocrystals could also be manipulated by controlling the molar ratio of the Pt and Pd precursors in the reaction solutions. The prepared Pd@Pt nanocrystals exhibited efficient catalytic activity and stability toward methanol electrooxidation, and their catalytic function was highly dependent on their Pt shell thickness due to the different synergism between Pt and Pd. We envision that this work will pave the way to designing novel metal nanostructures with unprecedented morphologies and functions.

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발표코드: **MAT.P-1112**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

THERMOELECTRIC PROPERTIES OF 3D-GRAPHENE

THIYAGARAJAN PRADHEEP 장지현*

울산과학기술대학교(UNIST) 친환경 에너지 공학부

Since the discovery of graphene in 2004, graphene has fascinated scientists with its exotic and unique properties. In our work, we have succeeded to synthesize three dimensional structure of graphene (3D-GN) using a simple templating technique. We have examined the structure by various characterization tools such as SEM, TEM, XRD, XPS as well as BET method. Our 3D-GN structure has pores in size of 10-20 nm which helps to reduce phonon transport without affecting the electrical properties. We have analyzed the thermoelectric properties of 3D-GN by means of laser flash apparatus and Ulvac ZEM-3 system. The 3D-GN shows promising results with a low thermal conductivity value of 0.90 W/mK at 773K and a maximum electrical conductivity value of 6660 S/m at 773 K. Our results indicate the possibility of separately controlling electrical and thermal conductivity, which enhances the thermoelectric figure of merit.

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

The enhanced electro-catalytic activity of PdPt@Pt core-shell nanospikes with roughened surface and multiple grain boundaries

윤지선 이광렬*

고려대학교 화학과

Core-shell nanostructures have recently attracted a great attention due to the high catalytic activity and durability. In addition to the core-shell effect, it is desirable to render other structural features such as high surface area and optimal shell thickness to the core-shell structure. Herein, we report the facile one-pot synthesis of a unique PdPt@Pt core-shell nanospike with catalytic performance elevating factors such as multiple grain boundaries,roughened surface, and a very thin catalytic Pt shell.

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Assembly of metal and functional polymers to fluorinated ultrafiltration (UF) membranes for anti-fouling and heavy metal removal

박성용 곽승엽*

서울대학교 재료공학부

Ultrafiltration membrane obtains high quality purified water through relatively easy and simple process than traditional water treatment methods such as sand filtration, coagulation and so on. However, practical use of UF membrane is limited because of occurrence of membrane fouling by undesirable deposition of retained organic or inorganic materials to membrane and penetration of toxic heavy metal ions due to its relatively large pore size. Thus, we developed functionalized fluorinated UF membranes with fouling resistance and heavy metal removal by surface modification with various functional materials, e.g. antibacterial silver nanoparticle (Ag NP), positively charged branched polyethylene imine (b-PEI), heavy metal ion chelatable hyperbranched polyamidoamine (HPAMAM). The effects of introducing Ag NPs and b-PEI to polyvinylidene fluoride (PVDF) membrane were enhanced anti-biofouling and inhibited inorganic fouling, respectively. The assembly of HPAMAM to polytetrafluoroethylene (PTFE) membrane was applied to removal heavy metal ions from contaminated water. As expected, the prepared membranes showed desired properties such as antifouling and heavy metal removal. These make them tremendously attractive in applications ranging from high-efficient membrane to eco-friendly water purification system.

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Facile synthesis of hollow Ru nanostructure via metastable nanotemplate

윤동환 박수현 이광렬*

고려대학교 화학과

Hollow nanostructures are receiving a great attention as promising materials for catalysis, optoelectronics, and nanobio applications. Hollow nanostructures are generally formed by multiple steps involving the formation and separation of template nanocrystals, hetero-phase growth on the surface of an existing nanotemplate, and subsequent removal of template, and this synthetic difficulty could greatly diminish the utility in the practical application of these interesting materials. Herein, we report a facile one-pot synthesis of a hollow Cu-doped Ru nanocage, which involves initial formation of a Cu@Ru core-shell nanooctahedron with the Ru phase localized on the surface and subsequent in situ destabilization and removal of the core Cu phase.

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Synthesis of octahedral Ir nanocrystals assisted by Cu

윤동환 방슬기 이광렬*

고려대학교 화학과

Iridium is one of major catalytic metal and therefore there is a strong interest to prepare facet-controlled Ir nanocrystals. However, synthesis of facet-controlled Ir nanoparticles has not been reported thus far, probably due to the difficulty in Ir atom packing; the Ir precursors are thermodynamically very stable and thermal decomposition of them usually lead to the formation of only very small spherical nanoparticles. In order to prepare facet-controlled Ir nanocrystal, it is utterly necessary to speed up the decomposition kinetics for the Ir precursor. Herein we report the successful synthesis of facet-controlled CuIr@Ir core-shell octahedral nanoparticle for the first time, by utilizing the facile Galvanic replacement of in situ formed Cu template by Ir.

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Unusual Rh nanocrystal growth control by space-confined heteroepitaxial growth on twinning boundary

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고려대학교 화학과

While nanocrystal growth is influenced by various reaction parameters, the atom packing motif of a pre-existing substrate, where a new phase can grow, is one of the strongest structure determining factor. Various nanocrystalline substrates have been employed for a heteroepitaxial growth, but little is known for the heteroepitaxial growth pattern on laterally crowded twinning boundaries. In this case, the surfactant-surfactant interaction between newly growing neighboring nanocrystallites would also play an important role in addition to the structure determining effect of the crystal packing motif of the nanosubstrate. We have recently reported the synthesis of coaxial Au@Pt nanowires with numerous adjacently placed twinning boundaries, and therefore the nanowires seem to provide the ideal opportunity for studying above mentioned issue. Herein, we report the successful dimension controlled vertical growth of Rh nanorods and nanoplates on a Au@Pt nanowire, which are not obtained in the absence of the Au@Pt nanowire substrate.

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Crystal growth behavior changing Zn-doping in Rh : morphological evolution in a set of novel Rh concave structures

이기웅 박종식 이광렬*

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Impurity doping has been extensively studied in materials science, because this methodology is particularly useful in the formation of shape controlled alloy nanoparticles for catalysis or optical applications. The successful formation of alloy nanoparticles, however, requires the synchronized decomposition of multiple precursors, and therefore the reduction potentials of precursors should allow the simultaneous decompositin of multiple precursors. Zinc has been rarely used as a dopant for the synthesis of noble metal alloy nanoparticles due to the difficulty in reduction. Although, we have strived to incorporate Zn atoms into Rh system, because such nanoparticle systems are expected to be metastable, prone to further structural transformations, potentially leading to novel nanostructures with useful material properties. Herein we report a simple synthetic strategy to incorporate Zn as a dopant into an alloy system and unusual role of dopant Zn in the structural evolution from 2D Rh nanoplate to 3D Rh concave nanotent, hierarchically stacked nanoframes, and hierarchical dendrites.

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Conductive carbon nanotubes attaced to Au nanoparticles as active elements in a field effect transistor

이명순 지성경 김돈*

부경대학교 화학과

Carbon nanotubes attached to gold nanoparticles (Au-CNTs) are prepared by decomposing $HAuCl_4$ at 503 K followed by carbonization of sucrose at 1173 K within an anodic aluminum oxide (AAO) template. The diameter of the Au-CNTs ($r_{Au\text{-}CNT}$) ranged from 40 to 250 nm, which corresponds to the channel diameter of the AAO template. The shape and crystallinity of the CNTs phase depends on the r_{CNT}. Highly crystalline, straight CNTs are observed when the $r_{Au\text{-}CNT}$ exceed 80 nm, and less crystalline, noodle-shaped CNTs are observed when the $r_{Au\text{-}CNT}$ are smaller than 80 nm. The crystallinity of the CNT phase is confirmed by analyzing the G and D bands in their Raman spectra and the electrical conductivities of the Au-CNTs. The electrical conductivity of the highly crystalline carbon phase of a Au-CNT ($r_{Au\text{-}CNT}$) = 250 nm) reaches ~10^4)S/cm. The side- and back-gated field effect transistors based on Au-CNTs, which are assembled using a dielectrophoresis technique, show that a Au-CNT may be a functional electronic material. Au-CNT devices can be promising candidates for future electronic and other sensing applications.

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Increase the graphene’s dispersion properties by amine substitution of graphene oxide

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고려대학교 화학과 [1]한국화학연구원 화학소재연구단 [2]한국화학연구원 신물질연구단 난치성 질환치료제연구센터

Graphene, consisting of a single layer of sp2 hybridized carbon atoms, has stimulated wide interests studied in high-tech engineering materials and energy-related materials due to its extraordinary electrical, mechanical and thermal properties. For the synthesis of graphene nanosheets, reduction of graphene oxide (GO) is one of the established methods for large-scale synthesis of graphene. Generally GO includes functional group such as epoxy, hydroxyl, carbonyl and carboxylic acid. By reaction of functional groups of GO with amine to increase dispersal in the water or organic solvent for printing techniques, we prepared amine substituted graphene compounds.

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Detection of prostate specific antigen by using multi wall carbon nanotubes deposited on the micropore filter paper

지성경 이명순 김돈*

부경대학교 화학과

The purpose of this study is fabrication of an inexpensive, simple and sensitive biosensor using multi wall carbon nanotubes (MWCNTs, diameter 20 nm length 5 μm) and micropore filter paper (pore size 0.45 μm). For detection of prostate specific antigen (PSA), the carboxylated CNTs were activated with anti-PSA antibody (monoclonal antibody of the prostate specific antigen) by using N-(3-dimethylaminopropyl)-N′-ethylcarbodiimide hydrochloride (EDC) and N-hydroxysulfosuccinimide sodium salt (NHSS). The activated CNTs were deposited on micropore filter paper, which were used for fabrication of biosensor with 2 × 5 ㎜^{2} size. Sensing signal of the biosensor increased to 55% of base signal along with the increased concentration of PSA.

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Lithium insertion into tungsten bronze β-$SrTa_2O_6$ and electrical property of $Li_xSrTa_2O_6$

김주영 김영일*

영남대학교 화학과

We attempted to incorporate Li^+ ion into the tungsten-bronze (TB) type lattice, by reationg orthorhombic TB-phase β-$SrTa_2O_6$ with Li_2CO_3 in the ratios of [Li]:[Sr] = 0～0.7. The Li-insertion into β-$SrTa_2O_6$ caused an evolution of crystal symmetry from orthorhombic ($x \leq 0.2$) to tetragonal ($x \geq 0.3$). Electrical properties of $Li_xSrTa_2O_6$ with x=0.2, 0.4, 0.6 studied by impedance spectroscopy from 27℃ to 260℃ in wet and dry atmospheres. Conductivity measured in wet atmospheres was always lager than that in dry atmospheres. $Li_{0.4}SrTa_2O_6$ possesses an ionic conductivity of ?10^{-6} S/cm at 260℃ in wet atmospheres.

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The use of plasmonic nanoparticles for efficient visible-light induced GO reduction and fluorescence quenching efficiency

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전북대학교 BIN 융합공학과 [1]Chonbuk National Uni BIN Fusion Tech.

Graphene was studied extensively for wide ranges of potential applications such as nano-electronics, energy storage materials, polymer composite materials, bio-sensing, and drug delivery due to its unique physical properties. Graphene can be synthesized by the reduction of graphene oxide (GO) which was mostly carried out with hydrazine or its derivatives or by thermal treatment (550?1100 °C) in inert or reducing atmosphere. Although, all these processes required either the use of toxic chemicals or high temperature or long time duration which in turn increased the energy demand. To overcome these shortcomings photo-irradiating reduction processes like UV-induced, photo-thermal reduction using a pulsed xenon flash, pulsed laser, and photo-thermal heating of camera flash lights were reported to produce reduced graphene oxide (r-GO). Except UV or pulsed laser that can deliver high photon energy, all other processes suffers low conversion efficiency. Therefore, the use of plasmonic nanoparticle as photo-catalyst would be one way to overcome the current shortcomings of visible light, which have low photon energy, induced r-GO synthesis method.In present study, an efficient photo-catalytic reduction of GO using visible light and plasmonic nanoparticles is reported. It has been found that the GO reduction progress was strongly reliant on the structure of plasmonic nanoparticles such as spherical gold nanoparticle (AuNP), gold nanorod (AuNR), and gold nanostar (AuNS). The quality of r-GO synthesized using visible light and plasmonic nanoparticles was as excellent as that of r-GO prepared by chemical reduction, which was demonstrated by a series of analysis (UV-Vis, FTIR, XRD, Raman, SEM and XPS) and DNA detection scheme based on fluorescence quenching.

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Rationally synthesized five-fold twinned core-shell Pt3Ni@Rh for selective reduction of a phenyl ring

김준 이광렬*

고려대학교 화학과

The preciseness of heteroepitaxial crystal packing transfer from Pt3Ni nanorod to Rh pentagons, finally to Rh nanostars and paddlewheel. All the Rh-covered pentagons, nanostars and paddle-wheels share the following structural features of 1) core-shell structure with Pt3Ni core and Rh shell and 2) five-fold twinning transferred from the Pt3Ni core. We demonstrated that all particles exhibit remarkable catalytic selectivity in the hydrogenation of tetrahydrophtalimide. The most active paddlewheel structure proceeds to further reduce one carbonyl group, indicating the sequential nature of phthalimide reduction by Rh nanoparticle catalysis.

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Preparation of Intercalative Layer Nanocomposites of Dipeptide Molecules and Montmorillonite

변미림 윤주영[1] 최진주[1] 한양수[1,*]

(주)세일에프에이 연구소 [1](주)나노스페이스 연구소

Intercalative layered nanocomposites of expandable clay (montmorillonite, Kunipia G, CEC = 119 mequiv./100g) and dipeptide molecules were prepared by intercalation reaction in an aqueous solution. 4 kinds of dipeptide compounds (KJ-A~D) were used as guest molecules. In the typical preparation, clay particles were preswelled at first in aqueous solution, then dipeptide molecules of 3 times excess of CEC were added into the clay suspension solution, and then reacted at 60 ℃ for 4 hours. It was observed that the dipeptide molecules are easily intercalated between the silicate layers to form dipeptide-silicate layer complexes with the basal spacing (d001) of 13.5 ~ 13.8 Å. Upon washing with deionized water a partial deintercalation of dipeptide molecules were observed, leading to a collapse of ordered stacking structure. It was also found that the solution pH played an important role in intercalation and deintercalation of guest molecules due to the zwitterionic nature of dipeptide molecules

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Preparation and Characterization of Nanoporous Composite of Ferromagnetic Fe_2O_3 and Layer Silicates

변미림 윤주영[1] 한양수[1,*]

(주)세일에프에이 연구소 [1](주)나노스페이스 연구소

Nanocrystalline ferromagnetic(r-Fe_2O_3) particles with spindle-type particle morphology are prepared by chemical hydrolysis using ferrous salt in the presence of layer silicate particle. In the chemical hydrolysis reaction route, ferrous sulfate, $Fe(SO_4)_2$, is forced hydrolyzed at 60℃ by the addition of NH_4OH solution to obtain ferrous hydroxide precipitate in silicate colloidal solution , followed by the aeration under an ambient atmosphere for the oxidation of Fe(II) to Fe(III), resulting in a ferromagnetic maghemite (r-Fe_2O_3) nanoparticle. The resulting maghemite-silicate composite powders are evaluated by powder X-ray diffraction, scanning electron microscopy, nitrogen adsorption-desorption isotherm. Thus prepared ferromagnetic Fe_2O_3-silicate layer nanocomposite exhibited high specific surface area of 250 ~ 280 m^2/g with the average pore size of ~ 50 nm, which are very promising features in the immobilization of enzymatic molecules.

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Single-crystal organic cross-junction nanowires for nanoscale electronics

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한양대학교 화학과

We use 6,13-bis(triisopropylsilylethynyl)pentacene (TIPS-PEN) and fullerene (C60) as p-type and n-type semiconducting materials, respectively, to fabricate single-crystal organic nanowires by a direct printing method, liquid-bridge-mediated nanotransfer printing (LB-nTM). By exploiting two different single-crystal organic nanowires in the form of cross-stacking geometries we show that high-performance organic p-n nanojunction can be realized by a consecutive printing of the nanowires. Cross-stacking of organic nanowires with single-crystalline nature will provide a generic possibility for fabrication of scalable high-density integrated devices with high-performance.

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Preparation of Binary Cu-Mn Oxide Catalyst Supported on Mesoporous Silicas

변미림 이희숙 김세희 한양수*

(주)세일에프에이 연구소

Nanoporous copper manganese oxide catalyst supported on mesoporous silica was prepared and the catalytic activity for carbon monoxide removal at ambient temperature evaluated. For the preparation of mesoporous silica tri-block copolymer was dissolved completely in acidic aqueous solution, at first, then TEOS was titrated into the solution at 40 ℃ and aged for 3 h, followed by hydrothermal treatment at 120℃ for 8 h. The precipitate was filtered, washed, dried, and calcined at 550 ℃ for 6 h in air, resulting in the mesoporous silica with the surface area (S_{BET}) of 1290 m^2/g and the pore volume of 2.2 mL/g. Deposition of Cu-Mn catalyst on the porous silica support was performed by a redox method in the presence of mesoporous silica particle and the catalytic activity for carbon monoxide removal at ambient temperature evaluated, which will be discussed in detail on the basis of XRD, XRF, nitrogen isotherm analysis, and CO removal activity test results.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

High Capacity Porous Hard Carbons as Anode Materials for Sodium Ion Batteries

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순천대학교 인쇄전자공학과

With significant efforts aimed at developing suitable sodium ion battery (SIB) anode, variety of options are being explored, among which, carbon based materials have distinguished themselves as a suitable and promising solution owing to their cost effectiveness, easily attainable and non-toxic properties. Hard carbon also known as disordered graphitic carbon has attracted immense attention in this regard [1] and presents enough reasons to pursue, aiming improvement. Here, we report the correlation between the degree of porosity and the reversible capacity from a sucrose derived hardcarbon (SHC) as an anode for SIB. The porosity in the SHC was regulated by varying the amount of bicarbonate salt added during the simple two stage synthetic process. Increase in porosity and surface area result in a sharp increase in reversible capacity. Conversely, a drooping effect is observed beyond an optimum level of porosity, suggesting that the pore size and material's structure are crucial in harvesting the best capacity response from SHC. With the optimal porosity, a reversible capacity of 324 and 289 mAh/g can be obtained for the 1stand 100th cycle at 20 mA/g, in contrast to 251 and 213 mAh/g for SHC, respectively. Appending to the above, a notable distinction in solid electrolyte interphase (SEI) between the pristine and modified porous SHC (MSHC) could be perceived; implying that the type of SEI formed on the hardcarbon (dependent on the surface functional groups) may have a crucial role to play in the electrochemical reversibility and dimensional stability. The diffusion coefficient measured by electrochemical impedance spectroscopy (EIS) and potentiometric intermittent titration technique (PITT) suggested that the ionic mobility in the material is strongly dependent on the porous texture. We suggest that, with the ideal type of porosity, which can hasten the Na ion transport, enhance storage sites and facilitate the formation of a dimensionally stable SEI, a high Na ion storage can be achieved in SHC.References[1]A. Ponrouch, A.R. Goni, M. Rosa Palacin, Electrochem. Commum., 25 (2013) 85.

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Preparation of Cu-Mn Oxide and Layer Silicate Porous Nanocomposite for Carbon Monoxide Removal

임동민 변미림 이희숙 김세희 한양수*

(주)세일에프에이 연구소

Porous nanocomposite of binary copper manganese oxides were prepared by a modified redox method in the presence of colloidal layer silicates and their catalytic activity for carbon monoxide removal at ambient temperature evaluated. At first, colloidal layer silicate were prepared by swelling synthetic layer silicate(Laponite RD) in de-ionized water, then potassium permanganate($KMnO_4$) was dissolved into the colloidal solution, subsequently a mixed aqueous solution of manganese(II) acetate and copper(II) acetate solution was added dropwisely to a solution of $KMnO_4$ under vigorous stirring. The resultant precipitate was filtered, washed, and dried at 120 ℃, and finally heat treated in air for 2 hours at 280 ℃. As the layer silicate particles exist in the coprecipitation solution, the resulting composite powders exhibited increased specific surface areas and pore volumes along with the enhanced activity of CO removal at ambient temperature.

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Synthesis of Hyperbranched Polyglycidol Derivatives and Their Application as PVC Plasticizers

이규원 곽승엽*

서울대학교 재료공학부

As commercial phthalate plasticizers for poly(vinyl chloride), such as DEHP, have been known as environmental hormones, the restriction on their use have been intensified recently. Also, their low molecular weight promotes migration from products when they contact with harsh environment. We estimated hyperbranched polyglycidol derivatives as alternative plasticizers to phthalates. Hyperbrnahced polglycidols with alkyl chains of 2 to 8 were synthesized and PVC films blended with 60 phr of plasticizers were fabricated. Miscibility and glass transition of plasticized PVC were measured by DSC analysis. Mechanical property, thermal stability, transparency and migration resistance were evaluated by tensile test, TGA, UV/Vis spectroscopy and leaching test, respectively. In addition, general toxicity of plasticizer was executed via oral rat toxicity. From the results, we confirmed hyperbranched polyglycidol derivatives are promising alternative plasticizers.

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발표코드: **MAT.P-1132**
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In silico Prediction of critical micelle concentrations for gemini surfactants

이민지 진은실 이성광*

한남대학교 화학과

Gemini surfactants are composed of two monomeric surfactant molecules linked by a spacer chain. gemini surfactants can self-assemble at concentrations almost a hundred-fold lower than that of corresponding conventional surfactants. Also, unlike conventional surfactants, gemini surfactants have unique properties because of the high surface tension lowering ability, good solubility for water. This study aimed to predict critical micelle concentration(CMC) of gemini surfactant by using a quantitative structure-property relationship(QSPR) method. The CMC dataset were collected from a series of 130 gemini surfactants. We tried to calculate each molecular descriptor using PreADMET program from gemini surfactants substructure which subdivided in a various of ways. The forward selection and bootstrap sampling method were applied to determine the optimum descriptor of the multiple linear regression(MLR). It was possible to know the applicable range of the prediction model by applicability domain(AD) of the results of each model. Y-scrambling was performed to confirm chance correlation of the model.

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A new smalll molecule for solution-processed in efficient photovoltaic devices

천예림 마재열 김형남 김란 김윤희[*] 권순기[1,*]

경상대학교 화학과 [1]경상대학교 나노신소재공학부

We synthesized a dithienobenzodithiophene based molecule with a planar molecular geometry, DTBDT-TTPD, for the fabrication of solution-processable organic solar cells. DTBDT-TTPD exhibited both a low optical band gap of 1.88 Ev and a low-lying highest occupied molecular orbital (HOMO) energy level of ?5.61 eV, indicating that DTBDT-TTPD is a promising electron donor for use in OSCs. OSCs prepared with DTBDT-TTPD as the electron donor and [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) as the electron acceptor were fabricated. An optimized power conversion efficiency of 4.98% with a high short circuit current of 10.6 mA/cm2 was achieved after finely tuning the morphology through an annealing step. These results indicate that DTBDTTTPD is an effective compound for producing very promising characteristics in small molecule solar cell devices.

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Crystallinity enhancement of 6,13-bis(triisopropylsilylethynyl) pentacene by nanoconfinement effect

백장미 성명모[*]

한양대학교 화학과

Organic single crystal have been interested for various devices, such as photonic devices and electronic devices, due to their improvement of performance compared to amorphous or poly-crystal statement. In our previous study, we fabricated single crystal nanowire with liquid-bridge-mediated nanotransfer molding. Fabricated organic single crystal nanowire device shown very high performance and have high crystallinity.

In this study, we analyzed that the crystallinity of 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-PEN) is depends on the pattern size of mold to make sure that the enhancement of crystallinity is from nanoconfinement effect. We fabricated various sized mold and synthesis TIPS-PEN wires with the molds. The synthesized wires have been investigated by scanning electron microscopy (SEM) and crystallinity of wires have been analyzed by selective-area electron diffraction (SAED).

We fabricate field-effect transistors (FET) to compare the performance organic film devices with nanowire devices, and show the nanowire devices have very high-performance. Also, we fabricate high-performanced nanowire inverter with fullerene (C_{60}).

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Optimization of Electrochemical Performance of SnO2-entrapped Graphene Framework

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SnO_2 의 환원 반응에서 Li_2O 와 Sn 이 생성되는 conversion 반응 이후 Sn 은 이론적으로 4.4 개의 Li 과 alloy 될 수 있어서 충,방전시 높은 capacity 를 갖을 수 있다는 장점이 있어 이차전지의 음극소재로 적용하기 위해 다양한 nanometric 형상 및 composites 에 대한 연구가 수행되어 왔다. 이는 SnO_2 의 방전시 리튬과의 alloy 반응으로 인한 비가역적인 부피팽창으로 야기된 pulverization 때문으로, 그 결과 cycle 이 진행됨에 따라 보이는 specific capacity 의 급격한 감소를 완화시키려는데 주 목적이 있었다. 본 연구실에서는 SnO_2 의 비가역적인 부피 팽창으로 인해 발생하는 crack 형성을 방지하기 위해 framework 를 형성한 graphene layer 사이에 SnO_2 를 담지시키는 실험을 실행하였다. 즉, graphene oxide 와 diboronic acid (BDBA)가 공유결합하여 형성된 graphene framework(GF)에 SnO_2 nanoparticles 을 담지함으로써 SnO_2 의 전기화학적 성능을 향상시키는 결과를 보고하였다.(Journal of Power Sources 240(2013)149-154) 그러나, cell test 시 coulombic efficiency 가 좋지 않아 충,방전이 진행될 수록 capacity 가 빠르게 감소하는 현상이 확인되었다. 이에 따라 본 연구에서는 SnO_2/GF (SGF)의 합성과정에서 BDBA 의 양을 조절함으로써 X-linking density 를 향상 (과량 사용시, 양끝단의 acid 가 모두 에스테르화 반응에 참여하는 것의 정도가 감소함) 시키고, 충방전 조건을 최적화하여 반복되는 충·방전에도 안정한 capacity retention 을 갖는 SGF 를 합성하기 위한 실험을 진행하고 있다.

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Shape-Dependent Catalytic Activity of Nickel particles in methanol and ethanol electrooxidation

백민욱 B.T.Huy PHAMQUOCTHAI 이용일*

창원대학교 화학과

AbstractCatalysis is becoming a strategic field of science because it represents a new way to meet the challenges of energy and sustainability. In the work, We successfully synthesized the Ni particles of various shape. The Ni particles are applied to methanol and ethanol electrooxidation in alkaline media. As results the Ni particles shows dependent shape activity for elecrooxidation The study reveals that Ni particles of various shape are promising electrocatalysts for alcohol oxidation in alkaline media. We used Ni particles of near spherical, hollow, Flower like hollow shape as catalyst. The Ni particles are characterized by scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS) X-ray diffraction (XRD).

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New limb structured blue light emitting material with bulky substituents on 2, 3, 9, 10-position of anthracene

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경상대학교 화학과 [1]경상대학교 그린에너지융합연구소

In this study, we designed and developed new blue-emitting material with high color purity and efficiency for OLEDs. The new blue-emitting material was synthesized via the Suzuki cross coupling reaction. The structure of new material was confirmed by using FT-IR, NMR, and mass spectroscopy. The optical, electrochemical and thermal properties have been investigated, and the molecular structure-property relationships were evaluated.The non-doped devices using EFPA displayed 2.55% maximum external quantum efficiency (EQE) with CIE color coordinates (0.166, 0.197). The doped device using 5% EFPA as a dopant showed maximum EQE of 2.90% and CIE coordinates of (0.142 0.107).

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Enhancement of photovoltaic property of $CH_3NH_3PbI_3$ hybrid solar cells by designing nanoporous TiO_2structures

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Recently, perovskite $CH_3NH_3PbI_3$ sensitizer has been recognized as a promising inorganic sensitizer on fabrication highly efficiency hybrid solar cells. In this solid state hybrid solar cells, the role of TiO_2 is accepting the electrons from the photo excited $CH_3NH_3PbI_3$ and transporting them to the TCO such as FTO. It is generally reported that highly porous TiO_2 film with a thickness of approximately 200nm showed the optimum photovoltaic conversion efficiency(PCE). We applied TiO_2 nanosphere and assembled structures in prepaparing the nanoporous TiO_2 layers. According to the applied TiO_2 or nanostructures, pore structures and the connectivity in the film have been modified, which greatly influenced on the photovoltaic property of $CH_3NH_3PbI_3$ solar cells. Resultantly, PCE of the fabricated perovskite solar cell was enhanced to over 13%.

