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장소: 대전컨벤션센터
발표코드: **목1A1기조**
발표분야: 기조강연
발표종류: 기조강연, 발표일시: 목 11:30, 좌장: 팽기정

Ionic Liquids in Separations and Mass Spectrometry, a New Frontier

Daniel W. Armstrong

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Room-temperature ionic liquids (RTILs), also known as liquid organic, molten, or fused salts, are a class of nonmolecular ionic solvents with low melting points. Most common RTILs are composed of unsymmetrically substituted nitrogen-containing cations (e.g., imidazole, pyrrolideine, pyridine) with inorganic anions (e.g., $C1^-$, PF_6^-, BF_4^-). ILs are also interesting because of their other useful and intriguing physicochemical properties. In this presentation an overview of the structure and properties of ILs and a description of their expanding use in various applications in separations, chromatography and mass spectrometry will be given. A number of studies have appeared indicating that ILs have exceptional promise as stationary phases. They have a dual nature selectivity in that they separate nonpolar molecules as would a nonpolar stationary phase and they separate polar molecules as would a polar stationary phase. Many ILs have exceptional thermal stability. They are being used increasingly in a variety of applications including 2-D GC and enantiomeric separations. ILs have proven to be the best liquid Maldi MS matrix since we introduced them as such a few years ago. The properties of ILs that make them effective will be discussed. Further, the dications developed for high stability ILs have found another novel use in electrospray MS as a reagent for ultra sensitive anion analysis.

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발표코드: **목1A1특별**

발표분야: 특별강연

발표종류: 특별강연, 발표일시: 수 17:00, 좌장: 김홍래

Beyond Genes

Roger D. Kornberg

Stanford University

Constant transcription of the genetic information in the DNA is a central process for all living beings. The DNA-molecule itself lies protected within the cell nuclei. The genetic information therefore needs to be copied and transformed into what is called messenger-RNA, which carries the information out into the protein-producing parts of the cells. It is the proteins that in their turn actually construct the organism and its function. If the transcription process is interrupted the organism will soon die, since all protein production in the cells ceases. This is what happens in cases of poisoning by certain types of toadstools, like the death cap. The toxin in the death cap blocks the function of a specific enzyme, RNA-polymerase, which plays a central role in the transcription process. Within a few days the toxin spreads from the bowels to the liver and kidneys, hence slowly destroying all these organs. Many illnesses – like cancer, heart disease, and different kinds of inflammation – are also linked to disturbances in the transcription process.

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발표종류: 특별강연, 발표일시: 목 10:50, 좌장: 김종승

화학물질 분류와 표지에 관한 세계조화시스템(GHS)

- 국내외 이행 경과와 전망

양정선

산업안전보건연구원 화학물질안전보건센터

화학물질 취급자에게 정확한 유해위험 정보를 알려주어 취급자 스스로 자신을 보호하여 불의의 사고에도 신속하게 대응하고 건강을 보호하기 위한 조치를 하도록 돕는 것은 매우 중요하다. 이를 위하여 체계적으로 화학물질을 분류하고 유해위험 정보를 이해될 수 있는 표현으로 전달하는 것이 필요하다. 그러나 각국의 화학물질 분류, 표지에 관한 기존의 법률 또는 규정의 차이 때문에 결과적으로 동일 제품에 대해서 나라마다 다른 분류나 경고표지를 작성해 왔다. 이러한 화학물질의 유해위험성 분류, 전달 체계의 차이는 국제적으로 화학물질의 교역 규모가 늘어남에 따라 상당한 혼란과 물류비용을 증가시켰다. 이와 같이 같은 물질에 대하여 나라마다 다른 분류기준을 적용하고 다른 형태의 경고표지를 하게 되어 정보혼란에 따른 위험성을 초래하게 되는 것을 막기 위하여, UN 에서는 1992 년 물질안전보건자료 (MSDS, Material Safety Data Sheet)를 포함한 화학물질의 분류 및 경고표지에 대한 세계조화 시스템(GHS, Globally Harmonized System of Classification and Labelling of Chemicals)에 합의하였다. UN 은 2003 년 통일된 GHS 지침을 발간하였고 2008 년까지 각국에서 GHS 를 이행하기로 합의하였다. GHS 는 화학물질 및 혼합물에 대하여 고유한 유해위험성을 확인하여, 물리적 위험성 (폭발성물질 등 16 개 항목), 건강 유해성 (급성독성물질, 호흡기 과민성, 피부 과민성, 흡인유해성 등 11 개 항목), 환경 유해성 (급성 수생환경 유해성 물질 등 2 개 항목)으로 분류하고, 그 유해성 정보를 통일된 표현으로 전달하는 것이다. 일단 각 나라가 수입 또는 자국에서 생산되는 화학물질에 대해 일관되고 적절한 정보를 얻을 수 있다면, 화학물질 노출 관리 및 사람과 환경 보호를 위한 인프라구축은 쉽게 확립될 수 있다. 비록 시행 초기에는 기존 분류체계와 GHS 분류차이로