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Mechanically durable superhydrophobic surface coatings using perfluorinated silica/silyl-modified methacrylate nanocomposites

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Superhydrophobic surface coatings with high static water contact angle (>150°) have been receiving tremendous attention in recent years. The applications of superhydrophobic coatings are diverse due to their unique water-repellency, self-cleaning ability, and anti-biofouling property. Various methods have been proposed to fabricate superhydrophobic surfaces mimicking the lotus surface structure, including lithographic patterning, plasma etching, electrochemical deposition, and chemical vapor deposition. However, these methods often require harsh synthetic conditions and complex fabrication techniques. Furthermore, the poor mechanical stability of superhydrophobic coatings formulated on the surface is generally another limitation in their widespread applications. Herein we demonstrate on a one-step facile spray-coating technique to prepare a superhydrophobic surface coated with perfluorinated silica/silyl-modified methacrylate nanocomposites. The superhydrophobic surface coatings are characterized in term of water contact angles, wetting hysteresis, and the surface roughness/morphology. Futhermore, abrasion resistance of the fabricated superhydrophobic coatings was evaluated by a home-made scratch tester, which was composed of a piece of sandpaper and weights of different masses.

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Superhydrophobic hollow silica nanoparticles: Highly efficient recyclable smart materials for oil/water separation

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Superhydrophobic hollow silica nanoparticles (SHSNPs) with great recyclability have been synthesized by simple sonochemical method. The contact angle (CA) of the SHSNPs was 163° on glass surface. It further showed 165°, 161° and 160° on superhydrophobic sponge, Cu mash and stainless steel screen, respectively. The obtained superhydrophobic sponge exhibited excellent oil-absorption performance including high capacity (upto more than 60 times of their weight), good selectivity and extraordinary recyclability. The metal screen filters (both the Cu and stainless steel) could selectively filter the oils from the oil-water mixture with high flux rate (upto 11022 Lm-2h-1). Our material offers great technological promise in the field of water remediation, clean-up of large-area oil spills, and oil recovery including selective absorption materials for environmental preservations.

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Hydrothermal synthesis and luminescence properties of NaYF4:Yb/Er upconversion phosphor under various synthesis conditions

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창원대학교 화학과

AbstractUp-conversion luminescent materials with anti-Stoke optical properties have received considerable attention due to their potential applications in luminescent nanodevices including flat panel displays, solid state lasers, optical fiber based telecommunications and solar cells. Recently, the attention of the nonscientists has been focusing more and more on biological applications. The up-conversion nanoparticles (UCNPs) have many good characteristics. The main materials are that they can emit visible or near infrared (NIR) light under NIR irradiation. In addition, these UCNPs show a sharp emission bandwidth, high photostability, tunable emission, long lifetime, and low cytotoxicity. These benefits make the UCNPs can be used as probes for intravital imaging which enables the investigation of physiological processes within the context of a living organism, and provides a more complete picture of disease pathology and development.NaYF4:Yb/Er phosphors were prepared by hydrothermal method. The preparation RECl3 and RE(NO3)3 (RE = Y, Er, and Yb) solutions. And various capping agent solution (malonic acid, olecic acid and EDTA) prepared at room-temperature. The selection of an appropriate capping agent is one of the key issues for preparing carboxyl-functionalized upconversion phosphors with controlled phase, size, and shape. And the 10 ml water solution of NH4F (4 mmol) and NaOH (4 mmol) was added capping agent solution and RE(NO3)3 solution dropwise under stirring for 1 hr. This solution put in the autoclave system running various temperatures (200, 240, 260, 280, and 300 oC) for 3 hr. The resulting nanoparticles were precipitated by the addition of ethanol, collected by centrifugation washed with ethanol several times. Their crystalline structures, surface morphologies and phase transitions were investigated according to annealing process by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and photoluminescence (PL).

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Formation of high voltage $CH_3NH_3PbBr_3$ solar cell by interface control

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Recently perovskite ($CH_3NH_3PbI_3$) solid state solar cell draws great attention due to its high photovoltaic conversion efficiency (PCE) and economical fabrication process. Herein we studied Br-based perovskite ($CH_3NH_3PbBr_3$) solar cell that offers ultra-high open circuit voltage (V_{OC}) because of its selectively wider band gap and higher conduction position.In this work, we prepared Au/$CH_3NH_3PbBr_3$/TiO_2/FTO cells, belonging to depleted heterojunction solar cell. Perovskite acts as not only an absorber but also a hole transport material (HTM). This solar cells without introducing hole-transporting layer exhibit ultra-high V_{OC} higher than 1.3V. By controlling the TiO_2 surface and optimizing the cell structure, the PCE over 5% was achieved in this work. TiO_2 surface was passivated by organic molecules with carboxylic functional group. By introducing organic molecular layer between TiO_2 and $CH_3NH_3PbBr_3$ layer, the electron transport from the perovskite to TiO_2 layer was significantly enhanced. Resultantly, V_{OC} and PCE were enhanced to 1.36 V and 5.3 %, respectively.

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Upconversion luminescence of Yb3+, Er3+-doped Y2SiO5

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AbstractUpconversion (UC) luminescence via energy transfer (ET) process between pairs of Yb3+ and Er3+ ions was investigated in Yb3+, Er3+-doped Y2SiO5 nanoparticles prepared by hydrothermal method. The morphology and structure of the nanoparticles were investigated by scanning electronic microscopy and X-ray powder diffraction. The different morphologies include rectangle cubic, boomerang-like form can be obtained by calcining temperature The up-conversion spectra were recorded using a near-infrared diode laser (λ=980 nm). Upon excitation with the NIR diode laser, UC luminescence with an intense emission band centered at ~660 nm, along with less intense emission bands at ~540 nm, was detected. The concentration of Yb3+ and Er3+ has a stronger influence on the relative intensities of the green (G) and red (R) UC bands. The upconversion process of Yb3+,Er3+-doped Y2SiO5 is a two photon process. The ET mechanism was discussed.

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A small molecule base on asymmetric Naphthalene-Thiophene for Organic Thin Film Transistor

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경상대학교 화학과 [1]경상대학교 나노신소재공학부

We designed and synthesized a new asymmetric semiconductor(NBTND) by the palladium catalyzed Suzuki coupling reaction for organic thin film transistor (OTFT). The structure of the material was assigned by NMR and IR and the performance of NBTND was characterized by UV-visible spectroscopy, cyclovoltammetry, thermogravimetric analysis, differential scanning calorimetry. The asymmetric molecule has high thermal stability and good oxidation stability as HOMO level of -5.35 eV. The thin film transistor using new asymmetric semiconductor exhibited the field effect mobility of 2.68×10-2 cm2 V-1s-1 .

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Fast Preparation of Highly Surface Enhanced Raman Scattering Active Silver Nanoparticles by Electrolysis

PHAMQUOCTHAI **B.T.Huy** 이용일*

창원대학교 화학과

Abstract The surface-enhanced Raman scattering (SERS) effect was first observed on silver electrodes roughened by oxidation reduction cycles. The advantages of the latter with respect to the electrodes in an electrochemical cell are due to the large adsorption capability and the simplicity in the preparation of the SERS-active substrate. In addition, different SERS-active substrates and metal colloidal suspensions have been successfully employed. Silver colloidal nanoparticles are probably the most studied and a variety of procedures have been developed to produce monodispersed nanoparticles characterized by relatively small size variations. In this work, highly efficient and large-scale synthesis of silver nanostructures for the SERS-substrate was produced by electrolysis using sodium sulfate as an effective electrolyte. The silver nanostructures obtained were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD). The SERS spectra for different analytes in the silver nanostructures substrate were investigated.

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Synthesis of carbon materials with controlled porosity and polarity for CO2 capture applications

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한양대학교 응용화학과

The increase of CO2 concentration in the atmosphere has been recognized as a major contributor to global warming, so people are greatly concerned about its environmental impact. CO2 capture and storage is therefore necessary to prevent the release of large quantities of CO2 into the atmosphere. Among the promising materials that could adsorb and store CO2, carbon-based materials such as activated carbon, carbon nanotubes, nanofibres and templated carbon materials have been focused due to low cost, high chemical and thermal stability, and low sensitivity to moisture. For realizing high CO2 adsorption property using carbon based materials, understand of structure-properties relations (i.e., microporosity, polarity and functionality) of carbon materials are essential. Herein, we investigate CO2 adsorption capacity of synthetic carbon materials (e.g. Resorcinol - Formaldehyde carbon, Phenol ? Formaldehyde carbon and etc.) in terms of structure-properties of synthetic carbon materials. Using various methods to control the microporosity and polarity (mainly the extent of oxygenates and nitrogen based moieties on the carbon), it is elucidated how CO2 capture on synthetic carbon materials is varied. Gas sorption measurements, SEM, IR, elementary analysis and CO2 adsorption experiments were carried out to prove the structure-properties relations of synthetic carbon materials for CO2 capture.

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Fabrication of Palladium Nano-raspberry using Peptide as a Template and its Application to C-C Coupling Reaction

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서울대학교 화학생물공학부

Peptide building blocks have biocompatibility, biological recognition abilities, and chemical versatility, and they can be easily synthesized. Therefore, many researchers have studied about using peptide to make nanostructures having various functional abilities. Peptide self-assembly process is important to regulate various functions such as bio-mineralization and catalytic activity. Recently, we have reported that series of tyrosine-rich peptides (TRPs) induced nano film formation at air-water interface and played a critical role as a catalytic scaffold. Here, through interactions between TRPs and metal ions, we have found that both peptide assembly and the formation of metal nanoparticles (NPs) can be easily manipulated. Especially, we have noticed that TRPs could induce the reduction of palladium (II) ion to Pd NPs (5-6 nm). The folding and conformational change of the peptides with Pd+2 ions made the Pd NPs to form a raspberry-like structure. Additionally, these raspberry-shaped Pd NPs showed good catalytic activities in copper-free Sonogashira cross-coupling reaction in water.

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Synthesis of Trimethylolpropane-cored Poly(ε-caprolactone) with Extremely Short Arms and Its Application to a Flexible PVC

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서울대학교 재료공학부

Trimethylolpropane-cored poly(ε-caprolactone) (TMP-PCL) with extremely short arms is succesfully synthesized using a facile pseudo-one-pot process. The well-defined molecular architecture of TMP-PCL are controlled with the consideration of monomer conversion, end-capping, and vacuum purification conditions. The arm number of TMP-PCL is 3 corresponding to the number of hydroxyl groups in TMP, and the degree of polymerization in one arm is 3. This TMP-SPCL is a transparent viscous liquid at room temperature due to its exremely short arms. Moreover, this TMP-SPCL exhibits an unentangled Newtonian behavior and biological nontoxicity. A flexible PVC prepared with TMP-SPCL with extremely short arms shows excellent stretchability, migration resistance, and good clarity. Consequently, well-defined TMP-SPCL with short arms can be useful for fabricating phthalate-free flexible PVC products.

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Optimization of TiO2 structure in cobalt electrolyte based Dye Sensitized Solar Cell

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Due to the lower redox potential of iodide/triiodide couple and corrosion towards the electrode iodide/triiodide redox shuttle has some limitation in photovoltaic performance of Dye sensitized Solar Cell. Electrolytes containing cobalt complexes are promising alternative to iodide/triiodide redox electrolytes. Due to bulkiness of the Co-complex diffusion through the TiO2 working electrode has been identified as limiting factor for dye sensitized solar cell based on cobalt redox electrolytes. TiO2 spheres of around 350nm with larger pore size ware synthesized and employed as photo anode to assist the diffusion of bulky electrolytes, such as cobalt bipyridyl [Co(bpy)3]2+/3+ with organic dye D35 and Y123. This tailored morphology of TiO2 material improves the efficiency of dye sensitized solar cell indicating better diffusion of electrolyte. Large pores generated in TiO2 spheres also reduce recombination and decrease the diffusion resistance, as revealed by electrochemical analysis.

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Nafion/Layered Silicate Composite Membrane with Low Vanadium ions Crossover for Vanadium Redox Flow Battery

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Microporous layered silicate AMH-3 has a 3D ordered porous structure that can be used as a permselective barrier and is therefore very promising as a solution for the vanadium ions crossover problem of Nafion in vanadium redox flow batteries (VRBs). Nafion was modified with delaminated AMH-3 (D-AMH-3) to reduce vanadium ions crossover. The composite membrane was investigated by FE-SEM and EDS. The composite membrane had sandwich-type structure that consist of double Nafion outer layers and a D-AMH-3 central layer. The VRB assembled with composite membrane exhibited a lower vanadium ions permeability compared to the neat Nafion, thereby improving the columbic efficiency and capacity retention. The VRB with composite membrane kept a stable performance after 100 cycle charge-discharge test.

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Encapsulation Layer Fabrication of Organic-Inorganic Hybrid Thin Film by Atomic Layer Deposition and Molecular Layer Deposition

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한양대학교 화학과

We fabricate organic-inorganic thin film for the purpose of encapsulation by molecular layer deposition(MLD) using Adipoyl Chloride(AC) and 1,4-Butanediamine. Ellipsometry was employed to verify self-limiting reaction of MLD. Linear relationship between number of cycle and thickness was obtained. We found that desirable organic thin film fabrication is possible by MLD surface reaction in monolayer scale. Purging was carried out after dosing of each precursor to form monolayer in each sequence. We also confirmed roughness of the organic thin film by atomic force microscopy(AFM). We deposit AC and 1,4-Butanediamine at 70 °C and investigated surface roughness with increasing thickness of organic thin film. We confirmed precursor's functional group by IR spectrum. We calculated WVTR of organic-inorganic hybrid super-lattice epitaxial layer using Ca test. WVTR indicates superlattice film can be possibly use as encapsulation in flexible devices.

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Development of a garphene heater for winter sports wear and its physiological evaluation

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Graphene has come into the spotlight as a new material for display, industry, and so on. The high electrical and thermal conductivity of graphene along with its remarkable chemical and mechanical properties attract researchers of various academic fields. Recently, it has been found that graphene is superior to any other previous material as a heating element because of its flexibility, transparency, fast-heating, and homogeneous temperature distribution. The graphene heater could be suitable for heating elements in winter sports wear because of its flexibility and well-distributed surface temperature. This study was aimed to explore ways to make the graphene heater for winter sports wear and investigate the physiological effect of the graphene heater when applied to winter sports wear.To make large-scale graphene films for a heater, chemical vapor deposition (CVD) method was used. One volunteer subject participated in a pilot test. The subject was exposed to a cold environment maintained at an air temperature of -6℃ and relative humidity of 20%. Subjective perceptions (thermal comfort, thermal sensation, shivering sensation, and humidity sensation) were assessed. Temperature of skin heated by the graphene heater was kept around 50℃. The results showed that rectal temperature was more stable and shivering sensation was lower in the graphene heater applied conditions when compared to Control. However, no significant difference was found among the surface temperature of the skin(AH, BH, and CH). These results indicate that the graphene heater was beneficial for maintaining body temperature during cold conditions and have implications for the development of cold protective clothing in extreme environments.

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Light-triggerd release from a dendrimer-nanorods comosite membrane

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삼육대학교 화학과

The development of a novel drug-delivery system with the ability to respond to a given stimulus has attracted much attention due to their enhanced therapeutic efficacy.We have developed the versatile delivery system using the dendrimer-nanorod composite membrane able to give a response to near-infrared (NIR) irradiation. The membrane was fabricated through dithiocarbamate (DTC) cross-linking of polyamidoamine (PAMAM) dendrimers to gold nanorods.The photothermal effect of a gold nanorod by NIR irradiation leads to rapid increase in temperature around the composite membrane, accelerating the release of drugs through the membrane.Scanning electron microscopy (SEM) was used to analyze surface morphology of the fabricated membrane and quantitative release of drugs by NIR irradiation was measured by UV-vis spectroscopy or fluorescence spectroscopy.

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Studies on the effect of ordered mesoporous carbon support structure on Na/SO_2 battery

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성균관대학교 화학과

Sodium based batteries are one possible alternative to the lithium-ion battery due to the low cost and comparatively higher natural abundance of sodium, particularly with regard to large-scale applications. In this study, we suggest that Na/SO_2 battery is made up of an inorganic electrolyte, sodium as the anode and carbon materials as the cathode. For a lithium ion battery, the risk of explosion is due to the use of organic electrolyte with vulnerable to heat and the oxide anode materials causing a decomposition reaction of oxygen at high temperatures. For a Na/SO_2 battery, whereas it is more safety due to this system was used a nonflammable inorganic electrolyte and the carbon materials instead of the oxide cathode materials. After discharge, the particle such as sodium chlroride (NaCl) is generated at the cathode and it has been caused a problem in the safety of the electrode and a reversible reaction. To solve this problem, we were synthesized the ordered mesoporous carbons (CMK8, CMK3) with high surface area by using impregnation and synthesized materials were introduced into the cathode material. The as-synthesized ordered mesoporous carbons were characterized by X-ray diffraction (XRD), Nitrogen-sorption isotherm and scanning electron microscope (SEM), and electrochemical properties were analyzed by charge-discharge profile, cycle performance.

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Facile synthetic route to reduced graphene oxide for electrochemical energy storage application

민영제 백승민*

경북대학교 화학과

Hydrogen have attracted much scientific interest as one of perfect energy sources because it is non-polluting and renewable. At first, graphene oxide (GO) was synthesized via a modified Hummer's method. And then, the prepared GO was reduced via polyol reduction process to develop effective defect sites for hydrogen storage applications. According to X-ray diffraction patterns, GO was fully reduced to graphene nanosheets. From X-ray photoelectron spectroscopic analysis, it confirmed that the bonding nature of GO was changed after polyol reduction. SEM and TEM images of reduced graphene oxide show that the inter-layer distance of these materials increased than that of graphite (0.34 nm). Also, Nitrogen adsorption-desorption isotherms confirmed that synthesized reduced graphene oxide could have much amount of micropore that is effective for hydrogen storage compare to GO. Therefore, the present reduced graphene oxide could be used as a new hydrogen storage material with enhanced properties.

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Efficient decomposition of organic pollutant under visible light irradiation by Double Heterojunction structure of FeWO4/TiO2/CdS

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인하대학교 화학과

Dark brown color FeWO4 nanoparticles of average size 50-70 nm was prepared by hydrothermal method which showed a profound absorption over the entire visible range. A heterojunction between FeWO4 and TiO2 was made by simple sol-gel method. The haterojunction shows notably high visible light photocatalytic activity in decomposing Isopropanol (IP) in gas phase and Salicylic acid in liquid phase. . 5/95 FeWO4/TiO2 shows 1.7 times higher CO2 evolution and 2.5 time high rate constant for decomposition of SA compare to N-doped TiO2 , a well known visible light Photocatalyst. The valence band (VB) position of FeWO4 (+2.8 eV vs NHE) is lower than that of TiO2 (+2.7 eV). The high photocatalytic efficiency of the FeWO4/TiO2 composite is caused by intersemiconductor hole transfer from VB of FeWO4 to VB of TiO2. Subsequently, a double-heterojunction FeWO4/TiO2 /CdS structure was prepared by loading CdS quantum dots (QDs) onto the surface of the FeWO4/TiO2, which dramatically enhanced the visible-light photocatalytic efficiency. The catalytic activity of FeWO4/TiO2 /CdS in evolving CO2 from IP, was ~ 2.6 times that of FeWO4/TiO2 .The unexpectedly high efficiency of FeWO4/TiO2 /CdS seemingly is due to the unique band matching among these semiconductors. With sensitization of FeWO4 and CdS, not only the holes but also the electrons are generated in the VB and CB, respectively, of TiO2 under visible-light irradiation.

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The Development of Hollow Nanostructure with Exfoliated Ruthenium Oxides for the Energy Storage Applications

장수진 백승민*

경북대학교 화학과

According to the current research activities, the transition metal oxides could have better energy storage properties as anodes in rechargeable lithium-ion batteries, in comparison with those of carbon-based materials. In particular, since ruthenium dioxides have high electrical conductivity, excellent chemical and electrochemical property, lithium-ion battery based on ruthenate could lead to the enhanced columbic efficiency and cyclability. In this study, we are quite successful in the development of ruthenate hollow sphere, which leads to nearly 96% coulombic efficiency along with enhanced discharge capacity. Scanning electron microscopic images of samples show ruthenium dioxides nanosheets were assembled in a controlled manner onto the polymer particles. The morphology of ruthenate hollow sphere can be confirmed by transmission electron microscopic images, supporting that ruthenate hollow sphere maintains its spherical morphology even after calcinations reaction.

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Soft chemical route to band gap engineering of layered perovskite via electron beam irradiation

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The transition metal oxides with perovskite phase have highly attracted research interests because of their promising application in photocatalysis. Especially layered perovskites such as Dion-Jacobson phase have wide application including photocatalytic degradation of organic pollutants. In this study, we demonstrated the intercalation of organic molecules into interlayer spaces of layered perovskites, and examined effect of electron beam irradiation. According to X-ray diffraction patterns, the basal spacing of layered perovskites was significantly increased upon the intercalation reaction. The UV-vis diffuse reflectance spectra and results of photocatalytic degradation show that the electron beam irradiation derived the change of band gap of layered perovskites, which led to the enhanced photocatalytic activities in degradation reaction of organic pollutants. The transmission electron microscopic studies indicate that the electron beam irradiated perovskites could be used new host materials with controlled band gap after exfoliation reaction. This synthetic methodology could be applicable to the fabrication of new photocatalysts with enhanced activities.

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High-performance Gold/Nickel hydroxide composites as supercapacitor electrodes

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울산과학기술대학교(UNIST) 친환경 에너지 공학부

We introduce a new method to improve the electrochemical properties of Ni(OH)2 in the specific capacitance value, rate capability, and cycle life by simply electrodepositing gold nanoparticles (Au-NPs). The doped Au-NPs decrease the resistance and improve the conductivity of the electrode, which decreases the “dead volume” in the active materials and increases the capacitance. Furthermore, Au-NPs act as a catalyst to improve the redox reaction an alkali electrolyte and cause the redox reaction reversibly, which induces high oxidation current and increases the capacitance of the electrode. As a result, the Au/Ni(OH)2 composites show the highest capacitance in 1,927 F/g at 1 A/g, and retain 66% and 80% of the maximum value at a high current density of 20 A/g and 5,000 cycles. Since this method is very simple and easy, it can be readily applied to other metal oxide supercapacitors.

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Exfoliated Metal Oxide Nanosheet as a Highly Efficient Additive in Optimizing Electrode Performance of Co_3O_4-Graphene Nanocomposites

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이화여자대학교 화학·나노과학과 [1]이화여자대학교 chemistry

Dramatic enhancement of the electrode performance of Co_3O_4-graphene nanocomposites can be achieved by adapting exfoliated layered metal oxide nanosheets as an additive for the synthesis of the nanocomposites. Mesoporous Co_3O_4-CoO_2-N-doped graphene nanocomposites are synthesized by the crystal growth of Co_3O_4 nanoparticles in the presence of the mixture colloidal suspension of exfoliated CoO_2 nanosheet and N-doped graphene nanosheet. The incorporation of layered CoO_2 nanosheet induces an increase of the surface area of the resulting nanocomposite, which would be related to the diminution of π-π interaction between graphene nanosheets. The present nanocomposites exhibit promising performance as anode materials with the huge discharge capacity, which is much superior to that of CoO_2-free homologue. The present study clearly demonstrates that the incorporation of inorganic nanosheets into the graphene-based nanocomposite can provide a powerful and universal methodology to design and synthesize novel efficient electrode materials for lithium secondary batteries.

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Mixed Colloidal Suspensions and Lithiated Nanocomposites of Layered MnO_2 and RuO_2 Nanosheets

이슬 JINXIAOYAN 구태하 황성주*

이화여자대학교 화학·나노과학과

Homogeneously mixed colloidal suspensions of layered MnO_2 and RuO_2 nanosheets are synthesized by mixing the exfoliated colloidal nanosheets of each metal oxide. According to zeta potential measurement and UV-vis absorption spectroscopy analysis, the obtained colloidal suspensions show negatively-charged state and good colloidal stability without any phase separation. The co-flocculation of these anionic colloidal nanosheets with lithium cations yields well-ordered intercalation compounds of Li-MnO_2-RuO_2 nanocomposites (LMR). Electron microscopy and N_2 adsorption-desorption isotherm measurements clearly demonstrate that the MnO_2 2D nanosheets in these materials are intimately coupled with the surface of RuO_2 2D nanosheets and the house-of-cards-type stacking of two kinds of 2D nanosheets is responsible for highly porous materials with remarkably expanded surface area. The resulting LMR nanocomposites display highly porous structure with expanded surface. In comparison with the RuO_2-free Li-MnO_2 nanocomposites (~251 F g^{-1}), the present LMR nanocomposites deliver larger capacitances with good cyclability upto the 5000th cycle. The present experimental findings clearly demonstrate that the mixed colloidal suspensions of MnO_2 nanosheets and RuO_2 nanosheets are very useful precursors for synthesizing high performance electrochemical capacitors.

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Self-Assembly of Layered Double Hydroxide 2D Nanosheets with Polyoxometalate 0D Nanoclusters: Efficient Hybrid-Type CO_2 Adsorbents

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이화여자대학교 화학·나노과학과

Efficient hybrid-type CO_2 adsorbents are synthesized via an electrostatically-derived self-assembly of cationic Mg-Al-LDH 2D nanosheets and anionic polyoxometalate (POM, $V_{10}O_{28}^{6-}$ and $W_7O_{24}^{6-}$) 0D nanoclusters. The electrostatically-derived self-assembly between exfoliated Mg-Al-LDH 2D nanosheets and POM 0D nanoclusters ($W_7O_{24}^{6-}$ and $V_{10}O_{28}^{6-}$) yields a high flexibility in the control of the chemical composition and layer-by-layer-ordered intercalation structure with porous structures composed of mesopores and micropores. The hybridization with POM leads to the remarkable enhancement of the CO_2 adsorption functionality of Mg-Al-LDH by almost 10 times. Of prime importance is that the CO_2 adsorption functionality of the nanohybrid is strongly dependent on the type of guest POM species. This finding strongly suggests that the CO_2 adsorption functionality of the LDH-based nanohybrid materials can be optimized via the selection of guest species. The present result clearly demonstrates that the exfoliation-reassembling method is quite effective in synthesizing new LDH nanosheet-based hybrid materials with improved CO_2 adsorption functionality.

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Large-Scale Synthesis of Ag Nanoparticle-Silica Hybrid Composites and Their Application for Antibacterial Agents on Air Filtration

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Ag nanoparticle-silica (AgNP@SiO_2) hybrid composites were synthesized on a large scale and were used as a coating material for an air filtration system exhibiting synergistic antibacterial activity. The AgNP@SiO_2 composites were obtained via the seed-mediated growth method. Monodispersed silica spheres (~400 nm in diameter) prepared by the Stober process were used as a substrate material for decorating AgNPs. The silica spheres were functionalized with aminopropyl groups to bind Ag seeds on the silica surface, which were grown up to ~30 nm in size.The AgNP@SiO_2 composites were coated on filter samples and tested for the antimicrobial activity on bacteria. The target bacteria are gram-negative bacteria, *Escherichia coli*, and gram-positive bacteria, *Staphylococcus epidermidis*. The electron microscopic analysis revealed that those bacteria were trapped by the AgNP@SiO_2 on filter fibers, eventually leading to death of bacteria. The antibacterial activities of the coated air filter samples were also evaluated quantitatively using the colony count method. The filter sample showed 99.99% antibacterial efficacies for both bacteria in bacterial solution. In these regards, the antibacterial effect of AgNP@SiO_2-coated air filters provides a future direction for their practical utilization in green environment applications.