혼란이 예상되나, 추후 안정적인 유해성 정보를 전달하여 사람과 환경을 보호하고, 생산 및 물류비용에 있어서 이득을 얻게 될 것으로 예상된다. 여기서는 국내외 GHS 이행을 위한 노력과 성과를 정리하고, 향후 GHS 의 국내 본격 도입 시 예상되는 문제점과 전망 등을 정리하고자 한다.

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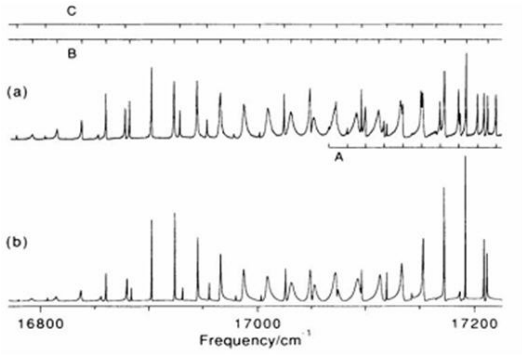
발표종류: 기념강연, 발표일시: 목 13:30, 좌장: 임만호

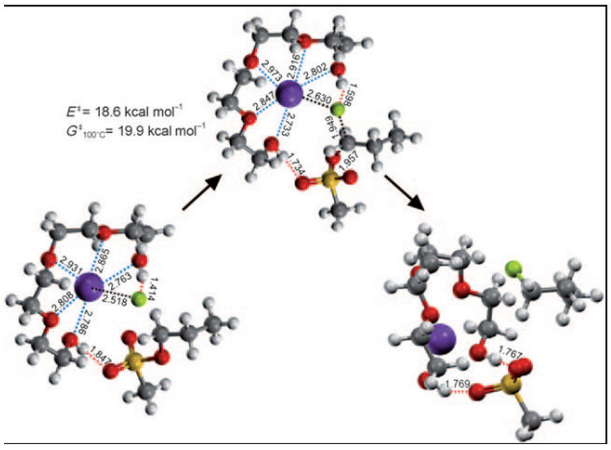
양자간섭으로부터 용매의 비대칭 촉매효과까지: 이론 및 계산화학의 새로운 지평

이성렬

경희대 응용화학과

간단한 분자의 광해리 과정에 있어서의 양자간섭 효과를 이용한 흡수스펙트럼 해석과 수동적 반응통제 가능성을 기술한다. (1+3) 반응통제이론에 나타나는 분자상(molecular phase)의 개념을 제시한다. 아미노산 및 핵산염기의 구조 및 반응에 대한 용매효과를 통하여, 열역학적 안정성뿐 아니라 속도론적 안정성이 생분자에 대한 실험결과를 해석하는데 있어서 매우 중요함을 강조한다. 화학반응에 용매가 촉매로 작용하는 경우를 기술하며, 특히 S_N2 불소화반응에 양성자성 용매가 매우 효과적일 수 있음을 보인다. 이 경우에 친핵체는 양이온과 함께 이온쌍(ion pair)으로 반응하며, 용매는 루이스 염기로 작용함을 제안한다. 이를 일반화하여 산, 염기 작용기를 동시에 보유한 유기용매 및 이온성액체(ionic liquid)가 S_N2 반응의 뛰어난 촉매일 수 있음을 메커니즘 연구를 통하여 보이며, 나아가서 입체화학적 선택성을 가진 용매촉매의 설계(solvent engineering)가 가능함을 제시한다.





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발표분야: Novel Functional Nanostructures: ㅡ Materials, Structures, Properties and Applications Ⅰ
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 박수영

연성소재 분자조립 나노기술

김상욱

KAIST 신소재공학과

연성소재란 고분자, 액정, 계면활성제, 콜로이드, 생체분자등 폭 넓은 소재들을 포함하는 개념으로서 이들은 전통적인 결정성 고체와 점성 액체의 중간에 해당하는 구조와 물성을 보이는 것으로 알려져 있다. 또한 이들 연성소재에 속하는 많은 물질들이 분자들의 자발적인 분자조립현상을 통해 기능성 나노구조를 형성하는 것으로 알려져 있다. 본 발표에서는 연성소재들의 분자조립현상을 원하는 형태로 조절하여 대면적에서 정형화된 나노구조를 만드는 다양한 방법들을 소개할 것이다. 블록공중합체나 카본나노소재와 고분자의 융합물질, 생체소재등의 분자조립 현상을 이용하여 다양한 형태의 기능성 나노구조를 제작하는 방법들을 소개할 것이다.

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발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김상율

Effect of space charge field on dynamic and steady-state photorefractive performance in polymeric composites

김낙중, 오진우, 최칠성

한양대 화학과

Today, polymeric photorefractive (*PR*) composites are considered to be promising for optical applications such as real-time holography; including optical correlation and real-time image processing, phase conjugation, neural networks, high-density holographic storage, and more. Space charge field (*Esc*) formation and chromophore reorientation are the crucial processes to perform the photorefractivity, since both the index contrast and the response time of PR grating are closely related with the *Esc* strength and electro-optic nonlinearity. In particular, the spatially varying charge distribution responsible for *Esc* formation depends on photoconductivity, including the dynamics of charge generation, transport, trapping, and detrapping in the materials.

In this work, we investigated the influence of key components for PR effect, such as photosensitizer, photoconducting polymer, *NLO* chromophore, and temperature, on the space charge field formation and discuss the effect of space charge field on the dynamic and steady-state photorefractive performance. At 632.8nm, photo-charge generation efficiencies, photoconductivities, space charge fields, four wave mixing diffraction efficiencies, gain coefficients, and phase shifts were measured as a function of external electric field and temperature. Then, on the basis of experimental results, the relation between the key parameters and the photorefractivity is analyzed and discussed.

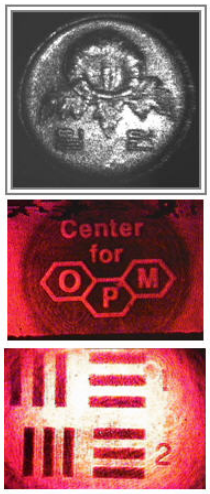
1. J.-W. Oh, W.-J. Joo, I. K. Moon, C.-S. Choi, and N. Kim, *J. Phys. Chem. B.* 113, 1592 (2009).
2. C.-S. Choi, I. K. Moon, and N. Kim, Appl. Phys. Lett. 94, 053302 (2009).
3. J.-W. Oh, C. Lee, and N. Kim et. al., *J. Chem. Phys.* 130, 134909 (2009).

4. J.-W. Oh, I. K. Moon, and N. Kim, *J. Photochem. Photobiol. A.* 201, 222 (2009).

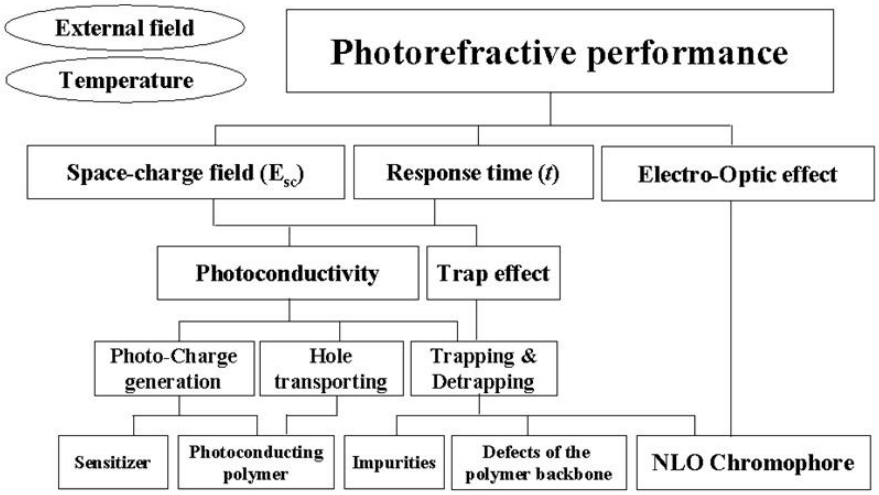
5. J.-W. Oh, C.-S. Choi, Y. Jung, C. Lee, and N. Kim, *J. Mater. Chem.* 9, 5765 (2009).