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Ferroelectric Polymer Films on Graphene: Molecular Dynamics Simulations and Density Functional Theory Calculations for Carbon-Based Switching Device Applications

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Graphene is a promising channel material for field-effect transistors and non-volatile memories owing to its high carrier mobility, but its zero band gap hampers the realization of such carbon-based switching devices. Doping graphene with a thin-film deposition of ferroelectric polymer such as polyvinylidene fluoride (PVDF) has been known to increase its ON/OFF ratio, but the origin of the amplified resistance switching is still unclear. In order to better understand the mechanism at a molecular level, we carried out density functional theory calculations on the doping characteristics of a single-layer graphene as a function of the polarization direction of a PVDF thin film deposited on it, related it to the carrier concentrations and the resistance states of the graphene channel, and then carried out non-equilibrium Green’s function calculations to confirm the switching between high and low resistance states of the PVDF/graphene device. Based on this understanding, we propose a new architecture for PVDF/graphene-based field-effect transistors and non-volatile memories. Finally, since the β crystalline phase is the only PVDF phase whose permanent polarization can make it useful for ferroelectric applications, we carry out molecular dynamics simulations to confirm the formation of β-like phases from amorphous PVDF under a shear stress often applied during device fabrication.

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Highly Stable and Sensitive Iodine-125 embedded Au-NNPs for Sensitive SPECT Imaging Probe

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Radio-labelled gold nanoparticles (AuNPs)have been investigated for sensitive CT, SPECT imaging probe because of excellent biocompatibility, facile synthesis, and easy surface chemistry of AuNPs. Due to the lack of robust modification chemistry of iodine on the AuNP, the sensitivity and biological stability of labelled Iodine(125) was not enough to be used as practical SPECT-based imaging modality. Here, we propose robust iodine modification chemistry achieved simply by use of adenine-rich oligonucleotide-modified AuNPs and additional chemistry with SHPP, which is similar functional group with tyrosine. Therefore, lots of radio-active iodine can be modified per single gold nanoparticle through the reaction with Na^{125}I, chloramine-T, and sodium bissulfite. To generate stable imaging probe, additional gold shell was formed on iodine labelled AuNP core and then the resulting particle (Au-NNP) was protected with mPEG-thiol. The efficiency of radio-labelling reaction on gold and radio-activities of resulting Au-NNPs depends on the core particle size were investigated by use of three different DNA-AuNP size (5 nm, 15 nm, 20 nm). The Au-NNPs showedgreatly improved stability of ^{125}I-labelling by preventing possible hydrolysis or enzymatic attacks in in-vitro performed with human serum at 37 °C and in-vivostudied with nude mice.

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X-ray Amorphous Manganese Oxide Nanocrystals as Promising Anode Materials for Lithium Ion Batteries

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Amorphous manganese oxide nanocrystals are synthesized by soft-chemical redox reactions using reducing agents of KBH_4 and LiI at room temperature, and applied as anode materials for lithium ion batteries. Both amorphous manganese oxides have a layered MnO_2 local crystal ordering with the mixed oxidation state of Mn^{3+}/Mn^{4+}. In comparison with the nanocrystalline manganese oxide prepared with LiI and well-crystalline $K_{0.45}MnO_2$, the nanocrystalline manganese oxide prepared with KBH_4 shows much smaller particle size (~10 nm) with larger surface area (> 200 m^2/g). This nanocrystalline manganese oxide with smaller particle size shows much better anode performance with much greater discharge capacity (~530 mAh/g for the 50th cycle) for lithium ion batteries, compared with homologues with larger particle size (~240 mAh/g for the 50th cycle). The present results clearly demonstrate the advantage of nanocrystalline and amorphous nature for optimizing the electrode performance of manganese oxide. The present solution-based redox reaction can provide a facile, economic, and scalable synthetic route to efficient manganese-based anode materials for lithium ion batteries.

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Universal Sulfide-Assisted Synthesis of M-Ag Heterodimers (M = Pd, Au, Pt) as Efficient Platforms for Fabricating Metal-Semiconductor Heteronanostructures

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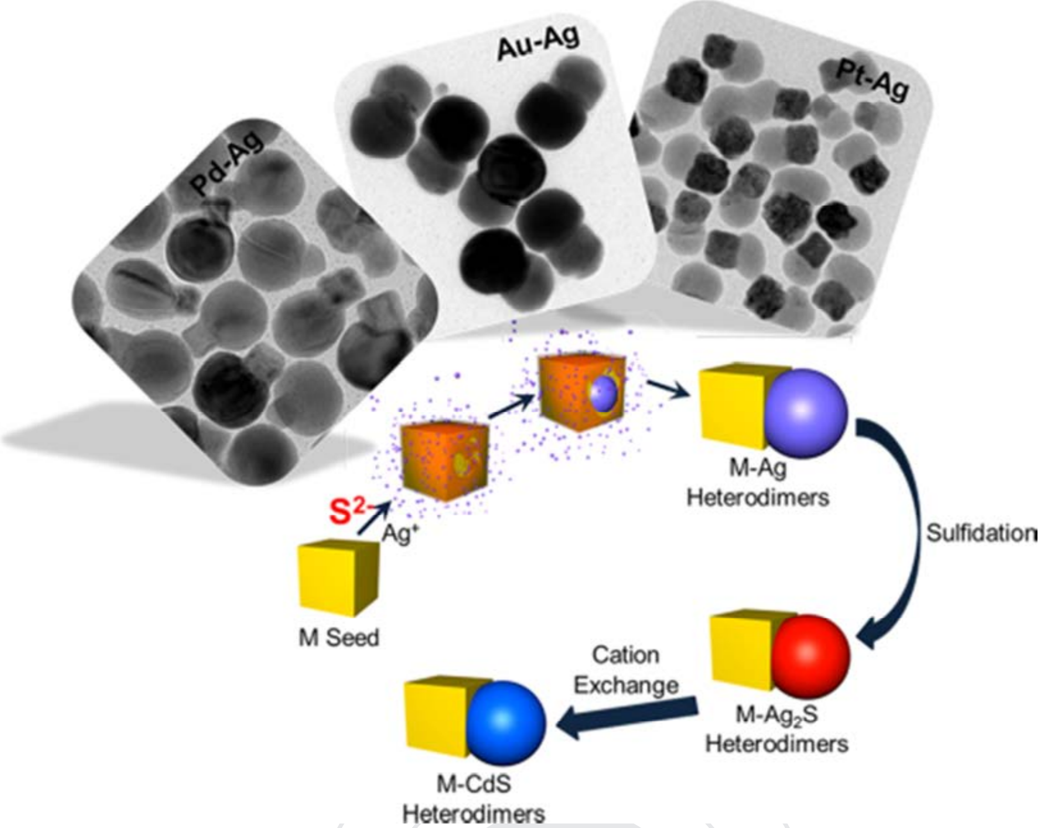
We report a universal sulfide-assisted synthesis strategy to prepare dumbbell-like M-Ag heterodimers(M = Pd, Au, Pt). Sulfide ions can give fine control over the reaction kinetics of Ag precursors, resulting in the anisotropic overgrowth of Ag to realize the dumbbell-like heterodimers irrespective of the surface facets or components of the M domain. The M-Ag heterodimers were facilely transformed to M-Ag_2S heterodimers via a simple sulfidation reaction. This study provides a versatile approach to realizing not only metal-metal heterodimers but also semiconductor-metal heterodimers and will pave the way for designing heteronanostructures with unprecedented morphologies and functions.


Pd-Ag
Au-Ag
Pt-Ag
S^{2-}
Ag^+
M Seed
M-Ag Heterodimers
Sulfidation
M-Ag_2S Heterodimers
Cation Exchange
M-CdS Heterodimers

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For smart window application: simple fabrication of infrared modulating VO_2 film

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부경대학교 화학과 [1](주)마프로 기술연구소

We could prepared a smart VO_2 window from the aqueous solution of VCl_4^+ by one step heating procedure. This procedure was very simple and more effective method to prepare the smart window: added PVP (10 %wt) into the VCl_4^+ mixture solution with V_2O_5, N_2H_4, HCl and water, coated over a piece of polished sapphire glass, and then sintered under Ar flow at 520 °C with a controlled heating history. At the low temperature, below the insulator to metal transition temperature (T_H = ~68 °C), the IR transmittance of the film was increased along with increased wavelength. However, in high temperature region (above T_H, metal phase), the transmittance was decreased upto 25 % in the long wavelength IR region (> 800 nm). The temperature dependence of IR transparency of the smart film, which observed by home made spectrophotometer, clearly shows the phase transition of the film near room temperature. The phase transition was also observed in electric transport measurement. These indicate the smart window can be used as energy save windows in modern green building.

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Novel Nanocomposite Anode Materials of 1D Ga_2O_3Nanostructure and Graphene Nanosheet Applicable for Lithium Ion Batteries

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이화여자대학교 화학·나노과학과

One dimensional (1D) nanostructured Ga_2O_3 is hybridized with reduced graphene oxide (rG-O) via the crystal growth of gallium oxyhydroxide nanorods in the presence of colloidal graphene oxide (G-O) nanosheets and the following heat-treatment at elevated temperature under inert atmosphere. Depending on the content of rG-O nanosheets in the nanocomposite, the heat-treatment induces a phase transformation from gallium oxyhydroxide to gallium oxide with its different polymorphs such as α-, β-, and γ-phase. In the obtained nanocomposites, layer-structured 1D Ga_2O_3 nanorods with the aspect ratio of ~5 are anchored over the surface of rG-O nanosheets. The house-of-cards stacking of sheet-like crystallites leads to the remarkable expansion of surface area to ~340 $m^2g^{-1}$and the formation of mesoporous structure with the average pore diameter of ~3-5 nm. The present nanocomposites show promising anode performance with discharge capacity (>750 $mAhg^{-1}$ after 40 cycles), excellent cyclability, and good rate characteristics, which is superior to that of Ga_2O_3 nanorods. The present study clearly demonstrates the usefulness of gallium oxide as new anode material for lithium ion batteries.

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Characterization of OLEFETs based on pentacene and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran doped tris(8-hydroxyquinoline) aluminum

김대규 오정도 최종호*

고려대학교 화학과

Organic light-emitting field-effect transistors (OLEFETs) are a class of next generation devices which combine the switching function with light emission properties in single devices. We present our application of the neutral cluster beam deposition method to fabricate bilayer heterojunction-based OLEFETs by superimposing two layers of pentacene and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) doped into tris(8-hydroxyquinoline) aluminum (Alq_3) as p-type and emissive layers, respectively. The OLEFETs with asymmetric electrodes (Au and Li:Al) show efficient charge injection of holes and electrons, good field-effect characteristics and electroluminescence under ambient condition. We observed the light emission enhancement using DCM.

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Low-Voltage, High-Performance OFETs with Cross-Linked Blend Gate Dielectrics

오정도 김대규 최종호*

고려대학교 화학과

Organic field-effect transistors (OFETs) were fabricated with cross-linked organic-inorganic blend dielectrics, consisting of Hf chloride precursor and 1,6-bis(trimethoxysily)hexane (BTMH) as a cross-linker. Various composition of cross-linked HfO_x/1,6-bis(trimethoxysily)hexane blend (CLHB) films were fabricated by solution-process methods at low temperature in air. The optimized CLHB films ($HfCl_4$: BTMH = 1 : 0.5) exhibit excellent dielectric properties (leakage current ~2×10^{-7} at 2 MV/cm and high capacitance ~137 nF/cm^2) and smooth surfaces. The OFETs fabricated with pentacene semiconductor using CLHB gate dielectric operated at low operating voltage (<-4V) and exhibited high hole carrier mobilities of 1.6 cm^2/Vs and current on/off ratio of 2×10^5.

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One-pot Green Synthesis of Poly(γ-glutamic acid) Capped Silver Nanoparticles and Their Application

박성빈 **Hiroshi Uyama**[1] **성문희**[2,*]

국민대학교 바이오발효융합기술연구소 [1]*Graduate School of Engineering, Osaka University* [2]*국민대학교 발효융합학과*

Nano-size silver particles are currently receiving increased attention for the wide range of new applications in various areas. To reduce environmental and biological risks, we have focused on the development of a green and simple synthesis of stable silver nanoparticles (AgNPs) without using hazardous chemicals. Poly(γ-glutamic acid) (γ-PGA) was used as a capping agent in this study because of its hydrophilic, anionic, and biocompatible properties. Here, we have successfully prepared γ-PGA capped AgNPs (γ-PGA-AgNPs) by one-pot green synthesis. The effects of the γ-PGA concentration and reaction temperature during the synthesis were investigated. The γ-PGA-AgNPs were characterized by UV-visible spectroscopy, scanning electron microscopy, and dynamic light scattering analysis. In addition, antibacterial activity against Gram-positive bacteria and Gram-negative bacteria has been assessed. Results suggest that the γ-PGA-AgNPs have high antibacterial activity against both Gram-positive and Gram-negative bacteria.

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Development of Organic Low Band-Gap p-type Semiconductors for Solar Cells

Mamun Muhammad Shamim Al 장성연[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

Harvesting energy directly from sunlight using photovoltaic cells is a very important way to address growing global energy needs with a renewable resource while minimizing detrimental effects on the environment. In the area of organic solar cells (OSCs), developing p-type semiconductors that can absorb wider spectrum of light with high absorbability has been an important issue. Constructing donor (D)-acceptor (A) conjugated structure is one of popular strategies to obtain such low band-gap organic semiconductors. In this work, low band-gap D-A conjugated small molecules (DR3TBDT and DB4TBBDT) were synthesized and their applications for solar cells were investigated. The characterizations to reveal their optical, electrochemical, and thermal properties were performed. The small molecules were applied as the photoactive p-type materials for OSCs and the hole-transporting materials (HTMs) for Perovskite solar cells respectively.

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Effect of ZnO encapsulation layer in P3HT/PCBM bulk-heterojunction solar cells

이린 성명모*

한양대학교 화학과

Organic photovoltaic (OPV) is promising candidate for low-cost and flexible renewable energy source. On the other side, OPV has problems from this organic material property which are unstable performance through time without encapsulation. For these reasons, interfacial encapsulation layer between photoactive layer and electrode to protect air corrosion and direct contact of inappropriate materials. In this study, thin ZnO film (10nm) was introduced as encapsulation layer on the top of P3HT/PCBM photoactive layer to air stable performance and also effective exciton separation. ZnO thin film is deposited by atomic layer deposition (ALD) method and thickness is observed using elipsometer. The photoelectric properties are investigated using solar simulator.

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Layer-by-Layer Assembled 3-Dimensional Electrocatalyst for Methanol Oxidation

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울산과학기술대학교(UNIST) 에너지공학과 [1]울산과학기술대학교(UNIST) 친환경에너지공학부

Layer-by-Layer (LbL) assembly has been widely developed as one of the most powerful techniques to prepare multifunctional films for various energy storage and conversion devices. In spite of recent progress in the LbL-based electrochemical devices, the precise control of electrochemical behavior is still challenging in 3-dimensional LbL structure. In this study, we report electrocatalytic thin films for methanol oxidation by adjusting the assembly sequence of LbL films based on the graphene nanosheets and metal nanoparticles. To investigate the structural effect on the electrochemical behavior, the gold and palladium nanoparticles are assembled into the graphene oxide (GO) with three different sequence of LbL process: $(GO/Au)_n(GO/Pd)_{6-n}$, $(GO/Pd)_n(GO/Au)_{6-n}$, and $(GO/Au/GO/Pd)_n$. The electrocatalytic activity of $(GO/Pd)_n(GO/Au)_{6-n}$ is higher than that of $(GO/Au)_{6-n}(GO/Pd)_n$ in most of the cases, indicating that the electrocatalytic activity can be highly affected by the position of metal nanoparticle in the LbL structure. This phenomenon also represents the structural dependence of ionic transport between the electrode and the electrolyte. In the case of $(GO/Au/GO/Pd)_n$ LbL structure, resulting in the increase of the contact layers between Au and Pd nanoparticles, the electrocatalytic activity shows higher than that of any other metal nanoparticle imbedded LbL structures. The X-ray photoelectron spectroscopy (XPS) analysis demonstrates that the enhanced catalytic effect of the LbL films can be induced by the electronic modification of metal nanoparticles without an alloy or direct contact between the heterogeneous metal nanoparticles, owing to the electronic conduction of graphene nanosheets within the LbL structure. It is expected that this work provide insights into the modulation of intra-layer of LbL thin film.

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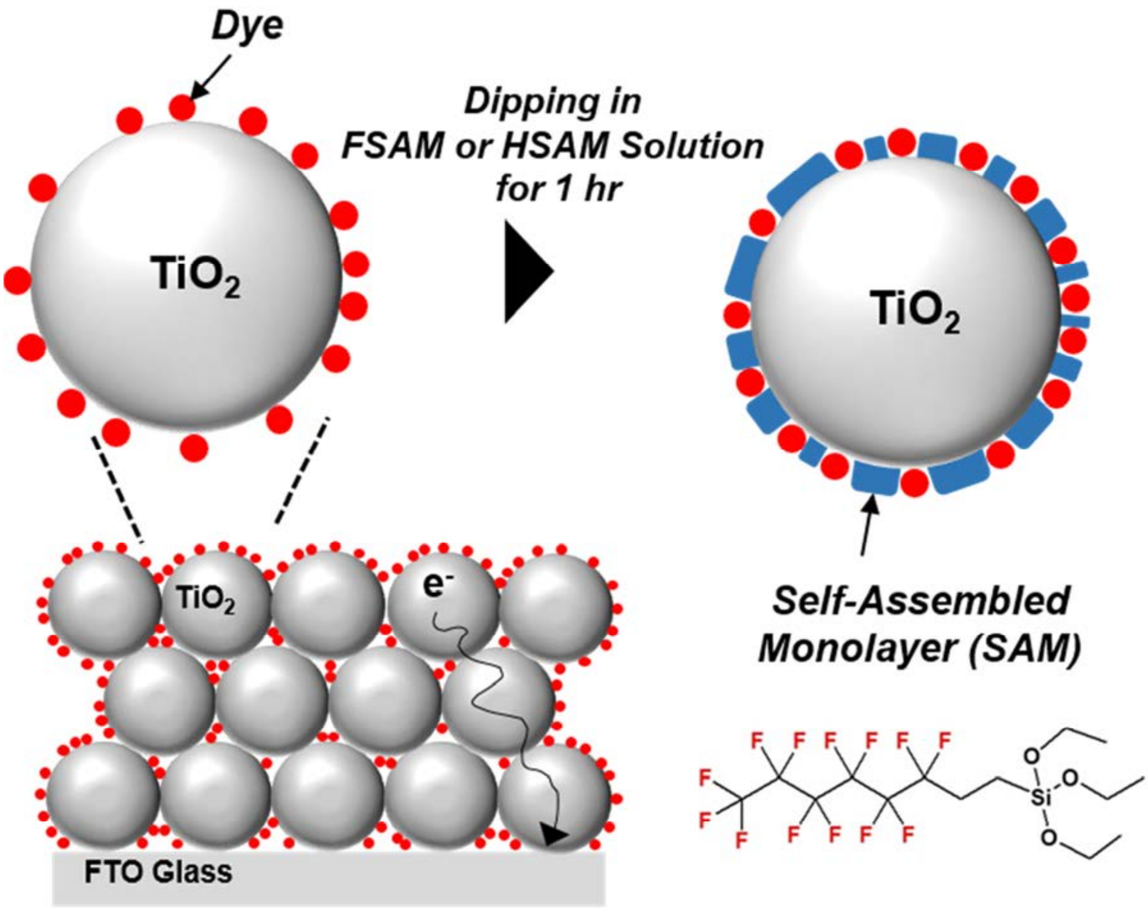
Surface modification of photoanode with superhydrophobic self-assembled monolayer for dye-sensitized solar cells

김태언 강용수*

한양대학교 에너지공학과

The superhydrophobic self-assembled monolayer (SAM) is introduced to increase the power conversion efficiency (PCE) on the surface of the TiO2 photoanode in dye-sensitized solar cells (DSCs). 1H,1H,2H,2H-perfluorooctyltriethoxysilane (FSAM) and triethoxyoctylsilane (HSAM) were deposited without loss of dyes via the sequential adsorption after dye (MK-2 organic dye) dipping process. The absorption spectra revealed that the aggregation peak of MK-2 dye at 370 nm decreased upon deposition of SAM, whereas the maximum peak at 480 nm increased in the order of reference < HSAM < FSAM. According to the chemical capacitance results collected by cyclic voltammetry, the SAM materials seem not to shift the TiO2 conduction band edge due to the small dipole moment of both FSAM and HSAM. Meanwhile, the impedance results imply that the SAM materials induced the reduction of recombination reaction rate in the order of FSAM > HSAM > reference attributable to their effects for TiO2 surface passivation. As a result, the FSAM-modified superhydrophobic photoanode exhibited a high PCE of over 9.5%, compared to 8.5 % for the reference without the SAM deposition, evaluated under 1 sun illumination, based on MK-2 and iodide redox couples in DSCs.


Dye
TiO2
Dipping in
FSAM or HSAM Solution
for 1 hr
TiO2
TiO2
e-
FTO Glass
Self-Assembled
Monolayer (SAM)
F F F F F F
F
F
F
F F F F
O
O
Si
O

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Electrochemical properties of TiO2 (001) plane photoanode in dye-sensitized solar cells with polymer electrolyte

편용범 김태언 강용수*

한양대학교 에너지공학과

Almost of (>94%) TiO2 structure consist of thermodynamically high stable (101) plane with low surface energy, 0.44 J/m2. However, (001) plane is more reactive because of higher surface energy of 0.90 J/m2 [1]. Therefore, the (001) plane is theoretically expected to increase photovoltaic conversion efficiency due to its more easily and tightly adsorbed dyes and reduced recombination by the high crystallinity [2]. In this work, we investigate the effects of the (001) plane in TiO2 photoanode on the photovoltaic performance in dye-sensitized solar cells based on polymer electrolyte. In particular, we emphasized the analysis of electrochemical properties of (001) plane in comparison with the (101) one in solid state dye-sensitized solar cells utilizing polymer electrolyte.[1] X. Q. Gong and A. Selloni, J. Phys. Chem. B, 2005, 109, 19560[2] H. G. Yang, C. H. Sun, S. Z. Qiao, J. Zou, G. Liu, S. C. Smith, H. M. Cheng and G. Q. Lu, Nature, 2008, 453, 638.

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Facile Electrochemical Deposition of Pd Flake Nanostructures and Their Superhydrophobicity and SERS activities

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충북대학교 화학과

나노 구조의 금속 표면은 벌크 금속과는 다른 독특한 물리적 및 화학적 성질을 가진다. 금속 나노 구조의 표면은 전기촉매, 초소수성 표면 및 표면 증강 라만 산란의 기판으로서 유용하게 응용되고 있다. 금속 표면의 특성은 구조의 모양과 크기에 의해 조절될 수 있기 때문에, 잘 정의된 모양과 크기를 가지는 나노 구조들을 형성시키려는 연구들이 많이 보고되었다. 본 연구에서는 형성되는 구조의 모양을 조절하기 위해 첨가해주는 계면활성제나 기판 표면의 전 처리 과정 없이, 금 표면 위에 직접 팔라듐 나노 구조를 전기화학적으로 석출하였다. 전기화학적 변수 중에서 구조의 성장 속도를 제어할 수 있는 전위를 조작하여 flake 타입의 모양을 형성하였고 전하량에 따른 구조의 성장과정을 검토하여 모양과 크기를 최적화시켰다. 구조의 성장과정에 따라 소수성을 나타내는 척도인 접촉각 및 표면 증강 라만 산란에 대한 활성이 다른 결과를 보였다. 가장 최적화된 0.04 C 의 전하량으로 형성된 나노 구조의 표면은 접촉각이 162° 으로 측정되면서 초소수성 성질을 가졌으며 표면 증강 라만 산란에서도 가장 높은 활성을 보였다. 본 연구의 결과를 통해 나노 수준에서도 세부적인 크기나 모양과 같은 요인들이 소수성 및 표면 증강 라만 산란의 활성을 결정한다는 것을 확인하였다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No.2012H1B8A2026112)]

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Effect of temperature and concentration on the Anodic Formation of Nanoporous Gold Films in Chloride Solutions

김민주 김종원*

충북대학교 화학과

나노다공성 금속 구조체는 균일한 표면 구조를 지니며, 매우 큰 표면적을 가진다. 전기화학적으로 구조가 안정하고 다양한 반응에서 높은 촉매적 활성을 보이기 때문에 많은 연구에 응용되고 있다. 나노다공성 구조를 형성하는 방법 중에서도 양극산화 반응은 비교적 간단하게 구조를 형성할 수 있다는 장점이 있다. 본 연구진은 염소 이온 존재 하에서 양극산화 반응을 이용하여 금 표면에 나노다공성 구조를 형성시켰으며, 가해주는 전위와 용액의 pH 가 구조에 미치는 영향을 관찰하여 보고하였다. 본 연구에서는 염소 이온 존재 하에서 양극산화 반응을 이용하여 나노다공성 금 구조를 형성할 때, 용액의 온도와 염소 이온 농도의 영향을 확인하였다. 온도와 농도가 증가함에 따라 AuCl4- 가 생성되는 양이 증가하였고, 금 산화물이 형성되는 정도가 달라진다. 각각 다른 조건으로 형성한 나노다공성 금 전극의 구조를 비교하여 생성 메커니즘을 자세히 알아보았다. 결과적으로, 온도와 농도 조건을 최적화시킨 후 시간을 조절하여 표면적이 매우 큰 나노다공성 구조를 형성시켰다. 주사 전자 현미경을 통해 형성한 나노다공성 구조의 표면을 관찰하였다. 또한, 각 조건에 따라 생성된 나노다공성 금 구조에 따른 글루코오스 산화 활성을 비교함으로써 나노다공성 금 구조의 인대와 구멍의 크기가 작을수록 글루코오스 산화 활성이 증가하는 것을 확인하였다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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발표코드: **ELEC.P-1180**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Shape-controlled Pt Nanostructures Prepared by Electrodeposition: Their Superhydrophobicity and SERS Activity

최수희 김종원*

충북대학교 화학과

Surface-enhanced Raman scattering and hydrophobicity have received much attention due to their applications as observe the vibrational modes of molecules and self-cleaning, respectively. SERS and hydrophobicity are both affected by metal surface structures. Therefore many researchers reported various metal nanostructures for highest activity of SERS and hydrophobicity. We investigate on the SERS activities and hydrophobicity at Pt nanostructure surfaces electrodeposited with different deposition charges on Au electrodes. The surface properties of Pt nanostructures depending on deposition charges were characterized by scanning electron microscopy and electrochemical surface area measurement, which were correlated to the SERS activities and hydrophobicity. SERS activity was investigated using 4-aminothiolphenol as a probe molecule. Pt nanostructures with deposited charge of 0.04 C exhibited the highest SERS activity. In addition, Pt nanotree structures exhibit excellent uniformity and reproducibility. The unique structure of Pt nanotrees results in a contact angle larger than 162°, so Pt nanotrees can be considered to be superhydrophobic substrates. The sharp sites of Pt nanostructure play a key role, whereas the electrochemical surface area does not significantly affect the SERS activities and hydrophobicity. [This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2012H1B8A2026112)]

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발표코드: **ELEC.P-1181**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Roles of graphene oxidation and their qualities in SnO2 /graphene composite anode materials for Li-ion batteries

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이화여자대학교 자연과학대학화학나노과학과 [1]이화여자대학교 나노과학부 [2]이화여자대학교 화학과

The various kinds of Li ion battery potential anode materials have been researched through combination of graphene and transition metal oxides. However, the degree of graphene oxidation in transition metal oxide/graphene composite anode is incomplete. We synthesized various kinds of carbon coated SnO2 nanoparticles by sol-gel method. It showed that the different performances followed by starting carbon sources (natural, artificial graphite) and oxidation rates. This phenomena is strongly related to Li ion diffusion time and initial discharge (litiation) capacities. These fundamental studies of oxidation rates of graphene and transition metal oxides hybrids can give help to boost up commercialization of next generation LIB anode electrodes.