6. I. K. Moon, C.-S. Choi, and N. Kim, *J. Pol. Sci. B.* 47, 1695 (2009)

7. S. J. Yoon, M. Joo, U.-J. Hwang, and N. Kim, *J. Phys. Chem. C.*, 112, 18592 (2008).



-Application-



-Requirements for photorefractive performance-

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발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 김상율

Detailed Analysis of Nanostructures in Thin Films of Block Copolymers using Synchrotron GIXS

이문호, 진상우, 노예철, 안병철, 정정운, *Hirohisa Yoshida, **Teruaki Hayakawa

*포항공과대 화학과 *Tokyo Metropolitan University **Tokyo Institute of Technology*

We quantitatively investigated nanostructures and phase transitions of several block copolymer systems in thin films using synchrotron grazing incidence small angle X-ray scattering (GISAXS): poly(ethylene oxide)-b-poly(11-[4-(4-butylphenylazo)phenoxy]undecyl methacrylate) (p(EO)-b-p(MAAZ)), poly(styrene)-b-poly(oligothiophene side chain modified isoprene) (PS-b-POTI), and poly(styrene-b-isoprene) (PS-b-PI). The quantitative GISAXS analysis showed that the p(EO)-b-p(MAAZ) in the homogeneous, isotropic melt state undergoes phase-separation near 190 °C and then forms a body-centered cubic (BCC) structure of spherical p(EO) domains in the p(MAAZ) matrix, at which point the p(EO) domains and the p(MAAZ) matrix are both in amorphous, liquid states. The BCC structure of spherical p(EO) domains is converted to a hexagonal cylinder structure near 120 °C, which is induced by the transformation of the isotropic phase of the p(MAAZ) matrix to the smectic A phase, which is composed of a laterally ordered structure of p(MAAZ) blocks with fully extended side groups. The resulting hexagonal cylinder structure is very stable below 120 °C. This microscopic hexagonal cylinder structure is retained as the smectic A phase of the p(MAAZ) matrix undergoes further transitions to smectic C near 104 °C and to a smectic X phase near 76 °C, while the amorphous, liquid phase of the p(EO) cylinders undergoes crystallization near -15 °C. These complicated temperature-dependent disorder-order and order-order phase transitions in the films were found to take place reversibly during the heating run. A face-centered orthorhombic structure of p(EO) domains was also found during the heating run and is an intermediate structure in the hexagonal cylinder structure to BCC structure transformation. PS-b-POTI is an interesting semi-rod coil diblock brush copolymer, At room temperature, the diblock copolymer molecules in thin films were found to form an alternately stacked structure comprised of amorphous PS and smectic-A POTI microdomains whose stacking direction is

parallel to the film plane. On heating, the films underwent a phase transformation to a hexagonal cylinder structure with cylindrical POTI domains in the PS matrix oriented normal to the film plane. This phase conversion is induced by the transformation of the POTI domains from a smectic-A phase to an isotropic phase, where the smectic-A phase is composed of a laterally ordered structure of interdigitated bristles in the POTI blocks. A PS-b-PI in our study showed a hexagonally perforated layer (HPL) structure, which is well known in polymer science. This diblock copolymer in film was confirmed to form ABC stacked HPL structure. The detailed analysis of the HPL with ABC stacking was conducted for the first time. Another PS-b-PI in our study showed to form gyroid structure in thin films and the gyroid structure was also analyzed in detail. The synchrotron GISAXS analysis has been extended for other interesting functional polymers including linear and brush polymers and block copolymers. These studies were supported by the Korea Science & Engineering Foundation (National Research Lab Program and Center for Integrated Molecular Systems) and by the Ministry of Education, Science and Technology (Brain Korea 21 Program and World Class University Program). Synchrotron GIXS measurements were supported by the Ministry of Education, Science and Technology and POSCO.

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발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김상율

Investigation of GAMA as a new ATRP method

노석균

영남대 디스플레이화학공학부

The use of air stable catalysts in their higher oxidationstate was successfully developed and used as a tool insynthesizing polymer materials. The reverse ATRP requiresa conventional radical initiator such as a peroxide or 2,2'-azobisisobutryonitrile (AIBN) to generate a lower oxidationstate of the transition-metal complex. The reducing agentcan reduce the higher oxidation state transition metal througha single electron process in activator generated by electrontransfer(AGET) ATRP. Compared to the reported reverseATRP or AGET ATRP methods, our catalyst systems weredeveloped by only using iron(III) or cupper(II) in the absence of additives.As a result, the reaction systems are less toxic and lessexpensive, which makes them attractive for potential practicalapplications. Herein we report the iron(III) and cupper(II)-catalyzedATRP["generation of activators by monomer addition (GAMA)] with phosphorus ligands in the absence of a radical initiator or reducing agent. The use of oxidativelystable catalysts overcomes the air-sensitivity problem which isassociated with lower oxidation state metals, and makes thepreparation and storage of the ATRP catalyst systems morefacile. Notably, there is no need to premix the transition metalwith the ligand and then isolate the catalyst complex. Theligand and Fe(III) and Cu(II) can simply be mixed and directly reactedwith the monomer. Therefore, isolating and purifying thecatalyst is not necessary, thus saving on cost.

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Self-assembly and Breath Figure of Small Molecules for Hierarchically Ordered Polymeric Materials

김정학, 서명은, 김상율

KAIST 화학과

We report the combination of the top-down and bottom-up approaches with small organogelators to produce dual-patterned honeycomb lines on nanometer scale. The BF technique was applied to a photopolymerizable small molecule, causing it to self-assemble into supramolecular fibrillar networks and further a hierarchically ordered honeycomb structure. The resulting structure was then patterned by exposure to UV irradiation through a photomask, which induced selective chemical crosslinking in the exposed region. After developing, honeycomb lines were obtained at predefined locations. Details of synthesis, pattern generation and their structures will be discussed.

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New Optical Functions and Applications of Poly(diphenylacetylene) Derivatives

곽기섭

경북대 공과대학/고분자공학과

Since Professor Toshio Masuda in Kyoto University synthesized poly[1-phenyl-2-(p-trimethylsilyl)phenylacetylene] [PTMSDPA] in 1991, many researches concerning its derivatives syntheses, physical properties, functions, and applications have been done up to date. The PTMSDPA possesses several unique qualities including (a) an ultrahigh molecular weight, (b) excellent mechanical property, (c) chemical and thermal stability, (d) good solubility in organic solvents, and (e) film-forming ability. Especially, because PTMSDPA has an extremely large fractional free volume (FFV) of 0.26 in film, it has attracted much attention as a highly gas- and vapor-permeable membrane. It should be also noted that this polymer emits an intense fluorescence in a visible region because of the effective exciton confinement within the main chain due to the intramolecular electron interactions of the phenyl rings. We have recently reported new potential applications of PTMSDPA as a useful material for 1) thermosensor, 2) electrospun optic nanofiber, 3) highly polarized fluorescent film, and 4) fluorescence image patterning. PTMSDPA is an amorphous, semi-flexible polymer. The combination of the fluorescence property of PTMSDPA and its high gas- and vapor-permeability served as the basis for a unique and practical application of PTMSDPA film to the optical detection of various organic solvent chemicals. When some solvents diffused into such a fluorescent polymer film with large FFV as PTMSDPA, the chemicals stimulated entangled polymer chains to affect the interchain distances and solid-state electronic structures. This indicated the highly potential applications of PTMSDPA as 5) VOC sensor, 6) latent fingerprint detective film, and 7) fluorescent viscosity sensor.

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발표분야: Novel Functional Nanostructures: ㅡ Materials, Structures, Properties and Applications Ⅰ
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 노석균

무기-유기 소재의 융합 및 미 구조 제어에 의한 광전소자 제조

석상일

한국화학연구원, 화학소재연구단, 소자재료연구센터

무기물과 유기물의 장점을 결합하고 미구조를 제어한 고기능성 소재를 이용한 많은 연구 중에서 최근 고효율의 저가 태양전지 혹은 포토디텍터 제조에 대한 관심이 크게 증가하고 있다. 상용화가 임박한 염료감응형 태양전지는 스위스 로잔공대의 그래첼(M. Gratzel) 교수가 1991 년 세계 최초로 개발한 태양전지로서 다공성 TiO_2 전극/염료/전해질 혹은 홀전도성 유기물로 구성되어 있다. 이것은 일반적인 반도체 접합 태양전지와 다르게, 가시광 영역을 효율적으로 흡수하는 염료 분자가 화학적으로 흡착된 나노입자 반도체 산화물 전극에 광을 조사함으로서 엑시톤(exiton)을 형성하고 이중 전자가 반도체 산화물의 전도띠로 주입되어 전류를 발생시키는 원리를 이용하고 있다. 태양전지 생산원가의 대폭적인 절감이 기대되며, 흐린 날씨 및 빛의 조사각도가 10°로 좁아도 전기 생산이 가능한 장점과 투명하면서 다양한 색상 구현이 가능하기 때문에 빌딩 창문, IT 제품의 자가 발전기, 군사용 등 여러분야로의 응용성이 기대 되는 태양전지기술이다. 또한 근적외선 영역의 포토디텍터는 저가 제조기술의 확보에 의하여 보안, 의료 등에 대규모적인 활용이 예상되고 있다. 본 발표에서는 발표자의 연구실에서 진행 중인 연구를 바탕으로 한 무/유기 광전소재/소자의 결과에 대하여 소개하고자 한다.