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발표코드: **ELEC.P-1182**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrodeposited WO3 Film on Various Metal Substrates for Photoelectrochemical Water Splitting

김윤옥 강순형*

전남대학교 화학교육과

Electrodeposited WO3 thin films were prepared on the W, Ti, and Nb metal substrates in strongly acidic solution containing a tungsten precursor of (0.025 M sodium tungstate dihydrate powder (Na2WO4?2H2O)) and by varying the applied potential. The applied potential determined the thickness and crystallite size of the deposited WO3 thin films, irrespective of the metal substrate. The thickness and crystallite size of the films, as well as the total consumed electric charge (Q), increased as the applied potential was increased from -0.27 to -0.47 V. Conversely, the photoelectrochemical (PEC) activity declined as the deposition potential increased; the optimal performance was achieved at a deposition potential of -0.27 V for all metal substrates. This potential generated a porous WO3 film or a very thin WO3 layer composed of small nanoparticles, both of which were favorable for electrolyte penetration leading to enhanced charge transport/transfer behavior and providing a large contact area for the electrolyte. Furthermore, the PEC performance of WO3 on the W substrate was higher than those on the Ti and Nb substrates because of the homogenous composition of the W substrate that resulted in the least lattice disturbance. Thus, the maximum photocurrent density of 1.68 mA/cm2 at 1.5 V (vs. saturated Ag/AgCl) with an IPCE of 31% at 330 nm was obtained with the electrodeposited WO3 film grown at a deposition potential of -0.27 V on the W substrate. The charge-transport and charge-transfer behavior of the electrodeposited WO3 film were respectively discussed based on linear sweep voltammograms and electrochemical impedance spectroscopy.

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발표코드: **ELEC.P-1183**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Inverse Opal SnO2 based sensitized solar cells

<u>윤건</u> 강순형*

전남대학교 화학교육과

Nowadays, the exploration of new photo electrode architectures to improve the light-harvesting and charge-collection properties of sensitized solar cells and related devices has been regarded as a challenging work. Here, we demonstrate the synthesis of the inverse opal SnO2 film for sensitized solar cells by gravimetric sedimentation method, subsequently followed by the spin-coating or drop casting method. Using 430 nm poly styrene (PS) beads, we synthesized the SnO2 inverse opal structure showing the photonic crystal effect. These results were confirmed using Field-emission scanning electron microscopy, X-ray diffraction and ultraviolet-visible spectrophotometer. Based on these results, SnO2 inverse opal film was applied to sensitized solar cell to identify their unique properties and evaluated exploring the photocurrent-voltage measurement.

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발표코드: **ELEC.P-1184**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Sonochemical Preparation of Pt/MoS_2 as Electrocatalyst for Methanol Oxidation Reaction

이은직 조승익[1] 곽진수[1] 김근오[1] 박현욱[1] 권영욱[1,*]

성균관대학교 나노과학기술협동학부 [1]성균관대학교 화학과

In this work, we synthesized molybdenum disulfide (MoS_2) supported Pt nanoparticles (NPs) by ultrasound-assisted polyol method. Through the structural characterization, we found that our Pt/MoS_2 sample has uniform sized Pt NPs (2~3 nm) and well-dispersion on support. Electrochemical analyses of Pt/MoS_2 were investigated by rotating disk electrode (RDE) measurement. Compared with commercial Pt/C, Pt/MoS_2 showed higher catalytic performance and CO tolerance for methanol oxidation reaction (MOR). As a result, we demonstrated that our materials could be novel electrocatalyst for direct methanol fuel cells.

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발표코드: **ELEC.P-1185**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Shape-controllable Pt nano particles modified ITO glass for making a Glucose sensor

김정현 손용근*

성균관대학교 화학과

Since 1990s, diabetes has become a highly prevalent disease in Korea. Unfortunately, almost half of the diabetics between 30 to 44 years old are not recognized themselves are patients. So, a fast and convenience blood glucose testing method in daily life is necessary. Platinum is the one of the most widely used material in various glucose sensors. Surface area of Platinum is a key point to influence the sensitivity of the glucose sensor. Therefore, we made various shape of controllable platinum particles on ITO glass by using pulsed electrodeposition method for making a glucose sensor. Pt nano particles were fabricated in the ITO glass by pulsed electrochemical deposition method. In our work, different shapes and sizes Pt nano particles could be obtained by only changing the pulse time at the same potential. After the Pt modified ITO electrode fabricated, glucose oxidase and nafion were dropped on the electrode in sequential to form the sensing and protecting layers. This work was supported by the Component and Material Technology Development Program (No. 10046641, Development of Electronic Ink and Coating Materials for Leak Monitoring of the Hazardous Chemicals), funded by the Ministry of Trade, Industry & Energy (MI, Korea)

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발표코드: **ELEC.P-1186**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Photoassisted enhancement of the electrodeposition of a Copper(I) Oxide film

정재구 김용국 김승훈 노영철 채원석*

대진대학교 화학과

Electrodeposition of a cuprous oxide (Cu2O) thin film was studied to find the optimum conditions under which the deposition temperature could be lowered. Cu2O films were electrochemically deposited on FTO using Chrono amperometry in an aqueous solution. It was confirmed that the characteristics of cuprous oxide (Cu2O) using linear sweep voltammetry(LSV). A simple and novel deposition cell was designed to allow simultaneous thermostating and polychromic illumination.Under illumination, the Cu2O film deposition was significant, even at a temperature lower than that used under dark conditions. X-ray diffraction (XRD) analysis have confirmed that these films were indexed as cubic symmetric structured pure Cu2O (JCPDS: 05-0667), and UV-visible absorption spectra measurements have shown an optical band-gap energy of 2.5 eV.

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발표코드: **ELEC.P-1187**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Improved electrochemical performance of $LiFeMnPO_4$ through boron polyanion substitution

신병철 이한솔 이영일*

울산대학교 화학과

Olivine cathode has been identified as an promising new cathode material for Li-ion batteries. Especially, $LiFeMnPO_4$ is a desirable cathode material for lithium-ion batteries, due to its high theoretical capacity and its favorable chemical component, which are abundant, inexpensive and non-toxic. The crystal structure of synthesized samples was characterized by SEM, EELS and transmission electron microscopy. The electrochemical measurement of the substituted materials are performed with half cell and structural investigations of cathode material XRD and XPS.

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발표코드: **ELEC.P-1188**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Determination of Bisphenol A at Graphene Titania-Nafion Composite Modified Electrode

김동환 이원용*

연세대학교 화학과

Bisphenol A(2,2-bis (4-hydroxyphenyl) propane, BPA) is used to make plastic products. It is also well known for applications on epoxy resin, plastic food containers, drink packaging and so on. Unfortunately, many studies confirm that BPA is an endocrine disruptor causing abnormal hormone activities. Therefore, it is important to develop a simple and highly sensitive detection method for the determination of BPA in food and the environment.Bisphenol A underwent a totally irreversible oxidation in this system. To maximize the oxidation current of BPA, we used graphene-doped titania-Nafion composite modified glassy carbon electrode. Due to its excellent electron transfer properties and high specific area, graphene has a variety of applications in electrochemical sensors. It is possible to modify a glassy carbon electrode with graphene by simple casting and drying. Compared to the bare glassy carbon electrode, the graphene modified electrode exhibited more facile electron transfer in addition to enhanced oxidation current. We used cetyltrimethylammonium bromide (CTAB) that exhibits enhancement effect on the oxidation current of BPA. Optimization of the experimental condition for the determination of BPA was conducted. This method indicates the potential of the application of graphene modified electrode in designing simple and sensitive sensors for a rapid on-site monitoring of BPA from food packaging materials.

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발표코드: **ELEC.P-1189**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly sensitive electrochemical hemoglobin A1c detection based on boronic acid functionalized nanoparticles

안광수 이원용*

연세대학교 화학과

As a chronic disease, diabetes mellitus requires continuous care including periodical glucose monitoring because there isn’t any cure and it depends on many complex factors. Several diabetes monitoring methods were reported and done with glucose in blood; many of them reflect short-term (real-time) glucose level and sometimes miss the peak concentration. To care diabetes patients, long-term glucose monitoring is also important. Hemoglobin A1c (HbA1c), the most effective marker for diabetes diagnosis and care, is formed through non-enzymatic addition of glucose to the HbA. It presents plasma glucose level of the previous 1-3 months and well-known relationship between HbA1c and plasma glucose makes possible to monitor long-term glucose level in blood stream. The biomarker has great advantages than the others, including convenience, preanalytical stability and less perturbation. By these reasons, American Diabetes Association recommends measuring HbA1c at least two times a year in patients who need stable glycemic control.In this study, we developed new method which can determine HbA1c concentration by electrochemical impedance spectroscopy (EIS) technique with high sensitivity. Boronic acid is introduced to make binding with two cis-diol groups at surface of the minor hemoglobin component. Furthermore, to ensure high sensitivity, boronic acid functionalized nanoparticles were used as signal amplifier.[1] Am. Diab. Assoc., Diabetes Care 37 (2014) S14?S80[2] A. -G. Sofronescu, L. M. Williams, D. M. Andrews, Y. Zhu, Clin. Chem. 57 (2011) 153-157[3] G. Liu; S. G. Iyengar; J. J. Gooding, Electroanalysis 24 (2012) 1509?1516[4] Y. -K. Lyu, K. -R. Lim, B. Y. Lee, K. S. Kim and W. -Y. Lee, Chem. Commun. (2008) 4771-4773

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

Amperometric Ion Selective Sensors for Sodium and Potassium Detection in Biological fluids

DIBAFARHANASHARMIN 이혜진*

경북대학교 화학과

Among the electrolytes present in human body, sodium and potassium hold utmost significance because of their involvement in a number of metabolic processes. In this presentation, we demonstrate the development of amperometric ion sensors for detecting sodium and potassium in diluted blood and urine samples. Our attempt is to investigate prospective biological application of ion selective sensors featuring a microhole-liquid/gel interface in conjunction with sodium and potassium selective ionophores. The detection of sodium and potassium in diluted biological fluids were carried out using cyclic and differential pulse stripping voltammetry.

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발표코드: **ELEC.P-1191**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Non Enzymatic Hydrogen Peroxide Sensor Based on Hierarchical Structure of Metal Alloy

이원철 심윤보* 문종민[1]

부산대학교 화학과 [1]부산대학교 생명과학과

A novel amperometric sensor for hydrogen peroxide was developed through a hierarchical structure of metal alloy (Au, Zn, Ni, Cu, Co, etc.) on the conducting polymer layer. Poly-3′-(carboxylic acid)-2,2′:5′,2″-terthiophene (pTTCA) and poly-3′-(benzoic acid)-2,2′:5′,2″-terthiophene (pTTBA) were used as conducting polymer. The sensor probe was fabricated by electrochemically depositing metal alloy using normal pulse voltammetry (NPV) and chronoamperometry (CA). The sensor probe was characterized using cyclic voltammetry, chronoamperometry, electrochemical impedance spectroscopy and X-ray photoelectron spectroscopy. SEM and EDS were used to determine the surface characteristics and the ratio of metal alloy. Experimental parameters were optimized in terms of pH, temperature, applied potential, deposition potential and deposition time. The proposed sensor exhibited stability and a linear dynamic range of 10 μM to 10 mM.

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발표코드: **ELEC.P-1192**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced stability of enzyme electrode for glucose sensor and biofuel cell as anode in screen printed carbon electrodes (SPCEs)

전원용 김기훈 조남현[1] 김수지[1] 최영봉[1] 김혁한[1,*]

단국대학교 나노바이오의과학과 [1]단국대학교 화학과

Stability of enzyme electrode for glucose sensor and biofuel cell as anode was enhanced by co-electro-polymerization after drying the enzyme and mediator on screen printed carbon electrodes (SPCEs). We report the enhanced stability of enzyme electrode using the cyclic voltammogram (CV) technique on SPCEs. The surface morphology of the co-electro-polymerized the enzyme and mediator on SPCEs was examined by scanning electron microscopy (SEM). The electrical signal for stability of enzyme electrode and catalytically current were monitored by I-T curve and CV. Our study have shown enhanced stability of enzyme electrode. Co-electro-polymerization method will provide enhanced stability of enzyme electrode for real time monitoring of glucose sensing. Also, it will increase lifetime of enzymatic biofuel cell.

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발표코드: **ELEC.P-1193**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrochemical Quantitative Analysis of Uric Acid using Direct Electron Transfer (DET) Method

이수정 오인돈 이성민 최영봉 김혁한*

단국대학교 화학과

High concentration of uric acid(UA ; $C_5H_4N_4O_3$) in human body have been exposed to many diseases, such as gout, hyperuricemia, Lesch-Nyhan syndrome, arthtitis, diabetes, high cholesterol, renal, neurological, cardiovascular and kidnet diseases. We report electrochemical quantitative analysis of UA using the chitosan-CNT adsorbed the indium tin oxide(ITO) electrode. Uricase was conjugated by EDC/NHS onto the chitosan-CNT adsorbed ITO electrode. Uricase-bonded chitosan-CNT/ITO electrode was observed by scanning electron microscopy (SEM). Electrochemical characterizations of uricase/chitosan-CNT/ITO electrode were measured by cyclic voltammograms (CV) and different pulsed voltammograms (DPV). The resulting currents were linearly related with range of 0 ~ 5mM as concentration of UA. The present fabricated uricase/chitosan-CNT/ITO electrode with a selectivity and sensitivity is promising for diagnosis early

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발표코드: **ELEC.P-1194**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

An Improved Dual Amperometric/Potentiometric Microsensor for the Real-Time Simultaneous Measurements of NO/K^+ or NO/Ca^{2+}

문정미 김이슬 이종목 이영미*

이화여자대학교 화학나노과학과

The development of a dual microsensor for simultaneous measurements of two closely linked biological species is demonstrated. In particular, the sensor targets nitric oxide (NO)/potassium ion (K^+) or NO/calcium ion (Ca^{2+}). Nitric Oxide is known to be closely related to K^+ or Ca^{2+} in biological system. For instance, NO/cGMP (guanosine 3’, 5’-cyclic monophosphate)/K^+ channel pathways have been reported to be involved in many biological processes including vasodilation. In addition, there is a basic pathway for the stimulation of cNOS (constitutive NO synthase), which involves the release of Ca^{2+} from subsarcolemmal storage sites. Endothelial receptors for a variety of ligands stimulate Ca^{2+} release and generate subsequent NO production. Due to these close linkages between NO and Ca^{2+}, as well as NO and K^+, it is of great interest to analyze NO/Ca^{2+} and NO/K^+ concurrently. A dual microsensor possesses two microdisks: one disk is used for amperometric NO measurement and the other is used for potentiometric ion(K^+ or Ca^{2+}) measurement. Sensor performances, such as sensitivity and selectivity, are characterized and the results show the possibility for the biological application. As-prepared sensor is applied for the NO/K^+ or NO/Ca^{2+} measurement at biological organ tissues, rat kidney. The level of NO and each ion are clearly location dependent over the kidney surface and it is considerably matched with results studied by various method reported previously. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (2014R1A2A2A05003769).

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Mechanism Study of Oxygen Reduction Reaction at Porous Pt Layer Depending on Its Porosity Using Scanning Electrochemical Microscopy (SECM)

조윤빈 이종목 이영미*

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The search for new catalyst material systems for high-performance oxygen reduction reaction (ORR) is important due to the wide range of its applications for amperometric oxygen sensing, fuel cell, etc. ORR, however, is a sluggish reaction and requires a high overpotential. The best ORR catalyst material today is platinum, and its various nanostructures have been fabricated and utilized to enhance the catalytic activity via the surface area increase.In this study, highly porous Pt layers with two different porosities are electrochemically deposited on Pt microdisk (diameter = 10 μm) electrodes, and the ORR at these porous structures is investigated in acidic solution using feedback and tip generation-substrate collection (TG-SC) modes of scanning electrochemical microscopy (SECM). While ORR takes place at the modified tip electrode, a constant potential enough to oxidize ORR intermediate is applied to the 76 μm Pt substrate electrode in order to investigate the ORR mechanism depending on the catalysts' porosity. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (2014R1A2A2A05003769).

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Measurement of Ascorbic Acid Using Various Metal Oxide Nanocomposites

유아름 김수진 이종목 김명화[1] 이영미*

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

In this study, two different metal oxide nanostructures were synthesized and characterized as electrocatalysts for electrochemical sensing of ascorbic acid (AA). AA has been realized as an important antioxidant, enzyme cofactor for biosynthesis, natural antihistamine, etc. Therefore, accurate quantification of AA in various samples is highly required for the better understanding of its function. First, highly crystalline iridium oxide nanofibers (IrO_xNFs) were synthesized by electrospinning process. Second, ruthenium oxide nanowires (RuO_2NWs) were grown on electrospun titanium oxide nanofibers (TiO_2NFs) by chemical vapor deposition (RuO_2NWs-TiO_2NFs). The morphology and structure of both materials were characterized by FE-SEM, XRD. For the electrochemical characterization, three-electrode cell was used with a glassy carbon electrode loaded with the synthesized IrO_xNFs or RuO_2NWs as the working electrode and a saturated calomel electrode (SCE) as the reference electrode, and a coiled platinum wire as the counter electrode. Electrochemical activities of these metal oxide materials for electrochemical oxidation of AA are characterized by linear sweep voltammetry (LSV), constant potential amperometric experiments (i-t). We also confirmed the selectivity over acetaminophenol (AP), dopamine (DA), glucose, NADH, and uric acid (UA) at their physiological levels using i-t and differential pulse voltammetry (DPV). In addition, these electrodes were applied for AA measurements in urine and vitamin tablet samples. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (2014R1A2A2A05003769).

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Optimized measurement of gaseous neurotransmitters with a needle-type electrochemical microsensor at inner cortex area of dysfunctional rat brain

하예진 이종목 이영미*

이화여자대학교 화학나노과학과

Nitric oxide (NO) and carbon monoxide (CO) play physiologically important roles as signaling molecules and their biological functions are similar to each other. Due to technical difficulties, however, exact functional relationship between NO and CO has not been explained clearly yet. To better understand the dynamic and close interactions of NO and CO in brain, we fabricate an improved needle-type amperometric dual microsensor. The sensor consists of a planar working electrode possessing two Pt microdisks (diameter of each disk = 50, 76 μm) electrodeposited with second metals (Pt black, Au) and a Ag/AgCl reference electrode. Each disk surface of the working electrode is covered with gas permeable polymer membrane to obtain the selectivity to only NO or CO over common biological interfering species. The NO/CO dual sensor is applied to monitor dynamic changes of NO and CO levels underneath of the rat brain surface under normal or epileptic conditions. The epilepsy is acutely induced by 4-aminopyridine (4-AP) injection into the brain tissue. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2014R1A2A2A05003769).

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Fabrication and characterization of an electrochemical triple microsensor for simultaneous measurements of CO, NO and O_2

김진후 나지선 이영미*

이화여자대학교 화학나노과학과

Carbon monoxide (CO), nitric oxide (NO) and oxygen (O_2) play important roles in regulating fundamental physiological functions. Endogenously produced CO and NO gases function as signaling molecules similarly to control a certain biological processes such as vasodilation and neurotransmission. In addition, the biosynthetic procedure of CO and NO is alike and enzymes in this synthetic system require O_2 and NADPH to be activated. In this study, we demonstrate the development of an amperometric CO/NO/O_2 triple microsensor which can measure these gases simultaneously. The sensor is made of a triple platinum working electrode (WE1, WE2 and WE3, with 76, 50, and 25 μm in diameter, respectively) and Ag/AgCl counter/reference electrode. The triple WE Pt disks are etched to form micropores in shape and then electrodeposited with porous platinum layer. The largest WE1 for CO sensing is modified additionally with electrodeposition of tin. Silanizing solution is dispensed over each disk, lastly. Modification of three sensing disks with different surface treatments gives apparently different selectivity to each gas at WE1, WE2, and WE3. Sensor performances, such as sensitivity and selectivity, are characterized and the results show the possibility of the triple sensor for the biological applications. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (2014R1A2A2A05003769).

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Amperometric Detection of Ascorbic Acid with Porous Ruthenium Oxide

양예진 이영미 이종목*

이화여자대학교 화학나노과학과

To control the chance of electron transfer (ET) between the electrode surface and electroactive species with slow ET rate might be possible by controlling the continuity of nano-structure. It is also well-known that glucose has relatively slow ET rate compared to ascorbic acid (AA). Previously, we have reported glucose sensing with porous ruthenium oxide. Here, we have tried to determine AA rather than glucose by controlling the continuity of porous ruthenium oxide. Ruthenium oxide on gold wire (d=25 μm) was prepared by electrodeposition with various deposition cycles (4, 10, 15, 30, 45, 60 cycles) and the morphology was characterized by field emission scanning electron microscope (FE-SEM). Among various RuOx-n (n: number of deposition cycles) RuOx-10 showed the largest current response ratio of AA vs. glucose in the amperometric experiments. In amperometric i-t curves of AA oxidation, RuOx-10 showed sensitivity of 990 μA $mM^{-1}cm^{-2}$ for the linear range of zero to 10.0 mM with response time of 0.2 s and detection limit of 0.04 mM without any response to other intereferences.

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Amperometric Ascorbic Acid Sensing Based on Single Crystalline Iridium-Ruthenium-Vanadium Mixed Metal Oxide Nanowires

김현영 조아라 정지혜[1] 이영미 김명화[2,*] 이종목[*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 수학교육과 [2]이화여자대학교 화학 나노과학과

In this presentation, we observe the electrochemical activity of $Ir_{1-x-y}Ru_xV_yO_2$ (x+y=1) on Au nanowires ($Ir_{1-x-y}Ru_xV_yO_2$ NWs) prepared through a vapor-phase transport process by adjusting the different mixing ratios of IrO_2, RuO_2, and V_2O_2 precursors. The $Ir_{1-x-y}Ru_xV_yO_2$ NWs show selective electrochemical activity for ascorbic acid (AA) oxidation at pH 7.4. The catalytic activities of $Ir_{1-x-y}Ru_xV_yO_2$ NWs for AA oxidation vary depending on the different ratio of precursors. The appropriate potential for AA oxidation was determined by linear sweep voltammetry (LSV). Amperometric measurement of AA shows the highest sensitivity of 245 $nAmM^{-1}$ in 0.1 M phosphate buffer solutions (PBS, pH 7.4) by immersing 300 μm depth of $Ir_{1-x-y}Ru_xV_yO_2$ NW, where the selectivity against possible interferents is observed including actamidophenol (AP), uric acid (UA), dopamine (DA), glucose and NADH.

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Fabrication of an acid warning sensor using Acetylene Black/Polyaniline composite

장혜림 손용근*

성균관대학교 화학과

Hydrochloric acid is the one of the most used acids. Leak accident of the acid has occurred frequently at many places in industry. Therefore it is important to detect even small quantity of the acid for protecting fatal disaster. Polyaniline has known to change its conductivity when it is doped with proton acids. Reduced polyaniline(R-PANI) shows good insulator character, but after doping with proton acid the doped polyaniline(D-PANI) present good electrical conductivity. Also, the solubility to organic solvent of R-PANI is better than that of D-PANI. So, in this work, we chose R-PANI to fabricate acid sensor. However, when low concentration acid attacks the R-PANI, the switching speed of conductivity change is not high enough to detect instantly. Therefore, we made acetylene black/R-PANI composite to improve the change speed in electrical conductivity appearing after doping hydrochloric acid. First, we made acetylene black/R-PANI composite solution with different concentration of the acetylene black and fabricated devices. We observe the change of electrical conductivity during hydrochloric acid doping process. We obtained dramatical changes in conductivity when it was doped with low concentration hydrochloric acid.

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Amperometric Irinotecan Sensors in Conjunction with a Microhole Interface Featuring Water/polymer Composite Membranes

김혜림 이혜진*

경북대학교 화학과

본 포스터는 irinotecan 항암제가 서로 섞이지 않는 두 전해질 (수용성 액체/유기성 젤) 계면에서 이동하는 반응에 따라 전류값의 변화를 측정하는데 기초를 둔 센서 개발에 관한 연구 결과를 나타냈다. 물과 polyvinylchloride-2-nitrophenyl octyl ether (PVC-NPOE) 고분자 젤을 이용하여 단일 마이크로홀 사이에 계면을 형성하고, 물에 존재하는 irinotecan 이온이 전이하는 정도에 따라 전류의 변화가 일어나는 것을 순환전압전류법(cyclic voltammetry)과 시차 펄스 벗김 전위법(difference pulse stripping voltammetry)으로 정량적으로 분석하였다. 또한, 개발한 센서를 실제 시료(세럼)에서의 미량의 topotecan 항암제 검출에 적용한 결과를 나타내었다.

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Electrochemical detection of B-type natriuretic peptide (BNP)

한혜연 김은미[1] 이혜진[1,*]

경북대학교 화학 [1]경북대학교 화학과

본 포스터에서는 표면샌드위치 복합체 형성을 통하여 BNP 단백질을 전기화학적으로 검출한 결과를 나타냈다. 이를 위해 금 나노입자를 도포한 탄소 칩에 BNP 와 특이적으로 결합하는 앱타머를 고정하고, BNP 와 alkaline phosphatase(ALP)로 컨쥬게이션한 항체를 반응시켜 복합체를 형성한 후 기질인 4-aminophenylphosphate monosodium salt (APP) 와 반응시켜 전기화학 신호를 측정한 결과를 나타냈다. 순환전압전류법과 시차펄스 전위법을 이용하였다.

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Electrochemical biosensor for simultaneous determination of dopamine based on electrochemically reduced GO-Ferulic acid

설희진 배시라 전승원*

전남대학교 화학과

Reported herein are the synthesis of graphene using the modified Hummers method and its application for the electrochemical detection of dopamine. Graphene oxide-ferulic acid (GO-FA) was formed from the condensation reaction of GO and ferulic acid. The GO-FA was characterized via Fourier transform infrared spectroscopy (FT-IR), ultraviolet-visible spectroscopy (UV-Vis spectroscopy), and scanning electron microscopy (SEM). The electrochemical reduction of GO-FA (ERGO-FA) can be employed for the electrochemical detection of dopamine (DA). The electrochemical detection of dopamine was verified through the CV, DPV, and amperometric techniques, in a 0.1 M citrate buffer solution (pH 6.0). The influence on the pH (3.99-9.02) of the 0.1M citrate buffer solution of ERGO-FA/GCE on the oxidation of DA was determined, and interference experiments using interfering substances such as serotonin (5-HT), glucose, ascorbic acid (AA), H2O2 and uric acid (UA) were conducted. The detection limit of DA was found to be 0.188 μM (where s/n=3), and the linear ranges were 0.6-1000 μM at the ERGO-FA modified glassy carbon electrode (GCE).Keywords: Ferulic acid, condensation reaction, electrochemical reduction (ER), electrochemical detection, dopamine

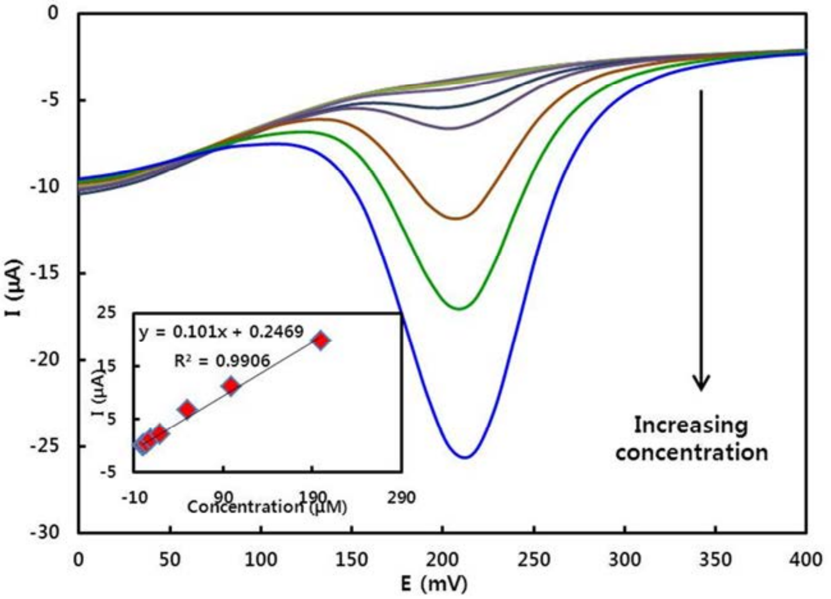

Figure. DPVs of ERGO-FA/GCE at various concentrations (0.5-200 μM) of DA in a 0.1M citrate buffer solution (pH 6.0), at a 50 mV/s scan rate. Plots of oxidation currents vs. concentrations

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Seaweed as a precursor for heteroatoms-containing highly porous carbon as a electrocatalysts for the oxygen reduction reaction

송민영 유종성* 양대수 박현열 김창기 배은진

고려대학교 신소재화학과

The oxygen reduction reaction (ORR) is one of the key reactions occurring in fuel cells, and to date mostly platinumbased catalysts or platinum alloys have shown the best electrocatalytic activity as cathode material for the ORR. However, wide-ranged applications of fuel cells are greatly hampered mainly as a result of the high cost and scarceness of platinum metal and its sluggish kinetics toward the ORR. To overcome these issues, much effort has been devoted to finding alternatives for platinum-based electrocatalysts by using nonprecious metals and various heteroatom-doped carbonaceous materials. we report the template-free pyrolysis of easily available natural seaweed, Undaria pinnatifida, as a single precursor, which results in “seaweed carbon” (SCup). Interestingly, thus-obtained SCup not only contains heteroatoms such as nitrogen and sulfur in its framework, but it also possesses a well-developed porous structure with high surface area. The heteroatoms in SCup originate from the nitrogen- and sulfur-containing ingredients in seaweed, whereas the porosity is created by removal of salts inherently present in the seaweed. These essential and fundamental properties make seaweed a prime choice as a precursor for heteroatom-containing highly porous carbon as a metal-free efficient electrocatalyst. As-synthesized SCup showed excellent electrocatalytic activity in the oxygen reduction reaction (ORR) in alkaline medium, which can be addressed in terms of the presence of the nitrogen and sulfur heteroatoms, the well-developed porosity, and the electrical conductivity in the carbon framework. The pyrolysis temperature was a key controlling parameter that determined the trade-off between heteroatom doping, surface properties, and electrical conductivity. In particular, SCup prepared at 1000 oC showed the best ORR performance. Additionally, SCup exhibited enhanced durability and methanol tolerance relative to the state of the art commercial Pt catalyst, which demonstrates that SCup is a promising alternative to costly Pt-based catalysts for the ORR.

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A Highly Efficient Pt Electrocatalyst Prepared by γ-Irradiation for Cathodic Oxygen Reduction Reaction

박현열 양대수 송민영 박종덕 강동현 유종성*

고려대학교 신소재화학과

A simple, efficient and scalable approach is developed for synthesis of Vulcan XC-72 (VC) supported Pt nanoparticles (NPs) that combines homogeneous deposition (HD) of Pt complex species through generation of OH^- ions by in situ hydrolysis of urea and subsequent reduction by the reducing species generated from radiolysis of water by γ-rays. This method not only avoids addition of any commonly used reducing agent but also offers more uniform homogeneous dispersion of Pt NPs with much smaller particle size. Thus when used as cathode catalyst for proton exchange membrane fuel cell, the synthesized VC supported Pt NPs demonstrated excellent electro-catalytic activity, higher Pt utilization efficiency, and considerably improved fuel-cell polarization performance compared to Pt catalysts prepared with other synthesis strategy such as conventional $NaBH_4$ reduction, HD-EG method and commercial Pt catalyst. The combined HD-γ-irradiation strategy is found to be simple with mild synthesis condition and hold promises to impact on synthesis approaches for preparation of Pt-based catalysts for fuel cells.

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Highly efficient metal-free phosphorus-doped platelet ordered mesoporous carbon for electrocatalytic oxygen reduction

양대수 송민영 박현열 김성수 유종성*

고려대학교 신소재화학과

Platinum-free electrocatalysts especially, various heteroatom-doped carbon nanostructureshave attracted particular attraction as plausible solution for commercializing fuel celltechnology. In this direction, novel phosphorus-doped platelet ordered mesoporous carbon(P-pOMC) is developed for the first time as metal-free electrocatalyst for alkaline oxygenreduction reaction. The P-pOMC is synthesized by nanocasting method using plateletordered mesoporous silica as template. Various characterizations reveal that the P-pOMCmaterials have covalently bound P atoms with carbon framework for facilitation of oxygenreduction reaction (ORR) and also have very high surface area with uniform distribution ofshort mesoporous channels for unhindered mass transfer. Combination of P doping andexcellent surface properties empowers the newly-developed P-pOMC catalyst to show highORR activity nearly equal to that of state of the art Pt catalyst along with superior long-termstability and excellent methanol tolerance.

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Simultaneous determination of Cd (II), Pb (II), Cu (II), and Hg (II) ions using Chronocoulometry

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부산대학교 화학과

The determination of Cd (II), Pb (II), Cu (II), and Hg (II) ions is performed with a blend of 3,4-diamine-5:2,5:2-terthiophene (DATT) and graphene oxide (GO) modified screen print carbon electrode (SPCE). Experimental variables that have an effect on the peak current, such as pH, deposition time, temperature, DATT concentration, GO to DATT ratio, and Nafion? concentration were optimized. Interference effects of other heavy metal ions were also tested at various electrolytes. Chronocoulometry (CC) was performed to analyze heavy metal ions by scanning the potential between -1.3 and +0.3 V after preconcentration in an acetate buffer solution. Calibration plots using DATT-GO/ Nafion? modified SPCE were obtained for each metal ion in the dynamic range from 1ppb to 10ppm. The detection limits for Cd (II), Pb (II), Cu (II), and Hg (II) ions were determined to be ~0.1 ppb. This method was investigated to analyze the heavy metals in real samples like tap water.

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High CO Tolerance Performance of Pt-Mesoporouos Metal Oxide Films for Methanol Oxidation Reaction by Strong Metal-Support Interaction

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We report a highly improved kinetics with superior CO tolerance in an electrocatalytic methanol oxidation reaction (MOR) on platinum-mesoporous metal oxide composite thin films. Pt-mesoporous metal oxide composite films were synthesized by two-step process. First, mesoporous tin oxide thin films (MSnTFs) and mesoporous gallium oxide thin films (MGTFs) with wormlike structure were prepared by sol-gel method. And then, Pt is deposited into the pores of MSnTFs and MGTFs by using electrochemical deposition method.In the results of electrochemical experiments as CO stripping and MOR, these samples showed the meaningful phenomena. Interestingly, we observed the high current pre-peak of CO stripping at 0.25 V, much lower potential than that of main peak, according to oxidation of weaker adsorbed CO molecules with Pt affected by mesoporous metal oxide thin film. In addition, these results were related to the explanations of effective enhancement of MOR. Pt-MGTFs and Pt-MSnTFs showed interesting MOR shape and much increased catalytic effiiency compared with only mesoporous Pt thin films. The properties of Pt-MSnTFs and Pt-MGTFs were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS) before and after deposition of Pt. From those analyses, we confirmed that strong metal support interaction (SMSI) between Pt and mesoporous metal oxides and significant changes of the electronic properties of Pt which could support the results of electrocatalytic activities.

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Electroreduction-based electrochemical-enzymatic redox cycling for detection of cancer antigen 15-3 using graphene oxide-modified indium-tin oxide electrodes

박선화 양해식*

부산대학교 화학과

We compare herein biosensing performance of two electroreduction-based electrochemical-enzymatic (EN) redox-cycling schemes [the redox cycling combined with simultaneous enzymatic amplification (one-enzyme scheme) and the redox cycling combined with preceding enzymatic amplification (two-enzyme scheme)]. To minimize unwanted side reactions in the two-enzyme scheme, β-galactosidase (Gal) and tyrosinase (Tyr) are selected as an enzyme label and a redox enzyme, respectively, and Tyr are selected as a redox enzyme label in the one-enzyme scheme. The signal amplification in the one-enzyme scheme consists of (i) enzymatic oxidation of catechol into o-benzoquinone by Tyr and (ii) electroreduction-based EN redox cycling of o-benzoquinone. The overall signal amplification in the two-enzyme scheme consists of (i) enzymatic conversion of phenyl β-D-galactopyranoside into phenol by Gal, (ii) enzymatic oxidation of phenol into catechol by Tyr, and (iii) electroreduction-based EN redox cycling of o-benzoquinone including further enzymatic oxidation of catechol to o-benzoquinone by Tyr. Graphene oxide-modified indium?tin oxide (GO/ITO) electrodes, simply prepared by immersing ITO electrodes in a GO-dispersed aqueous solution, are used to obtain better electrocatalytic activities toward o-benzoquinone reduction than bare ITO electrodes. The detection limits for mouse IgG, measured with GO/ITO electrodes, are lower than when measured with bare ITO electrodes. Importantly, the detection of mouse IgG using two-enzyme scheme allows lower detection limits than that using one-enzyme scheme, because the former gives higher signals at low target concentrations although the former gives lower signals at high concentrations. The detection limit for cancer antigen (CA) 15-3, a biomarker of breast cancer, measured using the two-enzyme scheme and GO/ITO electrodes is ca. 0.1 U/mL, indicating that the immunosensor is highly sensitive.

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Comparative study of stability of phosphonate self-assembled monolayers on indium-tin oxide electrode prepared using different method

김종찬 양해식*

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It is essential to obtain stable self-assembled monolayers (SAMs) for their applications to electrochemical (bio)sensors. Two commonly used methods for preparing phosphonate SAMs were compared in detail for the first time. SAMs of phosphonates with different alkyl chains were formed on indium?.tin oxide (ITO) electrodes using the dipping method and the T-BAG method (tethering by aggregation and growth). In addition, two different post-assembly washing methods were assessed. The stability of the SAMs measured by their charge-transfer blocking abilities were investigated using cyclic voltammetry and electrochemical impedance spectroscopy. The SAMs were tested to assess their stability against ultrasonic washing and their long-term stability in phosphate-buffered saline. Only the phosphonate with the longest alkyl chain (octadecylphosphonic acid, ODPA) was stable to the ultrasonic washing, with the charge-transfer blocking ability of SAMs prepared from decyl- and hexadecylphosphonic acid (DPA and HDPA) being significantly reduced after the process owing to damage of the monolayer. Moreover, the ODPA SAMs gave similar Xray photoelectron spectroscopic data, irrespective of the method of preparation and washing process used, providing further evidence of the stability of this monolayer. An increase in the length of the alkyl chain of the phosphonate (i.e., the length of the dielectric SAMs) decreased the double-layer capacitance and increased the charge-transfer resistance (blocking ability) against a redox reaction of $Fe(CN)_6^{3-}$ / $Fe(CN)_6^{4-}$. After 7 days of immersion in phosphate-buffered saline, the ODPA SAMs prepared by the dipping method maintained their blocking ability to a greater extent than those prepared using the T-BAG method.

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Adsorption of anionic ferricyanide ions on functionalized single-walled carbon nanotubes immobilized on a glassy carbon electrode

이현아 강찬*

전북대학교 화학과

Single-walled carbon nanotubes (SWNTs) were functionalized by attaching amino groups on their surfaces. A mixture of the amino group-functionalized SWNTs and poly(ethylene glycol) diglycidyl ether (PEGDGE) as a cross-linker was coated on the surface of a glassy carbon electrode and an amino group-functionalized SWNT modified electrode was prepared. The amino group-functionalized SWNT modified electrode is expected to show a new anion-adsorption property. Anionic ferricyanide ions were adsorbed on the modified electrode and fast electron transfer kinetics from the electrochemical reactions of the Fe(CN6)4-/Fe(CN6)3- couples were measured. It is hoped that the amino group-functionalized SWNT modified electrodes may extend the range of electrochemical applications.

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Washing-free Heterogeneous Immunosensor Using Proximity-Dependent Electron Mediation between an Enzyme Label and an Electrode

Dutta Gorachand 양해식*

부산대학교 화학과

Washing processes, essential in most heterogeneous labeled assays, have been a big hurdle in simplifying the detection procedure and reducing assay time. Nevertheless, less attention has been paid to washing-free heterogeneous labeled assays. We report a purely washing-free immunosensor that allows fast, sensitive, and single-step detection of prostate-specific antigen in serum with low interference. Proximity-dependent electron mediation of ferrocenemethanol (Fc) between an indium?tin oxide (ITO) electrode and a glucose-oxidase (GOx) label allows us to discriminate between a bound and an unbound label: a bound label offers faster electron mediation than an unbound one. The electrooxidation of Fc at a low applied potential (0.13 V vs Ag/AgCl) and a low electrocatalytic ITO electrode and the oxidation of ?-ascorbic acid by ?-ascorbate oxidase minimize the effect of the interfering species. A high concentration of glucose (200 mM) facilitates to obtain little dependence of the signal and background levels on the glucose-concentration variation in sample. The washing-free immunosensor can detect a concentration of ca. 1 pg/mL for mouse IgG in phosphate-buffered saline and a concentration of ca. 10 pg/mL for prostate-specific antigen spiked in female serum after an incubation period of 10 min. The concentrations measured with actual clinical serum samples are in good agreement with the concentrations measured with a commercial instrument, which renders the washing-free heterogeneous immunosensor appealing for practical use.

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An interference-free and rapid electrochemical lateral-flow immunoassay for one-step ultrasensitive detection with serum

Al-Monsur Jiaul Haque 양해식*

부산대학교 화학과

Point-of-care testing (POCT) of biomarkers in clinical samples is of great importance for rapid and costeffective diagnosis. However, it is extremely challenging to develop an electrochemical POCT technique retaining both ultrasensitivity and simplicity. We report an interference-free electrochemical lateral-flow immunoassay that enables one-step ultrasensitive detection with serum. The electrochemical?chemical?chemical (ECC) redox cycling combined with an enzymatic reaction of an enzyme label is used to obtain high signal amplification. The ECC redox cycling involving $Ru(NH_3)_6^{3+}$, enzyme product, and tris(3-carboxyethyl)phosphine (TCEP) depends on pH, because the formal potentials of an enzyme product and TCEP increase with decreasing pH although that of $Ru(NH_3)_6^{3+}$ is pH-independent. With consideration of the pH dependence of ECC redox cycling, a noble combination of enzyme label, substrate, and product [ß-galactosidase, 4-amino-1-naphthyl ß-D-galactopyranoside, and 4-amino-1-naphthol, respectively] is introduced to ensure fast and selective ECC redox cycling of the enzyme product along with a low background level. The selective ECC redox cycling at a low applied potential (0.05 V vs. Ag/AgCl) minimizes the interference effect of electroactive species (L-ascorbic acid, acetaminophen, and uric acid) in serum. A detection limit of 0.1 pg mL-1 for troponin I is obtained only 11 min after serum dropping without the use of an additional solution. Moreover, the lateral-flow immunoassay is applicable to the analysis of real clinical samples.

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Chemically oxidized porous carbon paper for the electrode of electroosmotic pump

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서강대학교 화학과

The functionalization of carbon paper by concentrated acid could create carboxyl, lactone, hydroxyl, phenol and quinone anchored over carbon surface that improve their activity in the electroosmotic pump. Chemical oxidation of porous carbon paper is carried out with acid mixture of sulfuric acid and nitric acid, and the effect of acid volume ratio (1:3-3:1) is investigated by means of different heat treatment condition. Among them, the best condition is at 110 ^{o}C for 10min. The specific electrochemical capacitance of carbon paper reached as high as 115 mF/cm^2, which is significantly greater value than that of 0.4 mF/cm^2 for air plasma treated carbon paper. The 8 mm pump assembled with the electrodes showed the flow rate of 27 μL min^{-1} at 1.5 V.

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Pd-Pt decorated carbon nanotubes for hydrazine oxidation

이슬기 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) have drawn particular attention on account of both their scientific interest and their potential for technological applications. Some researchers have reported that CNT supported catalysts (e.g. Pt, Pd, Au, ZnO_2 and TiO_2) exhibited good catalytic behaviors in various chemical reactions, involving hydrazine oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and hydrodehalogenation. In this work, we prepared the Pd-Pt decorated carbon nanotubes by thiol-functionalized CNTs. The obtained samples are characterized by transmission electron microscopy, X-ray photoelectron spectroscopy, cyclic voltammetry and chronoamperometry. For the hydrazine oxidation the Pd-Pt decorated CNTs exhibites higher electrochemical activity than thiolate CNTs.

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Spectroelectrochemical properties of newly synthesized terthiophene acrylic acids containing various conjugated linkers

Eswarreddy 심윤보*

부산대학교 화학과

Three new terthiophene acrylic acids, 3-(4-([2,2':5',2''-terthiophen]-3'-yl)phenyl)acrylic acid (TTPAA), 3-(5'-(thiophen-2-yl)-[2,2':3',2''-terthiophen]-5''-yl)acrylic acid (TTTAA) and 3-(5-([2,2':5',2''-terthiophen]-3'-yl)furan-2-yl)acrylic acid (TTFAA) were synthesized and characterized by FT- IR, 1H & 13C NMR, mass spectroscopy and elemental analysis. The synthetic route involves three steps including hydroboration, Suzuki coupling followed by knoevenagel condensation reaction, to give the title compounds (TTPAA), (TTTAA) and (TTFAA). The monomers were electrochemically polymerized on the Glassy Carbon and Platinum electrodes, then poly-TTPAA, poly-TTTAA and poly-TTFAA films were characterized by voltammetry using different scan rates, impedance spectrometry, and in situ UV-Visible spectroscopy. Thickness and surface morphology of polymerized electrode were characterized by using AFM analysis.

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Electrocatalytic oxidation of hydrazine by Pt-decorated graphene oxide

김지당 최현철*

전남대학교 화학과

Graphene is a two-dimensional material with a single atomic layer of carbon atoms arranged in a hexagonal lattice. Due to its unique structure, graphene exhibits unusual optical and electronic properties. In this study, we prepared Pt-decorated graphene by introducing thiol groups on graphene surfaces. Surface thiolation is an effective way to obtain dispersed metal nanoparticles on the surface of graphene. The samples were characterized by X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). Electrochemical characteristic of hydrazine oxidation is also investigated via Cyclic voltammetry (CV) measurement.

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Cytochrome c immobilized superoxide sensors based on electrochemically reduced graphene oxide and gold nanorod modified glassy carbon electrodes

장승철* THIRUMALAI DINAKARAN[1] Rajendran Baskaran[2]

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An electrochemical detection of superoxide (SO) free radicals by cytochrome c (Cyt-c) modified glassy carbon electrode (GCE), was introduced. For the Cyt-c modification, electrochemically reduced graphene oxide and gold nanorod (ErGO-GNR) composite was deposited onto the GCE. The ErGO-GNR composite modified electrodes showed an enhanced electro-catalytic activity compare with bare GCEs. In order to immobilize Cyt-c on the ErGO-GNR modified electrodes, in total of 3 different thiol mixtures were layered by using N-ethyl-N'-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC) and N-Hydroxysuccinimide (NHS) to allow the covalent binding between the protein and electrode surface. Electrochemical characteristics of each thiol mixture were investigated by using cyclic voltammetry and amperometric measurements were carried out to construct calibration plots for SO free radicals in PBS. The operation mode and the full performance details of the sensors will be described in the poster.

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Characterization of N, S co-doped active carbon by a thermal solid-state reaction for capacitors

권영탁 조미숙 이영관*

성균관대학교 화학공학과

Active carbon was doped with N and S by a thermal solid-state reaction. The doping degree and amount of active carbon were controlled by varying concentration of urea and sulfur. N, S co-doped active carbon was characterized and tested by X-ray photoelectron spectroscopy, Scanning Electron Microscope, Fourier Transform Infrared spectroscopy, and Brunauer-Emmett-Teller. The electrochemical properties of the co-doped active carbon were confirmed by cyclic voltammetry and charge-discharge test. Doped N and S provide to induce improved conductivity and capacitance of active carbon.

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Low-Potential Stable NADH Detection with Porous Gold Nanoparticles Modified Glassy Carbon Electrodes

정인택 심준호*

대구대학교 화학·응용화학과

We describe a simple one-pot approach for the synthesis of porous gold nanoparticles (AuNPs) without any extra surfactant, seed, control, and so on and their nonenzymatic electrocatalytic activity toward the electrochemical oxidation of beta-nicotinamide adenine dinucleotide (NADH). In contrast to the situation with non-porous AuNPs, amperometric low-potential stability of the NADH oxidation reaction was achieved by means of formation of porous AuNPs. The shape and structure of the porous AuNPs catalysts were characterized using scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and UV-vis absorption spectroscopy to examine the morphology and to analyze the optical properties of the synthesized products. To investigate the NADH detection, the porous gold nanoparticles were loaded on a glassy carbon electrode (GCE) with Nafion as the capping agent for the catalysts. The prepared electrode exhibited an improved performance at low overpotential in NADH detection. The greatly improved NADH detection indicates great promise for the design of amperometric biosensors, in connection to the immobilization of suitable dehydrogenase enzymes.

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Facile synthesis of core-shell Si/TiO2 anodes for lithium-ion batteries

<u>CHEN CHAO</u> 조미숙 이영관*

성균관대학교 화학공학과

A nanoparticle containing Si core and TiO2 shell was successfully prepared and demonstrated high cycle stability as an anode material for lithium-ion batteries. Amorphous TiO2 was coated on Si through sol-gel processing. Amorphous TiO2 were converted to anatase TiO2 by annealing at 500 oC for 4 h. X-ray diffraction, scanning electron microscope, and galvanostatic discharge?charge measurements were employed to characterize the structures and electrochemical performance of Si/TiO2. The Si/TiO2 core?shell electrode exhibited a reversible specific capacity of 480 mA h g-1 at 0.25 C over 50 cycles. This work suggests a facile and cost-effective strategy for the fabrication of a core-shell structure. The Si/TiO2 core?shell has the potential to be useful in energy storage devices.

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Pd-Pt bimetal on thiolated carbon natubes as electrocatalyst for methanol oxidation

이슬기 최현철*

전남대학교 화학과

Carbon nanotubes are receiving considerable attention as catalyst supports in both heterogeneous catalysis and electrocatalysis due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. These properties allow them to be applied for a wide range of promising applications in nanoelectronic devices, composite materials and sensors. In this work, we synthesized the Pd-Pt nanoparticles decorated CNTs. The obtained samples were characterized by SEM, TEM, and XRD. The electrochemical performance of prepared samples for methanol oxidation is evaluated by CV.

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Voltammetric Detection of Ammonium Ion Using Self-assembled Monolayers Modified with Ionophoric Receptors

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Thiazole benzo-crown ether ethylamine-thioctic acid (TBCEAT) was evaluated as an ammonium (NH4+) ionophore for the preparation of ion-channel sensors (ICSs) based on self-assembled monolayers (SAMs) on a gold electrode. A SAM film based on TBCEAT on a gold electrode was assessed as a NH4+-selective sensor, particularly the voltammetric response. The working principle of this voltammetric sensor conceptually mimicked that of the ligand gated ion-channel proteins with regard to the chemically stimulated changes in the membrane permeability. The response to various analytes is based on the change in the electron transfer rates of a redox reaction of the reporter ion [Ru(NH3)6]3+/2+ before and after the binding of NH4+ to TBCEAT on the electrode surface, where electrostatic repulsion between the NH4+-TBCEAT complex and [Ru(NH3)6]3+/2+ induced a decrease in the rate constant. The selective ion-recognition properties of TBCEAT were characterized fully in the conventional ion-selective electrode (ISE) configuration using plasticized polymeric membranes. The mixed monolayer formed with alkylthiol and TBCEAT could bind ammonium ion selectively, and effectively control the flux of the reporter ion [Ru(NH3)6]3+/2+, resulting in ammonium selective ICS with comparable performance (in terms of selectivity and detection limits) to conventional ISE.

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발표분야: 전기화학

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Nanoporous hematite nanorods for the highly efficient photoelectrochemical cell

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The hierarchical nanoporous hematite nanorod has been synthesized by treating boric aicd in the FeCl3?6H2O3 solution. The [FeB(OH)4]2+ complex is synthesized and decoupled slowly into Fe3+ during hydrothermal growth process. The slow release of Fe3+ ions due to the presence of [FeB(OH)4]2+ complex triggers the creation of the small dimension of FeOOH which is converted to the hierarchical α-Fe2O3 after annealing process. The hierarchical nanoporous α-Fe2O3 composed of ~ 15nm domains showed a photocurrent density of 1.41 mA/cm2 at RHE 1.23V which is 1.7 times higher than that of pristine hematite. The small domain of α-Fe2O3 increased the charge transfer rate between hematite and electrolyte by reducing recombination.

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Thiolated graphene oxide-supported Pd-Co alloyed nanoparticles as the high performance electrocatalyst for oxygen reduction reaction

윤미라 배시라 전승원*

전남대학교 화학과

Thiolated graphene oxide-supported Pd-Co alloyed nanoparticles (abbreviated as Pd-Co/tGO) with efficient electrocatalytic activity for the oxygen reduction reaction (ORR) were synthesized by a chemical reduction method in the presence of polyethylene glycol (PEG) as a stabilizing agent. The catalytic activity of the Pd-Co/tGO composite was significantly enhanced by electrochemical reduction at a potential range of 0 to -1.5 V in the pH 5 phosphate buffered saline (PBS) solution. The electrochemically reduced Pd-Co/tGO (ER/Pd-Co/tGO) was characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), and X-ray photoelectron spectroscopy (XPS). Electrocatalytic activities were verified by cyclic voltammetry (CV) and hydrodynamic voltammetry techniques. The ER/Pd-Co/tGO shows a higher electrocatalytic activity for the ORR than that of non-thiolated graphene compound, ER/Pd-Co/rGO. The Koutecky-Levich equation and plots confirm that oxygen reduction in the presence of the ER/Pd-Co/tGO catalyst follows a four electron transfer reaction.

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Electrochemical determination of dopamine and ascorbic acid using Pd nanoparticles supported on poly(3,4-ethylenedioxythiophene) functionalized graphene

최주은 전승원*

전남대학교 화학과

The electrochemical sensor based on poly(3,4-ethylenedioxythiophene) functionalized reduced graphene oxide with palladium nanoparticles (Pd/PEDOT/rGO) was constructed to simultaneously determine small biomolecules such as dopamine (DA) and ascorbic acid (AA). The structural features of the catalyst were characterized by transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDX) and X-ray photoelectron spectroscopy (XPS). Electrochemical determination of dopamine (DA) and ascorbic acid (AA) have been studied at a modified glassy carbon electrode (GCE) in 0.1 M phosphate buffer solution (PBS) using cyclic voltammetry (CV), differential pulse voltammetry (DPV) and amperometric response at pH 7.4. Linear analytical curves were obtained in ranges from 2.0 ×10-6 to 2.0 × 10-4 M and 2.0 ×10-6 to 4.8 ×10-3 for DA and AA, respectively. The low detection limit for DA and AA were 4.7 × 10-7 and 1.5 × 10-6 M, as well as no interference was observed from the common interfering species such as glucose, uric acid, serotonin.

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Enhancement of ORR activity of rGO/MnO2/Ag Electro-catalyst by electrochemical synthesis

이경미 전승원*

전남대학교 화학과

In this poster, we report the rGO/MnO2/Ag by electrochemical synthesis method. The physical properties of the rGO/MnO2/Ag were investigated via X ray-photoelectron spectroscopy (XPS), scanning electron microscope (SEM), transmission electron microscopy (TEM). This composition has a polycrystalline structure that Ag/MnO2 microsphere formation accompanied by Ostwald ripening process. The electrochemical properties of electro-catalyst samples were studied by cyclic voltammetry (CV), linear sweep voltammetry (LSV). The rGO/MnO2/Ag shows the current density and electron transfer number highly compared to that on the commercial 20% Pt/C at limiting diffusion zone, which has excellent electro-catalyst activity toward oxygen reduction reaction (ORR) in alkaline media.

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FeF_3/Reduced Graphene Oxide Microsphere Composites Synthesized Through Hydrothermal-Assisted Method as a Cathode Material for Lithium-Ion Batteries

제지운 김종식*

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In recent decades, rechargeable lithium-ion batteries (LIBs) are one of the most commonly used energy storage systems. The rapid growth of various electric devices market has been demanding LIBs with enlarged reversible capacities. FeF_3 is considered as an alternative cathode material for commercialized $LiCoO_2$, because FeF_3 has the high theoretical capacities of about 237 and 712 $mAh\cdot g^{-1}$ in the voltage range of 2.0-4.5 V and 1.5-4.5 V, respectively. However, FeF_3 has disadvantage of its low electrical conductivity exhibiting poor capacity retention and rate performance. In this study, we successfully synthesize FeF_3/reduced graphene oxide (r-GO) microsphere composites through a vapor-solid (VS) process. r-GO is used as a conductive agent to improve electrical conductivity of FeF_3. The size of FeF_3/r-GO microsphere composites is also controlled by varying the amount of r-GO which is 1.7 and 11 wt%. The prepared FeF_3/r-GO microsphere composites are characterized by XRD, FT-IR, EA, SEM, and TEM. FeF_3/r-GO11 exhibits an initial discharge capacity of about 174 $mAh\cdot g^{-1}$ in the voltage range of 2.0-4.5 V at 0.1 C rate (1 C = 237 $mA\cdot g^{-1}$) with a capacity retention of about 86.2 % after 50 cycles. In the wide voltage range of 1.5-4.5 V, FeF_3/r-GO11 also shows improved cycling performances compared to bare FeF_3, delivering the initial discharge capacity over 410 $mAh\cdot g^{-1}$ at 0.1 C rate.

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FeF_3/Activated Carbon Foam Nanocomposites as a High Electrochemical Performance Cathode Material for Lithium-Ion Batteries

김용경 김종식*

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Traditional cathode materials such as $LiCoO_2$, $LiMn_2O_4$, and $LiFePO_4$ have a limited actual specific capacity in the range of 120-160 mAh g^{-1}. Recently, the transition metal fluorides have been studied as a promising new class of cathode material, which exhibit large theoretical capacities and high discharge voltages. Iron trifluoride (FeF_3) is one of the most promising cathode materials due to its low toxicity, low cost, and high theoretical capacities of 237 and 712 mAh g^{-1} at 2.0-4.5 and 1.5-4.5 V, respectively. In spite of these advantages, wide band gap of Fe-F bonds is a fatal shortcoming for iron fluoride that leads a poor electronic conductivity, making the actual specific capacity far below the theoretical capacity. In this work, we prepare a mesoporous activated carbon foam (ACF) by resorcinol-formaldehyde carbon-gel method using a silica template. Through a wetness-impregnation method, FeF_3 nanoparticles are impregnated into the mesopores of ACF, which is a good electronic conductivity agent and a template. The structure and morphology are characterized by BET, FT-IR, XRD, SEM, and TEM. The electrochemical behaviors of FeF_3/ACF nanocomposites are analyzed by cycling performance, rate performance, cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS). The FeF_3/ACF nanocomposites show the excellent electrochemical performance with an initial discharge capacity of 195 mAh g^{-1} at a rate of 0.1 C in the voltage range of 2.0-4.5 V and exhibit a good capacity retention of about 93% during 50 cycles. The FeF_3/ACF nanocomposites show the improved electrochemical performances compared with bulk FeF_3.

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A highly sensitive lead-ion sensor based on peptide modified conducting polymer nanotube arrays

정유정 **Yangjiao** 조미숙 이영관*

성균관대학교 화학공학과

In this study, polypyrrole-co-polypyrrole-3-carboxylic acid (PPy-co-PPy-COOH) nanotube arrays were electropolymerized on ZnO nanorod arrays (as a template), which were electrodeposited by chronopotentiometry on ITO glass. The morphology of PPy-co-PPy-COOH nanotube arrays were verified by scanning electron microscopy, and their compositions were confirmed by ATR-IR and X-ray photoelectron spectroscopy. After that, TNTLSNN peptide, which has high affinity to lead, was immobilized on PPy-co-PPy-COOH nanotube arrays by covalent bonding between carboxylic acid group of the nanotube arrays and amine of the peptide. The sensing performance of the designed sensor was carried out by square wave voltammetry. The as-prepared peptide/PPy-co-PPy-COOH nanotubes sensor exhibits high sensitivity and selectivity due to fast ion transfer and high surface area of the nanotube.

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Synergistic effects of MnCo2O4 on capacitance and stability for supercapacitors

이창미 이상하 조미숙 이영관*

성균관대학교 화학공학과

Hierarchical hollow MnCo2O4 are synthesized by a facile hydrothermal deposition directly on zinc oxide nanorod arrays (as template), which are electrodeposited on stainless steel.The morphology of proposed hollow MnCo2O4 nanorods was characterized by scanning electron microscopy, transmission electron microscopy, and their compositions were verified by energy dispersive X-ray analyses, X-ray diffraction, and X-ray photoelectron spectroscopy. The hollow MnCo2O4 nanorods are further investigated as active electrode material for supercapacitors. Compared with individual component of Co3O4 and MnO2, the as-prepared MnCo2O4 exhibits better electrochemical performances such as, high specific capacitance, high energy density, and excellent long-term cycle stability.

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Facile preparation of hierarchical Ni(OH)2 hollow nanorod arrays and their application for non-enzymatic glucose sensing

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성균관대학교 화학공학과

Hierarchical nickel hydroxide hollow nanorod arrays (Ni(OH)2 HR) modified electrode was fabricated by chemical bath deposition of Ni(OH)2 nanoflakes on zinc oxide nanorod arrays as a template. The morphology of proposed Ni(OH)2 HR electrode was characterized by scanning electron microscopy and transmission electron microscopy, and its composition was verified by X-ray diffraction (XRD). The resulting modified electrode exhibited high electrocatalytic activity for glucose sensing due to the hierarchical hollow structure, which can provide large surface area and facilitate electron transfer and mass diffusion. Following the optimization of Ni(OH)2 deposition time, the as-prepared electrode showed excellent performance for glucose sensing in the alkaline solution, in which a high sensitivity of 1569.4 µA?mM-1?cm-2 was obtained in a wide linear detection range 2 - 3862 µM despite the presence of several interfering electro-active species, which indicated our sensor is a promising platform for further application on glucose sensing.

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The study for rechargeable zinc-air batteries using zinc or zinc hydroxide as anode

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울산대학교 화학과

Because zinc-air batteries have many advantages including high specific energy, competitive cost, abundant resources, and environmentally benign property, it is expected to be a promising power source and energy storage device in the near future. Zinc-air batteries has a theoretical specific energy of 1,085Wh/kg, and the theoretical cell voltage of 1.65 V. However, the practical working voltage of zinc-air batteries is less than 1.65 V due to the internal loss of the cell due to activation and ohmic and concentration loss. Primary zinc-air batteries have been widely commercialized as hearing aid. However, the utilization of rechargeable zinc-air batteries has been limited by some barriers related to the electrodes. These are problems originating from the zinc electrode, such as its low cycling stability, high degradation rate, passivation, and self-discharge. Thus, these problems must to solve for zinc secondary batteries. In this work, we totally study zinc anode reaction to solve problems caused by zinc anode for zinc secondary batteries. Thus, we estimated corrosion of zinc according to particle size of zinc. And, we investigated relationship between specific capacity and solubility according to zinc compounds such as zinc hydroxide (Zn(OH)2), zinc acetate ((CH3COO)2Zn), zinc chloride (ZnCl2) and zinc oxide (ZnO) powder. We confirmed improved electrochemical properties by containing electrolyte solution of high ratio and conducting agent in anode. In order to decrease corrosion of zinc anode and to make mixtures with high energy density (Zn 1,085Wh/kg, Mg 3,910Wh/kg, Si 8,470Wh/kg), zinc anode was made of zinc-magnesium-silicon mixtures.

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Graphene wrapped Mn_3O_4 composite by supercritical CO_2 fluid for supercapacitors

박승연 권영탁 조미숙 이영관*

성균관대학교 화학공학과

Graphene wrapped Mn_3O_4 nanocomposites were prepared by using a supercritical carbon dioxide ($scCO_2$) fluid. At first, composite of $MnCO_3$ and graphene oxide was prepared through $scCO_2$ and then, converted to Mn_3O_4/graphene by thermal oxidation under inert atmosphere at 500℃ for 4h. The oxidation of $MnCO_3$ and graphene oxide was determined by X-ray diffraction, energy dispersive X-ray spectroscopy, and thermo-gravimetric analysis. Spherical Mn_3O_4 particles (ca. 200~300 nm) were well dispersed in graphene, and the morphology of Mn_3O_4 was monitored by scanning electron microscopy. The electrochemical properties of Mn_3O_4/graphene composite were characterized by cyclic voltammetry and galvanostatic charging-discharging measurements. Graphene provide the conductive paths for Mn_3O_4 and lead to enhance the capacitance of Mn_3O_4. $ScCO_2$ make an ideal medium to fabricate carbonate minerals and to disperse graphene. This well wrapped Mn_3O_4 and its high electric conductivity indicated that the nanocomposites could be promising materials for supercapacitors.

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Simultaneous Determination of Heavy Metal Ions by a Chemically Modified Electrode with Comprising Graphene

백석호 심윤보* 김동민 박민욱

부산대학교 화학과

Functionalized polyterthiophenes comprising graphene were synthesized in a solution containing graphene and functionalized tertiophene monomer. Interaction between functional groups of graphene oxide (GO) and the monomers in an aprotic nonaqueous solution offers the formation of uniform and stable composited layer. Morphologies and compositions of the polymer materials were confirmed using SEM, FE-TEM, and XPS analyses, which show homogeneous and functionalized poly(terthiophenes-GO) composition. We observed that the heavy metal ions (Zn(II), Cd(II), Pb(II), Cu(II), and Hg(II)) can be deposited on the composited polymer layer via the complex formation reaction. Thus, stripping voltammetry was performed for the analysis of the ions in very low concentration by scanning the potential from -1.5 to +0.5 V after preconcentration. The results show the distinct anodic stripping peak of each ion at -1.1, -0.75, -0.49, -0.05, +0.15V, corresponding to Zn(II), Cd(II), Pb(II), Cu(II), and Hg(II) ions, showing detection limit of ~1ppb.

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Graphene/polyaniline composite paper-based supercapacitors by electropolymerization

박하빈 장병용*

부경대학교 화학과

Freestanding and scalable graphene/polyaniline composite paper-based supercapacitors were prepared by inserting a paper which is immersed in an acid solution between two Fluorine-doped Tin-oxide (FTO). The synthesis of graphene/polyaniline composite was conducted by one-step including electropolymerization. The morphology of the paper was confirmed by scanning electron microscopy (SEM). The electrochemical storage properties of the paper was characterized by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge/discharge measurements. The stability of the paper as a supercapacitor was also examined. In conclusion, the paper-based supercapacitors can be used for portable and flexible devices.

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물과 알코올 용액 조성이 전기삼투펌프의 구동에 미치는 영향

서아리 신운섭*

서강대학교 화학과

본 연구실에서는 전극과 다공성 멤브레인으로 이루어진 가장 간단한 전기삼투펌프(Electro-osmotic Pump)를 구현한 것을 보고한 바 있다 [1]. 펌프의 유량은 인가전압, 전류, 구동시간, 그리고 펌핑 용액의 종류에 따라 조성을 조절하여 변화시킬 수 있다. 본 연구에서는 펌핑 용액에 초점을 두고 실험하였으며, 그 중 물과 알코올 용액 조성 변화에 따른 펌프의 유량 및 압력 변화를 관찰하였다. 이 실험을 통해 물에서 보다 알코올의 농도가 진해질수록 전류가 감소하고, 이에 따라 유량 및 압력이 감소함을 확인하였다. 그러나 유량당 전력 효율은 농도 변화에 상관 없이 비슷함을 알 수 있었다.

Reference

1. a) W. Shin, J.M. Lee, R.K Nagarale, S.J Shin, A. Heller, *Drug Deliv. and Transl. Res.* 2011
b) W. Shin, S.J Shin, J.M. Lee, R.K Nagarale, A. Heller, *J. Am. Chem. Soc*. 2011, *133*, 2374

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Electrochemical properties of surface modified $Li_3V_2(PO_4)_3$/C cathode materials in lithium ion batteries

오례경 홍정의 류광선*

울산대학교 화학과

Rechargeable lithium ion batteries have been widely applied to the portable electronic devices, electrical vehicles, and energy storage systems due to its high energy density and rate capability. However, the current commercial cathode material, LiCoO2, suffers from several problems for large-scale applications due to its high cost and safety issues. From this aspect, the phosphate-based materials, which contain $LiFePO_4$, $LiMnPO_4$, and $Li_3V_2(PO_4)_3$, have been attracted. Among these things, $Li_3V_2(PO_4)_3$ (LVP) is most promising cathode material. Monoclinic LVP exhibits a theoretical capacity of ~197 mAh g^{-1} with three reversible lithium ions when charged to 4.8 V. However, low electronic conductivity of LVP induces its poor rate capability. To improve the electronic conductivity of LVP, many studies have been progressed such as carbon coating, metal doping, and surface modification. In this study, we studied about surface modified LVP/C to enhance the electronic conductivity and limit the direct contact with the electrolyte to protect side reaction in high voltage region. We selected Al_2O_3 and ZnO as surface coating materials. It can also repair the unconnected conducting pathways of carbon and improve the charge transfer process thorough the interface of active materials and electrolyte. X-ray diffraction and field emission-scanning electron microscopy were used to check the physical properties of pristine and surface modified LVP/C. Galvanostatic charge-discharge tests, rate performances, cyclic voltammetry, and electrochemical impedance spectroscopy were used to measure the electrochemical performances

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Synergistic effects of $Li_4Ti_5O_{12}$ and Co_3O_4 for enhanced capacities in lithium ion batteries

홍정의 오례경 류광선*

울산대학교 화학과

Spinel Li4Ti5O12 (LTO) material has an excellent reversibility of Li-ion intercalation and de-intercalation and exhibits zero strain volume change during charge and discharge cycles with an excellent safety performance. However, unfortunately LTO has a low electrical conductivity and also a theoretical capacity of 175 mAh g-1, which is lower than that of conversion-based anode materials such as Si or Sn. This disadvantage restricts its applications in high-power storage devices. In this work, we attempted to overcome the low theoretical capacity of LTO and the irreversible and poor cycling performance of metal oxides by synthesizing the LTO/Co3O4 composites. Composites comprised of LTO/Co3O4 were synthesized by solution combustion and solution precipitation methods. The diffraction patterns of LTO, Co3O4, and LTO/Co3O4 composite could be indexed as the cubic spinel structure corresponding to LTO with the Fd-3m space group and absence of any impurity-phase peaks. The surface and pores of LTO were covered with the Co3O4 particles. The Co3O4 particles existed in the composite are agglomerated less than pristine Co3O4. This structure is expected to prevent volume expansion and particle aggregation of Co3O4 particles in the pores of LTO. As expected, the LTO/Co3O4 composite had higher capacity than that of LTO, with a decreased slope and an extended plateau region over the voltage range of 0.01-3.0 V. Galvanostatic intermittent titration technique (GITT) and X-ray absorption near-edge structure (XANES) spectroscopy were also conducted to determine the relative contribution of LTO and Co3O4 to the characteristics of composite.


dispersion
Co^{2+}, NH_4OH
450℃/2h
heat treatment
LTO
LTO/$Co(OH)_2$
LTO/Co_3O_4
LTO
$Co(OH)_2$
Co_3O_4

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발표코드: **ELEC.P-1241**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

An electrochemical, straightforward HbA$_{1C}$ biosensor via use of electrochemically active nanoprobes

심승은 이정봉 현혜리 양현희 권지윤 차근식 남학현 신재호*

광운대학교 화학과

Diabetes mellitus, which is characterized by the defective regulation of blood glucose, is one of the major health concerns worldwide. The diagnosis and management of this disease require continuous monitoring of blood glucose level. However, glucose level is influenced by food or exercise and hence does not reflect the average glucose level over a prolonged period. To overcome such drawbacks, glycosylated hemoglobin (HbA$_{1C}$) presents a promising marker for performing long-term diabetes monitoring. HbA$_{1C}$ is formed by non-enzymatic glycosylation of hemoglobin when it was exposed to higher than normal level of blood glucose over time. The level of HbA$_{1C}$ reflects the average of the blood glucose concentration over the preceding 2-3 months. Herein we report a new concept of an electrochemical biosensor for the detection of HbA$_{1C}$ by using a specific reaction of HbA$_{1C}$ with boronic acids. Of note, the binding of HbA$_{1C}$ to boronic acids immobilized on the electrode surface may lead to change the electrochemical signal by blocking the access of redox probes. To emphasize such blocking effect, nanoparticular probes such as ferrocene (Fc)-modified silica nanoparticles will be employed. Furthermore, various types of boronic acid derivatives which are able to form self-assembled monolayer on gold electrode, have been studied to improve sensor performance (e.g., sensitivity, detection limit, and linear response range). In addition, the effect of pH was also investigated as it influences the formation of complex between boronic acids and HbA$_{1C}$. Finally, the optimized sensors will be employed to determine HbA$_{1C}$ concentrations in physiological specimen.

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An electrochemical aptasensor for selective and label-free detection of human lung cancer cells

TANVEER AHAMD MIR 심윤보*

부산대학교 화학과

Lung cancer is one of the leading cause of mortality among all types of cancer both in developed and developing nations, and has no effective cure, especially in later stages. Consequently, there is a critical need for the development of a tangible protocol for early detection of this disease. Conventional methods for lung cancer detection can be limited by the need for exogenous labels, time and labor-intensive protocols, as well as by poor sensitivity levels. In this study, we fabricated an electrochemical nanobiosensor for rapid, easy and label free detection of lung cancer cells. The proposed sensor showed a dynamic range between 15 to 1 × 106 cells with a detection limit of 15 cells.

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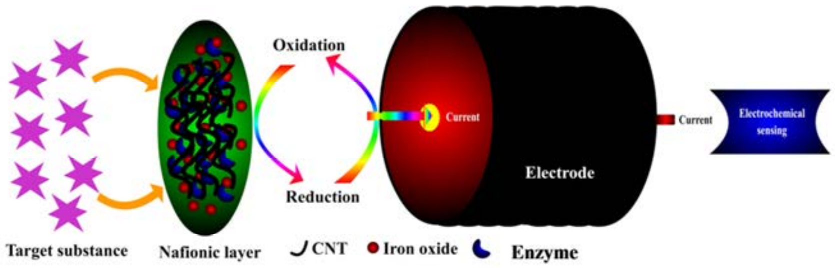
발표분야: 전기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

DEVELOPMENT OF NANOINTERFACED BIOSENSORS FOR DETERMINATION OF FOOD QUALITY AND AS CLINICAL BIOMARKERS

SAKTHIVEL KAVITHA 이용일*

창원대학교 화학과

Nano materials have been explored for various applications owing to their significant properties when compared with the bulk materials. Iron oxide nanoparticles (Nano Fe3O4), belongs to the class of metal oxide that is well known from ancient times. Carbon based nanomaterials, specifically carbon nanotubes are another interesting class of nanomaterial with unique properties like high surface area, superior mechanical strength, good electrical conductivity, high thermal conductivity, etc. Hence, they find applications in various diverse fields such as chemical & bio-sensing, fuel cells, solar cells, batteries, energy storage, electronic applications, etc. Highly sensitive and selective enzyme based biosensors have gained immense popularity due to their high specificity and high turnover numbers. Generally, redox mediators are used to improve the sensitivity and shorter the response time of the sensor but, it causes interferences. The incorporation of an appropriate nanointerface at the electrode can aid in faster transfer of electrons. Such superior sensitivity and specificity will be invaluable in assessing food quality and as disease diagnosis in the healthcare sector. In the case of food industries, the determination of hydrogen peroxide in milk can indicate the associated health risk while, the determination of freshness of fish can be utilized for the export industries. In the health care sector, detection of superoxide in biological samples can serve to diagnose various oxidative stress related disorders. The current topic of my presentation is based on the development of suitable nanointerfaced electrochemical biosensors for testing the quality of milk & fish and the clinical biomarker, superoxide.


Oxidation
Reduction
Current
Electrode
Current
Electrochemical sensing
Target substance
Nafionic layer
CNT
Iron oxide
Enzyme

일시: 2014년 10월 15~17일(수~금) 3일간
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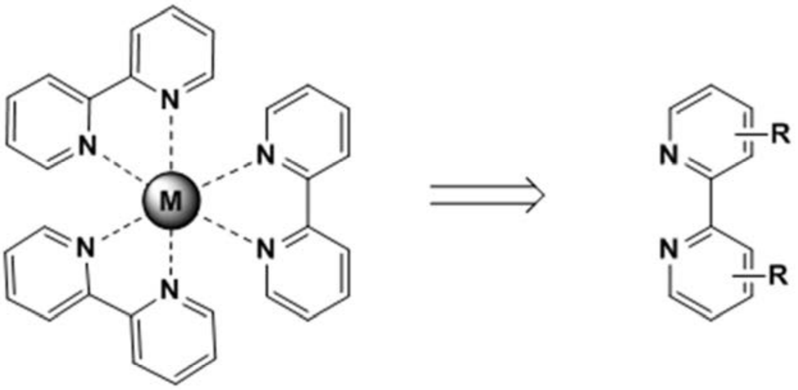
The convenient preparation of Bipyridine, Phthalimide and 4-Oxo TEMPO Derivatives : Application for Redox Flow Battery

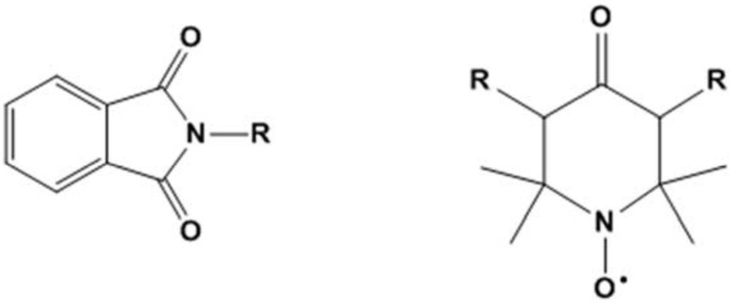
김기우 김은선 안철진*

창원대학교 화학과

Redox flow battery is a type of rechargeable flow battery that employs in different oxidation states to store chemical potential energy. To improve the energy density, we prepared metal complex including bipyridine ligand. Also, phthalimide and 4oxo-tempo derivatives was prepared for organic electrolyte. In this paper, we will present the efficient preparation of various bipyridine, phthalimide, 4-oxo tempo derivatives.



R= COOH, CO_2Et, Br, NO_2, OMe, NH_2



R= SO_3H, $CH_2CH_2CH_2SO_3H$

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Modification of glassy carbon electrode with poly-melamine film: An application for the detection of hydroquinone, catechol and resorcinol

김은경

서울대학교 사범대학 화학전공

Hydroquinone (HQ), catechol (CA) and resorcinol (RE) are known as dihydroxybenzene isomers. Due to their high toxicity, these isomers are considered to be environmental pollutants. Therefore, it is important to be able to detect these isomers in rivers and ground water. For this reason, we are working to develop dihydroxybenzene isomer sensors.Several dihydroxybenzene isomers sensors have been found effective in detecting the oxidation of hydroquinone, catechol and resorcinol. However, these sensors have some drawbacks, including a complicated modification process, high cost of materials and the instability of the modified electrode sensor. Herein, we share findings about the development of a sensor using poly-melamine modified glassy carbon electrode (GCE) that is capable of detecting dihydroxybenzene isomers in aqueous solution. We prepared poly-melamine modified electrodes by electro-polymerization of GCE in 0.1 M H2SO4 containing 1.0 mM melamine in the potential between 0 and 1.6 V for 20 cycles. The sensor displayed voltammetric responses with high electrocatalytic effects, good selectivity, wide linear range and high stability for the detection of dihydroxybenzene isomers in optimal conditions.

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Metal-free Counter Electrodes for Dye-sensitized Solar Cells Using Carbon Nanotube/Carbon Nanosheet Double Layers

강진현 장성연*

국민대학교 생명나노화학과

Dye Sensitized Solar Cell (DSSC) has been received as a next-generation solar cells. For the commercialization of DSSCs, the reduction of cost for materials and process has been one of the major issues. The development of cheap counter electrode (CE) is a very important prerequisite because the regular CE material is the Pt coated Fluorine doped tin oxide (FTO), which occupies almost half of the device cost. In this work, we developed a novel carbon based CEs by combination of highly conducting carbon nanosheet (CNS) and aqueous processable multiwalled carbon nanotubes (MWCNT). In the present CEs, the CNS mainly contributed as a charge collecting electrodes, while the MWCNT exhibited high electrocatalytic effects for the redox media (I-/I3- in this work). The electrocatalytic activity of the carbon based CEs and the performance of DSSCs using the CEs were investigated. The DSSCs using our carbon based CEs displayed a power conversion efficiency (PCE) of ~ 7%. This result can promise for the development of Pt and FTO free CEs for high performance DSSCs.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

어휘와 문장 수준에서 초등학교 과학 교과서의 이독성 분석

강석진

전주교육대학교 과학교육과

이 연구에서는 2007 개정 과학교육과정에 의거하여 개발된 초등학교 3 학년 과학 교과서와 6 학년 과학 교과서의 이독성을 어휘와 문장 수준에서 분석하였다. 어휘 수준의 분석에서는 어휘를 난이도에 따라 1-4 등급으로 분류하고, 등급별 빈도를 비교하였다. 문장 수준의 분석에서는 문장을 단문과 복문/중문으로 분류한 뒤, 종류별 빈도를 비교하였다. 또한 문장의 평균 길이, 즉 한 문장에 포함된 어휘의 수도 계산하여 비교하였다. 연구 결과, 2007 개정 과학 교과서의 어휘는 90% 이상이 1-3 등급에 해당되는 것으로 나타났다. 그러나 7 차 과학 교과서에 비해 어휘의 종류와 빈도가 증가한 것으로 나타났다. 특히, 이러한 증가는 6 학년에 비해 3 학년 교과서에서 두드러졌는데, 처음으로 과학을 공부하는 3 학년 학생들에게는 과학 교과서가 읽기 부담이 될 가능성이 있는 것으로 나타났다. 한편, 2007 개정 과학 교과서에서는 7 차 과학 교과서에 비해 복문/중문의 비율이 증가하였고, 문장의 평균 길이도 증가한 것으로 나타났다. 즉, 문장 수준에서도 2007 개정 과학 교과서의 이독성이 감소한 것으로 볼 수 있다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

예상하지 못한 현상의 관찰을 활용한 문제해결형 탐구 프로그램: 물과 에탄올 혼합시 기체 발생 현상에 대한 사례 연구

임민아 이현영 정대홍*

서울대학교 화학교육과

물질의 입자성을 지도하기 위한 대표적인 실험 중 하나인 물과 에탄올의 혼합 실험에서, 두 액체를 혼합했을 때 의도했던 부피 감소 현상뿐 아니라 용액의 온도 상승, 기체 발생 현상 등을 관찰할 수 있다. 학생들이 목표 지식 외의 이러한 현상에 관심을 가질 때, 적절한 지원을 통해 추가 탐구로 이어지는 기회를 제공할 수 있다. 물과 에탄올 혼합 시 발생하는 기체의 정체와 발생 원인에 대한 배경 지식을 탐색하는 과정에서, 가설 연역적 탐구 과정에 따라 실험값과 이론을 바탕으로 한 계산값을 비교하고, 주사기 등의 간단한 실험 도구를 사용하여 진행하였다. 가설 검증 결과, 발생하는 기체의 주성분은 혼합 전 액체에 용해된 대기 중의 질소와 산소이며, 두 용액의 혼합으로 인해 용액의 조성이 변함에 따라 기체의 용해도가 변화하는 것이 원인이었다. 이 현상은 binary system 에서의 용해도가 tertiary system 에서 유지되지 않고 달라지기 때문인데, 중등 교육과정을 벗어나는 이론적 배경을 갖고 있어 직관적으로 원인을 예상하기 어렵지만, 간단한 실험을 통해 가설연역적으로 해결하기 쉬운 주제이므로, 문제해결형 교육자료의 소재로 가치가 있다고 판단하였다. 이러한 측면을 고려하여 이 과정을 학교 과학의 관점에서 진행하여, 학생들이 실질적인 탐구를 경험할 수 있는 프로그램으로 개발하였다. 물과 에탄올의 혼합 소재는 위험성이 낮으면서도 기체 발생을 비롯하여 기존에 알려진 부피 감소, 발열 반응 등 관찰할 수 있는 현상이 다양하다. 또한 실험결과가 학생들이 관찰, 측정할 수 있을 정도로 명확하기 때문에, 학생이 가설 설정에서 실험 설계, 결론 도출에 이르기까지의 탐구 과정을 직접 수행하기에 적합하다. 물과 에탄올의 혼합시 관찰되는 현상을 통해, 물질의 입자성, 기체의 용해도 등

관련 지식을 학습할 뿐 아니라, 학생들이 실질적인 과학 탐구 과정을 경험할 수 있는 문제해결형 탐구 프로그램을 개발하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

한국-동티모르 과학교사 세미나: 과학교육을 통한 봉사활동

한재영* **정대홍**[1]

충북대학교 사범대학 화학교육과 [1]*서울대학교 화학교육과*

해방 후 혼란과 전쟁으로 세계 최빈국에 속했던 한국은 과거 1960-70 년대 외국으로부터 과학교육 원조를 받았다. 이를 기반으로 하여 과학교육은 한국의 경제발전에 지대한 공헌을 하였다. 이제 한국은 OECD 회원국으로 선진국 대열에 올라 있어 정부 차원의 수많은 해외 원조 사업(Official Development Assistance: ODA)을 수행하고 있으며, 정부 차원의 공적 원조 이외에 민간 차원에서도 봉사활동 등을 통해 원조를 제공하고 있다. 2004 년부터 한국의 과학 교사들은 개인적 봉사활동을 시작으로 현재는 전국과학교사협회(Korean Science Teachers Association: K-STA) 차원에서 동티모르에 8 년째 봉사활동을 이어가고 있다. 이 연구에서는 동티모르 과학교사를 대상으로 한 이 과학 봉사활동을 소개하고자 한다. 동티모르는 2002 년에 독립한 작은 나라로 최빈국에 속하며, 전쟁 후 한국의 모습과 비슷한 상황에 있다. 동티모르 제 2 의 도시인 바우카우에 있는 한 신부의 헌신적인 노력으로 한국과 동티모르 과학교사들이 참여하는 중등 과학 실험 연수 활동이 매년 이루어졌다. 동티모르 현지 여건을 고려한 실험 연수 프로그램을 구성하여 실험실이나 실험 기구, 시약이 거의 없는 동티모르 중고등 학교에서 과학 실험을 통한 과학교육이 이루어질 수 있도록 노력하고 있다. 한국 과학교사들의 열정이 동티모르 과학교사들에게 전해져서, 현재 동티모르에 자생적인 과학교사 연구모임이 만들어지고 있으며, 이 같은 변화가 지속적으로 일어나도록 계속 지원하고자 한다. 그러나 교사들의 자비로 수행되는 이 봉사활동은 경제적인 한계나 언어적인 문제 등 많은 어려움을 가지고 있으며, 이런 어려움이 극복될 수 있도록 기관과 학계의 관심과 지원이 요구된다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

창의적 사고력 신장 지향 PPC 쓰기 기법을 활용한 일반 화학 탐구 실험

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본 연구에서는 창의적 사고력을 신장시키는 다양한 교수전략으로 PPC 쓰기기법을 개발하였다. 개발한 수업전략은 탐구 실험 수업의 가설 설정 단계에서 그럴듯한 점(Positive) 발전시킬 점(Possibilities) 우려되는 점(Concerns) 생각해 볼 수 있도록 설계하였다. 일반 화학 실험을 수강하는 서울소재 사범대학 과학교육과 학생들을 대상으로 하여 한 학기동안 실시한 후 이 교수전략이 협의의 창의적 사고력인 발산적 사고력과 탐구 능력 측면의 비판적 사고력에 미치는 효과를 알아보았다. 이 연구를 적용한 결과, 발산적 사고력이 통계적으로 유의미하게 신장하였다(p

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

창의적 사고력 모형인 MH/SV/CV 모델을 적용한 탐구 화학 실험에서의 창의적 사고력과 비판적 사고력

정솔 강순희*

이화여자대학교 과학교육과

본 연구에서는 서울 소재 사범대학에 다니는 예비 과학 교사들이 수강하는 탐구 화학 실험 수업에 적용할 수 있도록 가설 설정을 MH/SV/CV 모델로 강화한 교수 전략을 개발하였다. 학생들은 창의적 사고력과 비판적 사고력을 향상시키는 측면으로 개발된 교수 전략에 따른 한 학기 동안의 실험을 경험하였다. 이 연구 결과, 본 연구에서 개발한 MH/SV/CV 모델 기법을 적용한 실험 교수 전략을 경험한 학생들의 창의적 사고력이 통계적으로 유의미하게 향상되었다(p.05). 또한 비판적 사고력의 5 개의 하위 요소 중에서 가설 설정 능력은 통계적으로 유의미하게 향상되었다으나(p.05).

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

초등과학교육에서 소집단 과학상상화 그리기의 유용성 탐색 연구

강훈식

춘천교육대학교 과학교육과

지금까지는 과학상상화 그리기와 관련한 연구가 거의 없어 이 활동의 효과성에 대한 정보나 과학교육에서의 효과적인 활용 방안이 구체적으로 제시되지 못하고 있는 실정이었다. 더군다나 과학상상화 그리기 대회가 2013 년부터 2 인 1 조 형식으로 변경되어 일선학교에서 지도 방법의 변화가 불가피함에도 불구하고, 그 효과에 대한 근거 자료나 실행에 있어서의 어려움에 관한 연구는 거의 없는 실정이었다. 이에 초등과학교육에서 소집단 과학상상화 그리기의 유용성 탐색 연구의 일환으로, 이 연구에서는 짝 활동이 과학상상화 그리기의 효과에 미치는 영향을 과학상상화의 특성, 과학상상화 그리기의 교육적 효과 및 어려움에 대한 인식, 짝 과학상상화 그리기의 장단점 측면에서 조사하였다. 연구 결과, 개별보다 짝 집단 환경에서 학생들은 '과학' 항목을 주제로 한 과학상상화를 약간 더 많이 그렸다. 학문 분야에 따라서는, 두 집단에서 모두 '기계' 분야가 가장 많이 나타났으며, '건설/교통', '지구과학', '환경', '에너지/자원' 분야도 비교적 많이 나타났다. 특히 '환경', '지구과학' 분야의 경우에는 개별보다 짝 집단 환경에서 더 높은 비율로 나타났으며, 3 개 이상의 학문 분야가 통합되어 나타난 경우도 개별보다 짝 집단 환경에서 더 많았다. 장소에 따라서는 두 집단에서 모두 '육지'와 '우주'가 주로 나타났고, '바다'가 나타난 경우도 적지 않았다. 시제의 경우에는 두 집단에서 모두 '미래', '현재' 순으로 나타난 반면 과거는 나타나지 않았으며, 특히 개별보다 짝 집단 환경에서 미래와 현재의 발생 비율 차이가 더 적었다. 전반적으로 개별보다 짝 집단 환경에서 그린 과학상상화가 좀 더 정교한 편이었다. 짝 활동이 인지적, 정의적, 심미적 측면에서 과학상상화의 교육적 효과에 대한 인식을 긍정적으로 변화시키지는 못하는 반면, 정의적 측면 중 과학에 대한 흥미 유발과 친근감 유발에는 긍정적으로 작용하는 것으로 나타났다. 짝 활동은 학생들이 개별적으로 과학상상화를 그리는 과정에서 겪는 상상하기, 주제정하기, 표현하기 측면에서의 어려움을

감소시키지는 못하였다. 많은 학생들이 짝 과학상상화 그리기에 대하여 서로의 단점 보완, 친구와의 친근감 유발, 과학상상화 그리기에 대한 흥미 유발, 과제수행시간 단축, 양질의 아이디어 생성 등과 같은 다양한 인지적, 동기적 장점을 언급하였다. 하지만 의견 불일치나 역할분담의 부재 등과 같은 협동기술 부족에 관한 단점을 지적한 경우도 적지 않았다.이런 결과는 짝 과학상상화 그리기의 효과성과 제한점을 밝혀 과학상상화 그리기 지도 방법의 다양화를 꾀하고, 짝 집단 형식의 대회 운영과 지도나 일반 과학수업에서 과학상상화 그리기의 효과적인 활용 및 지도 방안에 다양한 시사점을 제공할 수 있을 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

중학교 과학 및 고등학교 화학 ⅠⅡ 교과서에 제시된 실험 중 안전기호 및 안전에 관한 내용 분석

이재환* 류재정[1,*]

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과학교육에서 오래 동안 강조해 온 탐구는 교과서 내에서 여러 가지 형태로 나타나지만 그중 실험은 과학교과의 가장 기본적인 활동이자 동시에 안전사고의 위험이 항상 수반된다.교과서에 각 실험활동을 수행하기 전에 숙지해야 할 실험 안전에 관한 내용이 많이 부족하고 실재 교사와 학생 모두 안전에 관한 인식이 많이 부족하다는 것이 선행연구를 통해 인지하였다. 교과서에 제시된 실험마다 실험 안전에 대한 내용이 충분히 반영되었는지에 대한 연구의 필요성을 바탕으로 본 연구에서는 2013 년도에 발행된 교과서를 기준으로 과학 및 화학수업에서 요구되는 실험들 중에 특별히 안전에 유의해야 하는 실험부분 중 특별히 안전에 유의해야 하는 실험을 중심으로 실험의 종류 및 사용 도구 및 시약, 실험 방법 등을 분류하고 실험안전 기호 및 실험 안전 표시 내용이 충분히 제시 되었는지 비교 분석하였다. 본 연구를 토대로 실험 안전의 중요성을 교사와 학생 모두에게 고취시키고 차후 교과서 개정에서 실질적이고 효과적인 실험 안전 내용을 수록할 수 있도록 기초자료를 제공하고자 한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

과학관 전시에 사용된 디지털 매체 분석

차정호[*] 김학범

대구대학교 과학교육학부

학교밖 과학 학습을 위한 학습 공간으로서 최근 들어 과학관이 많은 주목을 받고 있다. 이 연구에서는 박물관을 포함하는 과학관에서 활용되고 있는 다양한 디지털 매체를 조사하고 분석하였다. 과학관에서 사용되고 있는 디지털 매체는 1) 전시물 제작, 2) 전시 설명, 3) 창작 및 체험 공간, 4) 과학관 통합 관리 측면으로 구분하였다. 전시물 제작에는 그래픽 패널, 모형, 영상, 테이블 탑 인터페이스 등이 사용되었고, 전시 설명을 위해서는 휴대용 단말기와 모바일 앱이 사용되었다. 창작 공간을 위해서는 아두이노와 3D 프린터 등의 도구가 일부에서 사용되었고, 과학관 통합관리를 위해 웹사이트가 광범위하게 사용되었다. 발표를 통해 국내외 여러 박물관 및 과학관의 구체적인 사례가 소개될 것이다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

미래사회 핵심역량에 대한 과학교사들의 인식

박혜진

용인홍천고등학교 1학년부

지식이 폭발적으로 증가하고 지식의 변화 주기가 짧아지면서 학교교육을 통해 학생에게 모든 지식을 전수하는 것이 불가능해졌다. 최근 학생들이 학교교육을 통해 단순히 지식을 축적하기보다는 실제로 무언가를 할 수 있는 능력 즉 역량을 높일 수 있는 방안에 대한 연구가 많이 이루어지고 있다. 또한 전세계적으로 교육과정 자체를 역량중심으로 개편하려는 움직임도 많다. 하지만 현장 교사들은 미래사회 핵심역량에 대해 잘 모르고 역량과 관련된 수업 자체를 어렵다고 인식하는 경우가 많다. 이에 과학교사들이 역량에 대해 어떻게 인식하는지 역량 관련 수업에 대해 무엇을 어려워하는지 정확하게 조사할 필요성을 느꼈다. 경기도 중등 과학교사들을 대상으로 역량에 대해 구체적인 설문 조사를 실시하였다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 수 16:00~19:00

Social Emotional Learning(SEL)의 관점에서 본 2009개정 교육과정 중학교 과학교과서 분석

김건희 신선희[1] 박현주[2,*] 모란[3]

조선대학교 화학교육과 [1]조선대학교 과학교육학과 [2]조선대학교 과학교육학부 [3]조선대학교 화학교육학과

“청소년 범죄, 단순 일탈 넘어서” ‘무서운 아이들'..촉법소년 범죄 연평균 1 만건 '카톡 왕따' 언어폭력 심각‥여고생 자살 “학교폭력 하루 평균 267 건” 나날이 청소년 문제는 증가하고 있으며, 우리나라 뿐만 아니라 다른 나라 또한 청소년 문제에 대한 문제가 대두되고 있다. 이러한 문제의 원인으로는 학생들에게 대해 지적 성과만을 바라며 사회적 정서적 교류와 참여에 대해서는 괄시하고 있는 기존의 교육 환경을 요인으로 꼽으며, 이에 대한 해결방안의 최우선 추진분야로써 인성교육의 강화에 대한 목소리가 매년 높아지고 있다. 이와 같은 문제로 고민하고 있는 해외에서는 최근, 보다 효과적이라고 제시되고있는 학습모델인 Socail Emotional Learning(사회정서학습)에 집중하고있다. 현재 우리나라 과학 교육은 인지적 영역과 탐구적 영역에 치중하고 있는 반면 SEL 관점에서는 인지적, 탐구적 영역과 더불어 다양한 영역을 필요로하고 있다. 이에 SEL 관점에서의 역량을 정의하고 2009 개정 교육과정 중등 과학교과서에서 SEL 역량이 얼마나 내재되어 있는지를 분석하고자 한다.

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논의 기반 일반화학실험에 의한 학생들의 모델링 능력 변화

이동원[*] 남정희 강여은[1]

부산대학교 화학교육과 [1]부산대학교 교육대학원

모델링이란 관심의 대상이 되는 현상에 대해 구체적인 형태로 자신의 생각을 표현하고 이를 수정해 나가는 과정을 말한다. 모델은 이론과 실제를 이어주는 다리의 역할을 수행할 수 있으며, 과학수업에서 모델링을 활용함으로써 학생들은 좀 더 과학을 실재적인 방법으로 이해하는데 도움을 받을 수 있다. 모델링 활동에서 학생들은 자신의 모델을 수정, 보완하기 위해 각자의 모델에 대해 의견을 교환한다. 모델링 활동에서 모델과 논의는 서로 긍정적인 영향을 줄 수 있다. 모델은 구체적인 설명을 제공함으로써 논의의 폭과 깊이에 영향을 줄 수 있으며, 모델에 대한 논의는 더욱 정교화 된 모델을 만드는데 도움이 될 수 있다. 논의 기반 일반화학실험에서 학생들은 논의를 통해 문제 상황이나 관찰 결과에 대한 자신의 생각을 표현하고 수정하게 된다. 학생들은 논의 기반 일반화학실험을 수행하는 과정에서 현상에 대한 각자의 설명체계를 만들고 정교화 한다. 이러한 점에서 학생들은 모델링을 수행한다고 볼 수 있다. 이 연구에서는 논의 기반 일반화학실험 활동이 학생들의 모델링에 미치는 영향을 탐색하여, 학생들의 설명체계에 어떠한 변화가 나타나는지 알아보고자 하였다. 연구를 위해 대학교 1 학년 21 명을 대상으로 1 학기 동안 6 개의 프로그램을 투입하고, 학생들이 작성한 실험 보고서를 수집하였다. 또한 전체 프로그램 실시 전, 후에 모델링 검사를 실시하고 사후에 인터뷰를 통해 모델링에 대한 학생들의 생각을 조사하였다. 수집된 자료들을 바탕으로 프로그램 진행과정에서 나타나는 학생들의 모델링 능력의 변화를 분석하고 인터뷰 내용으로 그 변화의 이유를 유추해 보았다. 프로그램이 진행됨에 따라 학생들은 학습한 내용을 여러 종류의 표상으로 표현하며, 풍부한 개념을 일관성 있게 조직한다. 또한 독자를 고려하여 글을 구성하고 실제 수행한 실험에서 획득한 경험을 바탕으로 설명하는 모습을 보인다. 인터뷰에서 학생들은 초기에 모델링이 무엇인지와 이를 작성하는 방법에 대한 지식이 부족하여 어려웠다는 의견을 많이 표현하였으며, 프로그램을

수행하는 과정에서 다른 학생들이 작성한 글을 보고 의견을 나눈 피드백과 실험과 관련하여 수행한 학급 토론이 모델링에 대한 어려움을 해소하는데 도움이 되었다고 진술하였다.

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Flipped Learning Education Model in General Chemistry Course

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The flipped learning education model inverts the traditional model by delivering instruction online (outside of the classroom) and moving “homework” into the classroom. It consists of three parts: pre-class, in-class, and after-class sessions. In the pre-class session, all the learning materials are provided on the blackboard (BB) system, a learning management system (LMS), so that students can take online quizzes and solve assigned problems. During the in-class session, an instructor delivers a summary lecture and students solve more advanced problems. In the after-class session, students review both the learning materials and the solutions provided on the BB. In addition, the recitation class or the tutorial session is offered to help students. This model was adopted jointly at UNIST and POSTECH to stimulate the learning in General Chemistry courses.

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일반계 고등학생들의 화학 반응속도와 평형의 개념형성과 개인차 요소간의 상관성

유왕선 김봉곤[1,*]

경상대학교 대학원 과학교육학과(화학교육전공) [1]경상대학교 화학교육과

고등학교 화학Ⅱ에서 화학평형과 화학반응속도 단원은 미시적이고, 동적이며, 수리능력이 요구되는 단원의 특성 때문에 학생들이 개념의 습득에 많은 어려움을 겪고 있으며, 따라서 다른 단원에 비해서 많은 오 개념을 파지하고 있는 것으로 조사되어 있다. 최근 우리나라 학교교육은 학생들의 창의성 계발과 자기주도적 학습능력의 향상에 지향점을 두고, 범국가적 차원에서 이를 강조하고 있다. 이러한 교육목표의 달성은 교과목/단원의 특징과 학생들의 개인적 특성을 고려한 학습지도의 설계와 실행이 동반되었을 때 가능하다. 따라서, 본 연구의 목적은 학생들의 개인적 특성을 고려한 화학Ⅱ 개념의 효과적인 학습지도방안을 마련하는 기초자료를 제공하기 위해서, 전남지역 일반계 고등학교 2 개교 3 학년 학생을 대상으로 화학Ⅱ에서 화학평형과 화학반응속도 단원의 개념 형성과 오 개념 유형을 파악하고, 지역, 성별 및 학생들의 개인차 요소(학습양식, 사고양식)과 같은 개인차 요소와 연관시켜 해석하고자 하였다.

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DFT study on the conformational isomerism of Schiff base as N,N'-bis(3,3'-dichlorosalicylidene)-2,2'-ethylenedianiline

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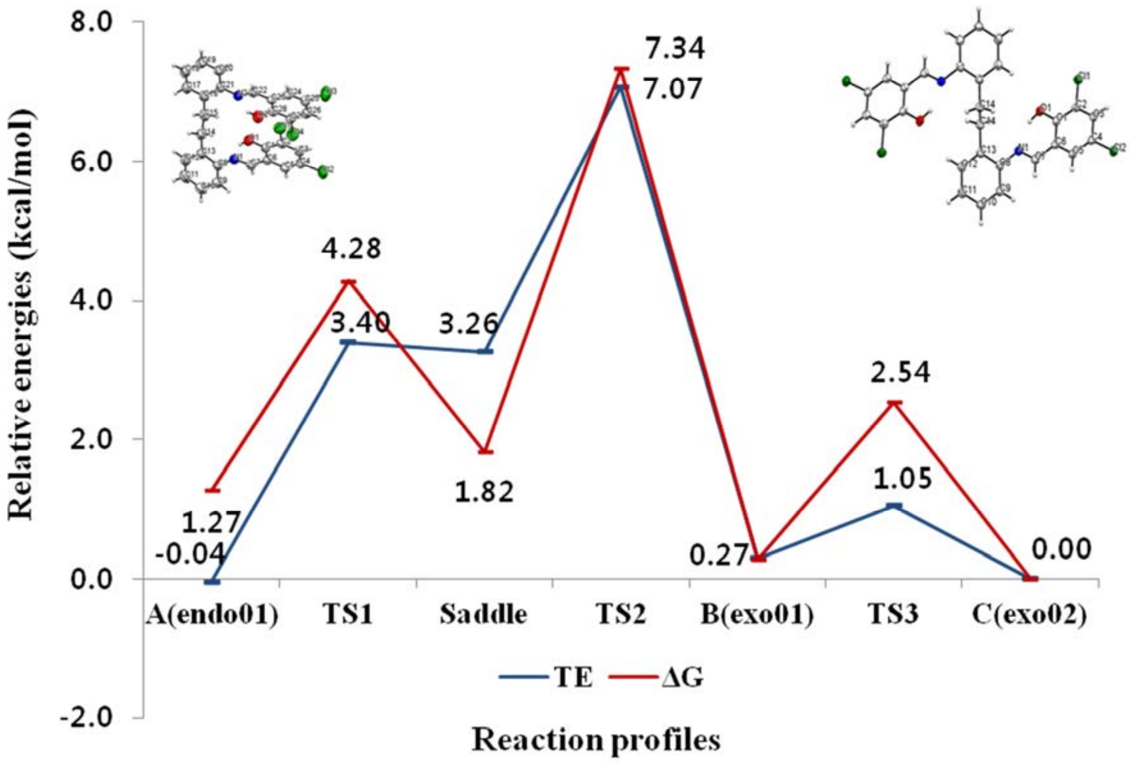
We had synthesized and characterized the Schiff base as N,N'-bis(3,5-dichlorosalicylidene)-2,2'-ethylenedianiline(L) by X-ray diffraction, FT-IR, and UV-Vis spectra. It was identified that the L can be exist Syn and Anti isomer as conformer in solid state. In this papers, To explore the molecular characteristics of two occurring conformers of N,N'-bis(3,5-dichlorosalicylidene)-2,2'-ethylenedianiline(L), DFT and TD-DFT calculations with density functional (B3LYP, PBE1PBE, and M11L) have been employed in a study of the conformational isomerism of N,N'-bis(3,5-dichlorosalicylidene)-2,2'-ethylenedianiline(L).According to the DFT calculation result, it was found that the conformational isomers of title compound can be exist six representative conformer according to torsion angle of main skeleton. The geometries of conformer Syn01 and Anti02 were in good agreement with X- ray crystal structure analysis. And also, We have identified that the overall reaction profiles of conformational isomerism proceeds through the three step reactions. In the second step, the higher energy barrier is shown that the conformational isomerism of the saddle compound is more proceed to the endo01 than to the exo01 isomer at a relatively low temperature.


8.0
6.0
4.0
2.0
0.0
-2.0
Relative energies (kcal/mol)
7.34
7.07
4.28
3.40
3.26
2.54
1.82
1.27
-0.04
1.05
0.27
0.00
A(endo01)
TS1
Saddle
TS2
B(exo01)
TS3
C(exo02)
TE
ΔG
Reaction profiles

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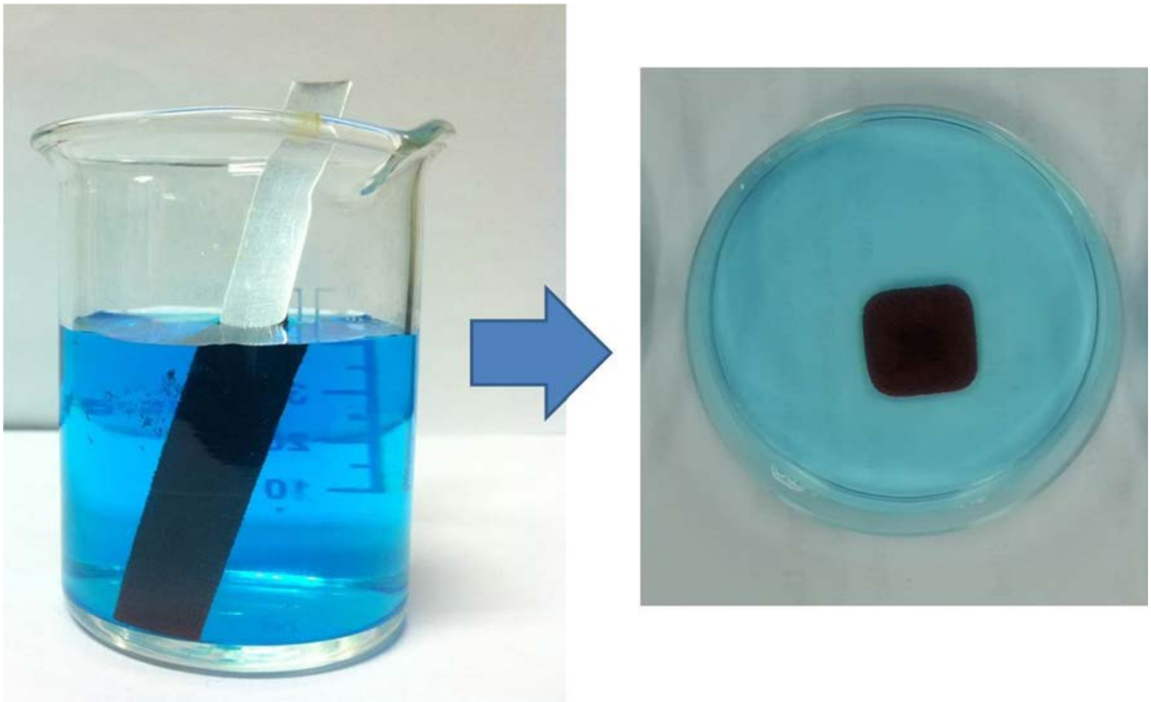
산화-환원 반응과 전위차 실험의 시각적 교재화 자료 개발

박진희 신동선[1] 유왕선[2] 김봉곤[3,*]

경남과학고등학교 [1]경남과학고등학교 과학교육부 [2]경상대학교 대학원 과학교육학과(화학교육전공) [3]경상대학교 화학교육과

산화-환원반응은 산-염기반응과 함께 화학반응에서 매우 중요한 개념이지만, 학생들은 개념의 습득과정에서 매우 어려움을 호소하고 있다. 특히, 황산구리 수용액과 금속아연의 반응에서 초기 환원 생성물은 실험조건에 따라서 검은색, 붉은색으로 얻어진다. 이처럼 실험조건에 따라서 다른 실험결과가 얻어지는 것은 학생들의 새로운 궁금증을 유발하기도 하지만, 불완전한 결과해석으로 화학교과에 대한 모호성이 증대되고 산화구리의 생성이라는 오개념을 유발하기도 한다.따라서, 본 연구에서는 구리(Ⅱ)이온과 금속간의 산화-환원반응에서 환원제(아연, 알루미늄, 철), 금속 염(염화 구리, 황산구리, 질산구리)의 종류에 따른 반응생성물의 확인과 반응속도 측정의 시각화 학습도구를 개발하고, 학습단계에 적절한 학습지도 자료의 표준화 방안을 개발하였다.



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중학교 물질분야의 검·인정 교과서에 따른 비교·분석

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2009 개정 교육과정에서는 세계화 시대에 대비한 교육과정으로의 전환이라는 정책기조를 반영하고, 21 세기에 적합한 인간상으로 새로운 지식을 창출하는 인간으로 규정하였다(교육과학기술부, 2009). 이에 따라 과학과 교육과정은 미래 지식 기반 사회에서 요구하는 인간상을 분석한 결과 가장 중요한 요소가 창의적 문제 해결력을 가진 인간이라고 확인하여 교육과정의 기본 정신을 학습자의 개별성 중시 및 과학적 창의성 함양으로 개정하고 '창의적 신장'을 과학교육의 목표에 포함시키는 것이 무엇보다 중요하다고 인식하였다. 또한 정부는 '2010 교과서 선진화 방안'을 도입하였다. 이러한 발표의 배경은 현재의 교과서는 방대한 분량의 지식이 요약, 압축된 형태로 수요자인 학생들에게 적합하지 않고, 현행 교과서 체제 내에서 출판된 교과서는 학생들의 자기 주도적 학습을 효과적으로 지원하지 못할 뿐만 아니라, 학습에 대한 흥미와 즐거움을 부여해주는데도 한계를 보여 왔다는 데에 있다. 한계의 원인으로 국정과 검정 교과서가 중심을 이루는 교과서 체제로 보고 이를 교과서 인정제도의 확대 실시하였다. 이 연구는 과학교과서에서 국정과 검정 교과서 체제가 점차 인정 교과서 체제로 변화하고 있는 시점에서 교육과정의 변화에 따른 교과서 변화가 얼마나 잘 반영되고 있는지 알아보기 위한 것이다. 중학교 과학의 물질 분야에 대해 2007 개정 교육과정의 중학교 과학과 2009 개정 교육과정의 과학 교과서를 구성체계, 내용체계, 탐구, 읽을거리측면에서 분석틀을 준비하고, 비교·분석한다. 인정 교과서 제도가 확대되어가는 시기에 실효를 거두기 위해서는 교과서 질 관리에 대한 점검이 우선시 되어야 하는데 이 논문은 교육과정 개편에 따른 교과서 개발 시 기초자료로 유용하게 쓰일 것이며, 현장 교사들의 교수학습의 지침서로 활용될 수 있을 것이다.

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환경교육에 대한 초등교사들의 요구

강석진

전주교육대학교 과학교육과

이 연구에서는 환경교육에 대한 초등교사들의 요구를 조사하였다. 환경교육에 대한 요구를 조사하기 위하여 환경교육 지원과 환경교육 연수의 2 가지 범주 총 22 문항으로 구성된 설문지를 개발하였으며, 환경교육 연수 범주의 경우 원격 연수와 현장 연수에 대한 선호도를 추가로 조사하였다. 교사들의 배경 변인에 따른 요구를 분석하기 위해 교육 경력, 학위, 환경수업 여부 등의 배경 변인도 조사하였다. 초등교사 155 명에게 설문을 의뢰하여 113 부를 회수하였다. 연구 결과, 초등교사들은 환경교육 지원 범주의 모든 문항에 대하여 필요성을 인식하고 있었다. 그 중에서도 새로운 정보 제공, 현장학습 기회, 야외학습장 제공에 대한 지원 등에 대한 요구가 높게 나타났다. 반면, 환경수업 전문가 강연, 학생 동아리 모임, 웹사이트 운영에 대한 요구는 상대적으로 낮았다. 환경교육 연수 범주에서도 모든 문항에서 연수의 필요성에 대하여 요구가 높게 나타났다. 그 중에서도 교사의 요구가 상대적으로 높았던 문항은 지역 내 환경교육 장소 정보 제공, 환경교육 이슈에 대한 교육, 환경교육 수업 전략 등이었다. 환경교육 연수 방법에 따른 선호도 조사에서 대부분의 문항에서 현장 연수보다 원격 연수에 대한 선호도가 높았다. 그러나 지역 내 환경교육 장소 정보 제공, 학교 밖 환경교육 장소 개발 및 사용에 대한 문항에서는 현장교육 연수를 상대적으로 선호하는 것으로 나타났다. 경력 교사들은 초보 교사보다 현장 연수에 대한 요구가 상대적으로 높았으며, 환경 수업을 실시하는 교사들은 현장 연수를 상대적으로 많이 요구하고 있었다.

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Catalytic mechanism of the outer-membrane species of anerobic microorganisms

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The redox potentials of possible redox species at the microbial cell surface and anode interface at pH 7 are -0.32 V for NAD+/NADH, -0.28 V for CO2/acetate, -0.20 V for FMN/FMNH2, and 0.254 V for c-type Cyt(Fe3+)/c-type Cyt(Fe2+) (vs. NHE). Here, NAD and FMN are nicotinamide adenine dinucleotide and flavin mononucleotide, respectively. The latter two species are bound to the outer-membrane (OM), which are involved in DET to the anodes. The former two species, in particular, the first species, are expected to be coupled for their oxidation to be catalyzed by the latter two OM species. According to cyclic voltammetric data of the present study, it is found that there exist two pairs of redox reactions with substrate turnover (ST) condition; one at E1/2 of -0.29 V and the other at E1/2 of -0.20 V. In particular, it has been found in the present study that the E1/2 of -0.29 V under the ST condition was shifted from the E1/2 of -0.19 V under the substrate non-turnover (SNT) condition, presumably to catalyze NAD+/NADH coupled redox reaction by an outer-membrane-bound FMN/FMNH2 (OMF) or c-type Cyt(Fe3+)/c-type Cyt(Fe2+) (OMC) redox reaction. The E1/2 under SNT of this study was closer to that of OMF. However, it has been known that the redox potential for the OMC has a range of -0.420 V to -0.060 V, and many researchers have reported that OMC is a main agent for DET in the mixed-culture bio-film. Therefore, the OMC mechanism should be further studied until the clear mechanism is resolved.

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Efficient Capture of CO2 by Aqueous Hydrazine

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서강대학교 화학과

We report that aqueous hydrazine (32 wt %) can be a promising absorbent for carbon dioxide (CO2) capture. We carefully evaluated the viability of aqueous hydrazine in terms of its absorption capacity, overall mass transfer coefficient, cyclic capacity, thermal stability, and viscosity. The results obtained from lab scale experiments are compared to those of a benchmark monoethanolamine (MEA, 30 wt %). Aqueous hydrazine exhibited excellent mass transfer performance and had comparable cyclic capacity in comparison to the MEA sorbent. Cyclic experiments of CO2 absorption and desorption yielded nearly identical values for CO2 absorption capacity, suggesting that aqueous hydrazine has high thermal stability. In addition, the 32 wt % hydrazine solution possesses low viscosity, which is beneficial especially for making the blended solvent system. The lab scale data reported here provide important information towards the industrial use of aqueous hydrazine for post-combustion CO2 capture applications.

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Effects of E-beam on struvite crystallization

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Nitrogen is an essential nutrient for living organisms; however, it can provoke water eutrophication when it is present in excess. Therefore, ammonia?nitrogen removal from wastewaters is of importance to prevent environmental pollution. Struvite ($MgNH_4PO_4?6H_2O$) is a white crystalline compound composed of magnesium, ammonium, and phosphate in an equal molar ratio. Removal of ammonia as struvite has been widely investigated on the treatment of wastewaters. Since the amount of $PO_4^{3-}$and Mg^{2+} in wastewaters are usually inadequate, a great amount of phosphate or magnesium salts are required for the effective removal of ammonia. This leads to a high operating cost, which hampers the widespread application of the struvite process. To solve this problem, we studied the effects of electron beam (E-beam) on the struvite crystallization. The formations of struvite as produced under different reaction conditions were confirmed by SEM, EDS, XRD, and wet chemical analysis.

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Hybrid Carbon-Metal Oxide Electron Transport Layers in Organic Solar Cells

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One of the major issues on inverted organic solar cells (OSCs) is to use the electron transport layers (ETLs) for increasing electron collection efficiency and suppressing carrier recombination. Several factors should be met to obtain favorable ETLs for an efficient photovoltaic device, such as good transparency, high electron mobility, favorable morphology, and high electron affinity to collect the electrons. For example, n-type semiconductors and carbon materials have been used as the ETLs for increasing the electron collections in solar cells. ZnO and TiO_2 have drawn attention because of their good transparency, environmental stability, simplicity of process and low crystallization temperature. Carbonaceous materials have been reported to increase the electron collection capability in OSCs owing to high electrical conductivity. From these known advantages of carbon and metal oxide, here in, we try to combine both materials with synergistic features.Carbon-metal oxide hybrids could serve as effective interfacial layers for poly(3-hexylthiophene) (P3HT):(6,6)-phenyl-C_{61}-butyric acid methyl ester ($PC_{61}BM$) based OSCs. Metal oxide precursors mixed with triblock copolymers are spin-coated on substrate and carbonized in Ar atmosphere. This method creates mesoporous carbon-metal oxide films with high surface area and controllable pore size. We demonstrate highly efficient OSCs by integrating mesoporous carbon-metal oxide in comparison with the devices without pores or the ones with neat mesoporous metal oxide.

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Design and assessment of bimetallic oxygen reduction catalysts as applied to microbial fuel cells

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Although main focus has been made on anodes where microorganisms function as biocatalysts oxidizing various organic and inorganic substances, more and more attention has been pouring on cathodes. Like chemical fuel cells, microbial fuel cells (MFCs) also use oxygen as a cathodic fuel and thus it is of paramount importance to develop cost effective, reliable oxygen reduction reaction (ORR) catalysts that can replace precious metal-based catalysts. Here we present our preliminary results of ORR catalysts development using bimetallic combination. We designed the catalyst system based on thermodynamic principles in which each metal plays different roles. In addition to that, we also investigated the effect of nitrogen atoms on ORR as they have been known to greatly increase ORR activity. To incorporate N into bimetallic systems, we synthesized M-Pd (M=V or Zn) systems from a mixture of metal salt precursor with a nitrogen-donating compound (N) and carbon nano powder (C) and heat-treated them at high temperature. Catalyst performance was evaluated by rotating disc and rotating ring-disc (RRD) techniques. From RRD experiments, the onset potential of ORR and the percentage of hydrogen peroxide were calculated. It turned out that bimetallic systems have better ORR activities than individual components. When applied to MFCs, power enhancement was observed.

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Investigation of current collector material and construction for enhanced microbial fuel cell performance

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Microbial fuel cells (MFCs) are electricity generating devices that use microorganisms as a biocatalyst. The chemical energy stored in organic materials is converted into electrical energy by microorganisms. During oxidation process, electrons are generated and collected by current collectors. The current collectors transfer the electrons to electrode which then flows to the external circuit. In this process, electricity is generated and can be used for useful work. But MFCs face challenging issues that have to be solved for critical application. Current collector is one of the key factors that affect the efficiency and cost of MFCs. In this study, the effect of contact area between anode and current collector using Titanium wire (Ti-wire) and Titanium mesh (Ti-mesh) and the effect of Titania (TiO_2) 1D nanostructure were investigated. Glucose (1 g/L) is used as substrate and microorganisms were obtained from wastewater taken from Hyeonpung sewage treatment plant. The MFC with Ti-mesh based anode showed the highest maximum power density (16.3 W/m^3).

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CuO-TiO$_2$ heterostructured composite for CO$_2$ reduction by solar irradiation

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CuO-TiO$_2$ hetero-structured composite were prepared by novel synthetic method and its photo-catalytic effect were evaluated with a methylene blue degradation and CO$_2$ reduction by gas chromatogram (GC) under simulated solar irradiation. Copper (II) oxide, a p-type semiconductor with narrow bandgap (E_g=1.2 eV), have received much attention in recent years as a good catalyst due to its high selectivity and activity in CO$_2$ reduction. In particular, CuO is a good candidate in the field of CO$_2$ reduction because of its valence band position that lies near the CO$_2$/O$_2$ potential. A strategy to enhance the CO$_2$ reduction efficiency is to couple CuO with TiO$_2$ to form p-n heterojunction that can enhance a charge separation efficiency of photogenerated charge carriers, stability against photocorrosion, and suitable band alignment for direct CO$_2$ reduction.

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CuO-TiO_2 nanostructure for CO_2 conversion to methane

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One of the major problems concerning environmental pollution and global warming is a rapid escalation in the level of carbon dioxide in atmosphere. The atmospheric CO_2 level can be reduced by converting it into useful products via thermochemical and photochemical processes. Amongst these conversion processes, the photochemical conversion is a cost effective and preferred process for the photoreduction of CO_2 into useful liquid fuels like methanol, formaldehyde, and methane gas. Here, we synthesized CuO-TiO_2 nanostructure, a hybrid material photocatalyst and tested for CO_2 photoreduction. The synthesis process involves the formation CuS nanostructure using electrochemical anodization followed by embedment of titanium isopropoxide as Ti precursor. The oxidation of the nanosctuctre is performed at temperature of 400 °C oxidizing Cu and Ti to form CuO-TiO_2 nanostructures.

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Cu_2ZnSnS_4 (CZTS) nanocrystal/TiO_2 composites for efficient photocatalytic reduction of CO_2

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CO_2 emissions is one of the largest political causing global warming. A variety of approaches for addressing CO_2 emissions are currently under research. Photocatalyst is one of the effective strategies to solve this issue. TiO_2-based materials are the most stable and preferred photocatalysts. But TiO_2 are only active under ultraviolet (UV) irradiation, because TiO_2 has a demerit of wide bandgap (3.3eV). For the efficient use of TiO_2 photocatalysts, one of the approaches is to couple it with another small bandgap photocatalytic material focused on broadened light absorption region. The band alignment between Cu_2ZnSnS_4 (CZTS) nanocrystal and TiO_2 favors charge separation across the interface, eliminating inefficiencies associated with direct carrier recombination.In this work, an attempt was done to fabricate hybrid photocatalyst based upon p-n heterojunction and applied for CO_2 photoreduction. CZTS, a well-known p-type semiconductor with a narrower direct band gap of 1.5eV, was synthesized and coupled with n-type TiO_2. The synthesis of hybrid photocatalyts was confirmed by numerous characterization techniques such as XRD, TEM, and UV-Vis spectroscopy.

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QSAR studies for predicting the chemical toxicity to the bioluminescent photobacterium (Vibrio fischeri)

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Quantitative structure-activity relationships (QSARs) attempt to relate statistically the biological activity of compounds to their chemical structure. The Vibrio fischeri bioluminescence assay which are rapid, cost effective and reproducible are gaining popularity. In this study, QSAR studies on Vibrio fischeri were derived using 2D molecular structure and several data mining methods. A dataset of effective concentration (pT50) for Vibrio Fischeri marine bacteria was assembled to develop a QSAR models from Kasier and Palabrica's publication. QSAR studies based on multiple linear regression and support vector machine were applied to estimate the ecotoxicity, expresssed as pT50 (Vibrio fischeri). All these models have been statistically validated (both internally by cross-validation and bootstrap and externally by blind testing).

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Salinity intrusion decreases monomethylmercury accumulation in the Mekong Delta food web via resuspension of fine-sediment particles

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The Mekong River Delta plays an important role in the sustainability of Southeast Asian fisheries and aquacultures. Annually, approximately 2,000,000 tons of fish are harvested from the Mekong River Delta, which provides 75% of the animal protein consumed by the rural Vietnamese population. Despite this importance, geochemical investigation of monomethylmercury (MMHg) bioaccumulation has been largely understudied. In the current study, we identified important biogeochemical factors affecting MMHg accumulation in Mekong Delta invertebrates and fish, focusing on the influence of salinity intrusion on the MMHg accumulation. Dietary carbon source as well as trophic position of the organism was identified as an important feature in determining MMHg bioaccumulation. In particular, freshwater carbon-feeding fauna, indicated by δ^{13}C depletion, showed a greater MMHg accumulation than coastal carbon-feeding fauna, which seems to be caused by enhanced trophic position (δ^{15}N = 5.9±1.0%) and MMHg concentration (5.9±3.0 pM) of freshwater microseston than those of estuarine microseston (δ^{15}N = 4.8±0.3%; MMHg = 1.9±2.4 pM). We suggest that resuspension of surface sediment, depleted in organic carbon and MMHg, in the estuarine mixing zone, decreases bioaccumulation of MMHg in the Mekong River Delta.

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Development of treatment and recycling techniques of waste nutrient solutionsfor hydroponics system

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During the last few decades, the soilless cultivation of vegetables and ornamentals has been increasingly shifted to closed hydroponics systems which are considered as environment-friendly cultivation systems. The main advantage of hydroponics systems is the reduction of water pollution by recycling the nutrient solutions used for hydroponics. In general, waste nutrient solutions contain relatively high concentrations of major ions (e.g., K+, NH4+, Mg2+, Ca2+,Cl-,NO3-, PO4-, SO42-) compared to those in municipal and industrial wastewater. Many developed countries have extensively investigated and developed the recycling and treatment technologies for the waste nutrient solutions. For example, several horticultural industries in Japan have examined the re-use techniques of waste nutrient solutions by the simultaneous reduction of pathogenic bacteria and heavy metals with activated carbon and excessive nutrients (e.g., NO3-) with Watercress. In Korea, a few studies have been conducted for sterilizing nutrient solution. A study showed that the passive flow-through system with sand and activated carbon layers is effective in sterilizing microorganisms (fungi, bacteria and some viruses). However, it required relatively long time for the successful outcomes and was difficult to maintain. In this presentation, we compare the physical, chemical and biological methods for the reduction of pathogens and excess nutrients in hydroponic systems in Europe, Japan and domestic. Also, we will present alternative, eco-friendly and efficient strategies for recycling and treatment of the waste nutrient solutions.

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In silico prediction of the degradation of pharmaceuticals and personal care products(PPCPs) by water treatment process

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Pharmaceuticals and personal care products(PPCPs) have been detected at low levels in water resources around the world. These compounds create challenges to water treatment since the number of compounds detected is large and keeps increasing and their physicochemical properties are highly diversified. Thus, in this study, quantitative structure-property relationship(QSPR) models for UV and O_3 water treatment processes are explored as a potential tool to prescreen these compound. Forward selection method were utilized to select significant descriptors from 2D descriptors in combination with multiple linear regression(MLR) and support vector machine(SVM) method. The models were evaluated by internal validation, external validation, Y-scrambling.

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Long-term and spatial variation of elemental concentrations in local streams impacted by abandoned mine drainage treated with limestone

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Spatial and temporal distribution of the elements in streams impacted by acid mine drainage (AMD) was investigated to determine controlling factors affecting local aqueous chemistry and changes in the concentration and distribution of metals before and after long-term limestone treatment. Water samples were collected in 2011 in Young Dong (YD) stream, Imgok Creek (IC), and adjacent streams, S. Korea. Young Dong AMD contributed to high concentrations of major and trace elements including Ca, Mg, Fe, Mn, Co, Li, Ni, Pb, Sr, and Zn in the YD stream. The spatial distribution of these elements was mainly controlled by redox processes, dilution on mixing with streams entering YD stream and IC, and co-precipitation/adsorption with Fe (hydr)oxides. Addition of limestone in 1999 lead to an increase in pH, and with the exception of Ca, the concentrations of the elements monitored in YD stream and IC generally decreased compared to data collected before limestone addition. However, the pH did not increase from 2008 to 2011 in the YD stream, suggesting the reactivity of the added limestone was reduced and that an alternative approach is needed to maintain effective long-term treatment. In contrast, K and Na levels temporally increased likely due to increases in agricultural activities along IC. This study suggests that physicochemical processes including dilution by mixing, redox reactions, co-precipitation/adsorption, and increases in pH were major factors controlling the spatial distribution of major and trace elements. However, even though the impacts of AMD can be countervailed by inputs from IC, the impact of other land use issues (e.g., agricultural activity) needs to be considered to assess regional water quality.

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A study on the diffusion coefficients of mercury complexes in agarose gels used for diffusive gradients in thin films

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A diffusive gradient in thin films (DGT) technique was applied to measure pore water Hg and monomethylmercury (MMHg) concentrations in lake and coastal sediments. DGT is one of the in situ passive sampling techniques, based on diffusion and adsorption of contaminants onto resin gels, that can be installed in experimental sites. To calculate Hg and MMHg concentrations in sediment pore water from DGT resins, determination of the diffusion coefficients of Hg(II) and MMHg for an agarose gel is required. Here, Hg and MMHg diffusion coefficients were determined under different concentrations of dissolved organic matter (DOM). In case of MMHg, the diffusion coefficient was found to be $3.7 \pm 0.6 \times 10^{-6}$ cm^2 s^{-1} for lake water and $3.4 \pm 0.4 \times 10^{-6} cm^2$ s^{-1} for coastal water. The total percentage of MMHg-DOM species increased as DOM concentration increased, and diffusion coefficients decreased; therefore, the MMHg diffusion coefficient seemed to be affected by the complexation of MMHg by organic ligands. The MMHg concentrations measured by DGT and centrifugation were comparable for pore water MMHg depth profiles, suggesting DGT applicability at the experimental sites.

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Reductive dechlorination of tetrachloroethylene by mackinawite in cement slurries with cobalamin

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Degradative solidification/stabilization (DS/S) is a modification of conventional solidification/stabilization (S/S) to degrade organic contaminants and immobilize inorganic contaminants simultaneously. This study investigates reductive dechlorination of tetrachloroethylene (PCE) in iron-based DS/S process by using mackinawite (FeS) and cobalamin (Cbl(III)) as an reductant and electron transfer mediator (ETM), respectively. FeS and Cbl(III) are naturally formed by microbial activity in the sulfate-reducing environment easily found at groundwater system. Cement has been found to enhance the reductive dechlorination kinetics of PCE by catalyze or participate in reactions. Cbl(III) has played a critical role as an electron transfer mediator (ETM) for reductive dechlorination of PCE in the DS/S-FeS system. The reductive dechlorination kinetics of PCE was significantly enhanced as concentration of Cbl(III) increased. The DS/S-FeS-Cbl(III) system was significantly dependent on pH. As pH increased, the dechlorination kinetics of PCE increased. To investigate the factors which catalyze or participate in PCE degradation reactions, X-ray diffraction, X-ray photoelectron spectroscopy spectra and Transmission electron microscopy image were obtained. Present studies can provide basic knowledge for enhanced reductive dechlorination of PCE by FeS in cement slurry with Cbl(III) in the sulfate-reducing environment.

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Geochemical Characteristics and Microbial Community Composition in Toxic Metal-rich Sediments Contaminated by Au-Ag Mine Tailings

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The effects of extreme geochemical conditions on microbial community composition were investigated using two distinct sets of sediment samples collected near weathered mine tailings. One set (SCH) showed extraordinary geochemical characteristics: As (6.7-11.5%), Pb (1.5-2.1%), Zn (0.1-0.2%), and pH (3.1-3.5). The other set (SCL) had As (0.3-1.2%), Pb (0.02-0.22%), and Zn (0.01-0.02%) at pH of 2.5-3.1. The bacterial communities in SCL were clearly different from those in SCH suggesting extreme geochemical conditions affected microbial community distribution even on a small spatial scale. The clones identified in SCL were closely related to acidophilic bacteria within the taxa Acidobacterium (18%), Acidomicrobineae (14%), and Leptospirillum (10%). Most clones in SCH were closely related to Methylobacterium (79%) and Ralstonia (19%), both of which are well-known metal-resistant bacteria. Although total As was extremely high, over 95% of it was in the form of scorodite (FeAsO4?2H2O). Acid extractable As was only ~118 and ~14 ppm in SCH and SCL, respectively, which is not known to be toxic to bacteria. Meanwhile, acid extractable Pb and Zn in SCH were above concentrations toxic to bacteria. Because As was present in an oxidized and stable form it is likely that Pb and/or Zn released from the sediment were mainly responsible for the differences in microbial community structure.

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Nano-QSAR approach for predicting the metals toxicity to Daphnia magna

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Nano-sized particles possess astonishing physical and chemical properties and have a number of fascinating potential applications in a wide range of industrial sectors such as electronics, magnetic and optoelectronics, biomedical, pharmaceutical, cosmetics, energy, environmental, catalytic, space technology and many others. However, since some nanoparticles can have a negative impact on human health and the environment, the design of nanoparticles should be always accompanied by a comprehensive nanosafety assessment. Thus, the development of model, complementary to experimentation, and sometimes even capable of replacing empirical testing, is of high interest. In this study using quantum-mechanical methods the calculations have been performed at the semi-empirical level of the theory for the 23 metals. The properties calculated from quantum-mechanical method were selected and model was developed using Multiple Linear Regression(MLR) and Support Vector Machine(SVM) method.

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Stable nitrate reduction over multiple recycles by eco-friendly bimetallic catalyst

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Potable water resources have been facing sever threats due to anthropogenic activities. Consequently, nitrate pollution is one of the most critical problem causing deterioration of surface and groundwater resources. Nitrate pollution potentially causes serious issues to environmental ecology and human health. Among denitrification techniques, catalytic nitrate reduction form water/wastewater has proven to be efficient, faster and reliable method. However, more studies are required to formulate eco-friendly catalyst and catalytic process to treat real groundwater for stable and selective nitrate reduction. In this study, we demonstrated stable nitrate reduction in real groundwater samples over multiple recycles using Cu-Pd bimetallic catalyst supported by hematite (Cu-Pd/hematite). All the experiments were performed in batch mode. More than 95% nitrate reduction was observed over four recycles by Cu-Pd/hematite catalyst. Nitrogen selectivity was observed in the range of ? 60% in all recycling batches. Nitrite selectivity was negligible (>1%), while about 40% ammonium selectivity was observed in all recycling experiments. Inductively coupled plasma mass spectrometry (ICP-MS) analysis revealed that negligible Cu and Pd leaching occurred during all recycling batches. The results from this study showed that Cu-Pd-hematite is a stable catalyst with respect to recycling and nitrate reduction, with relatively higher nitrogen selectivity

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Effects of soil particle size and micropore volume on TPH removal from contaminated soils

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To remediate soils contaminated by petroleum hydrocarbons, a variety of physical, chemical, and microbiological techniques have been investigated. However, it has been frequently reported that remediation efficiency decreased in the presence of the large portion of soil fine particles. Thus, it is important to understand how soil micro-environments (mainly microparticles and micropores) affect the release of total petroleum hydrocarbons (TPH) in contaminated soils. In this study, we investigate 1) distribution of TPH in contaminated soils with various particle sizes, 2) the rate and extent of TPH release during physical and chemical extraction, and 3) variation of TPH in in-situ contaminated sites where surfactant was injected for TPH removal. Six contaminated soils were separated based on various particle sizes (i.e., >2mm, < 0.38 mm) sharply decreased in 0.5 min and slowly decreased to 0.002 cc g-1 in 10 min. These results imply that physical (sonification) and chemical (solvent extraction) impacts can enhance TPH release from contaminated soils by destructing soil micropores and TPH desorption from microparticles. A strong correlation between TPH and soil micro-environments suggests that TPH can strongly bind to micropores as well as the surface of microparticles. A field study by employing in-situ samplers in monitoring wells in a diesel contaminated site is also ongoing to examine the effect of soil microenvironments on in-situ TPH distribution. The effects of soil micro-environments on TPH removal should be investigated to better understand TPH behavior in contaminated soils and to develop an effective solution for oil-contaminated lands.

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Photocatalytic degradation of methylene blue and hexachlorobenzene with laser induced ZnO nanoparticles

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Zn plate were ablated by a pulsed Nd:YAG laser to produce nanoparticles ZnO compounds in deionized water in the absence of any surfactants or catalysts. The structural and morphological properties of the ZnO nanoparticles were characterized by X-ray diffraction (XRD), field-emission scanning electron microscope (FE-SEM), transmittance electron microscope (TEM). The photocatalytic degradation of methylene blue (MB) and hexachlorobenzene (HCB) was carried out on including the calcination temperature of ZnO, irradiation time and the intensity of light were optimized. The products of dechlorination reaction and reaction paths were analyzed by gas chromatography (GC).

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Efficient Dechlorination of 4,4'-DDT using Fe/C/Pd Nanoparticles Produced by Pulsed Laser Ablation in Liquid (PLAL)

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Persistent organic pollutants (POPs) have concerned public due to their toxicity, bioaccumulation and persistency in the environment and human health. Bimetallic catalysts have recently appeared significant effect for the remediation of groundwater and sediment contaminated with chlorinated organic compounds. Fe nanoparticles were produced by pulsed Nd:YAG laser (1064nm, 10Hz, 7ns) ablating onto an Fe plate immersed in methanol with a reducing agent, ascorbic acid. The morphological and optical properties of Fe/C/Pd catalysts via PLAL were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), Ultraviolet-visible spectroscopy (UV-Vis). Fe/C/Pd catalysts were used to the dechlorination of 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (4,4'-DDT) under various conditions. The products of dechlorination reactions were analyzed by gas chromatography (GC). This study suggested that Fe/C/Pd catalysts could be potentially employed to rapidly degrade 4,4’-DDT in the contaminated environment.

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Chemical degradation of endosulfan by Fe(0) and toxicity test of its product

안삼영

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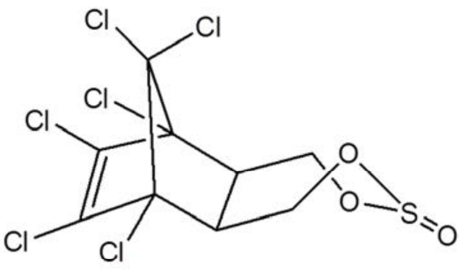
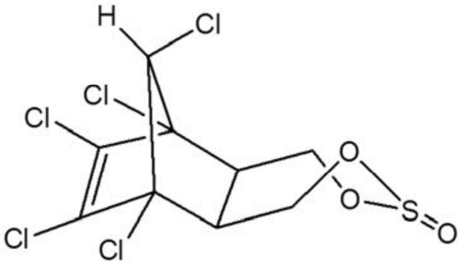
Treating endosulfan with Fe(0) resulted in the complete removal of endosulfan and the formation of 1-CRE(one chlorine reduced endosulfan) as a main product. According to the instrumental analysis, such as LC-MS, GC-MS, 1H-NMR and 13C-NMR, only one chlorine at the bridge carbon was replaced by hydrogen and the orientation is syn to the double bond as shown in Fig. 1. Further reduction of 1-CRE by Fe(0) proceeded much more slowly than endosulfan. Endosulfan and 1-CRE were tested for mutagenicity by bacterial reversion-assay with 5 strains (TA100, TA98, TA1535, and TA1537) of Salmonella typhimurium and a strain (WP2 hcr) of Escherichia coli.



α-endosulfan



1-CRE