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발표분야: Novel Functional Nanostructures: Ⅰ Materials, Structures, Properties and Applications Ⅱ
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 김범준

Novel liquid crystal block copolymers and their applications as sensors

박수영

경북대 고분자공학과

The amphiphilic liquid crystalline block copolymers of LCnP-b-PAA (n = 3, 6, 11, LCnP = poly(n-(4-cyanobiphenyl-4'-oxy)(CH2)n acrylate), PAA= poly(acrylic acid)) were synthesized by using a RAFT polymerization method. A TEM grid on the octadecyltrichlorosilane (OTS) coated glass was used for a sensor frame. The monolayer films of the block copolymers on the 4'-pentyl-4-cyanobiphenyl (5CB) were made by spreading the block copolymer solution on the water to make monolayer film, adsorption of the monolayer of the block copolymer on the 5CB filled TEM grid, sealing the sensor frame with epoxy, and filling water to control pH. 5CB on the OTS coated glass and at the interface with water was oriented perpendicular to the glass and parallel to the interface, respectively, making 5CB bright when the TEM grid was observed through polarized optical microscopy. LCnP-b-PAA at the interface with 5CB made 5CB to be aligned perpendicular to the interface at higher than pH = 10 but 5CB became parallel to the intersurface at lower than pH = 10. The shrinkage of PAA block at low pH changed the homeotropic to planar orientation by cooperative motion of 5CB at the interface. These cooperative motions were strongly dependent on the spacer length of the liquid crystal block copolymer. These results indicate that these LC TEM cells may be used as sensors which can detect environmental stimuli.

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Self-assembled Nanostructures of Non-conventional Block Molecules for Material Applications

조병기

단국대 화학과

Non-conventional block copolymers bearing different types of building blocks would be an interesting subject in the macromolecular assembly, in order to create novel functional nanostructured materials. For several years, our group has studied on newly designed block copolymers by molecularly hybridizing branched dendron, linear coil, mesogenic rod and disc. In this talk, our presentation will focus on the recent results regarding dendritic block copolymers, so-called dendron-coil and block codendrimer. The details in their assembling properties and material applications via molecular engineering will be addressed.

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발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 김범준

Structured Colloidal Materials from Block Copolymers

이기라, *이광렬, **Ed Kramer, ***David Pine

*충북대 공업화학과 *고려대 화학과 **UC Santa Barbara ***New York Universtiy*

Block copolymer particles with nanostructures were prepared by evaporation-induced self-assembly of block copolymer inside droplet. Organization of symmetric block copolymers inside emulsion with surfactant have produced onion-like structures. Then, by adding homopolymers in emulsion phase with block copolymers, we have succeeded in controlling the morphologies inside particles from lamellar to cylinders and spheres. Depending on particle size, we found that morphologies were dramatically changed inside block copolymers. Also, by using amphiphilic block copolymers or mixtures, both of particle shapes and internal structures were controlled well.

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Thermally Stable Au Nanoparticles via Photo-crosslinkable Polymeric Stabilizers

방준하

고려대 화공생명공학과

Polymer nanocomposites consisting of polymers and inorganic nanoparticles (NPs) have attracted many interest due to their applications such as solar cell, sensors, catalysts and ferroelectric devices. To integrate NPs into polymer matrix in the controlled manner, thiol-terminated stabilizers have been used to tune the surface property of NPs such as Au, Pt, CdSe, etc. However, a practical use of such particles in the nanocomposites is very limited by thermal instability even at ~90 ^{o}C, leading to the agglomeration of NPs. To impart the thermal stability of NPs, we modified Au NPs surface using UV-crosslinkable polymeric stabilizers. After UV-crosslinking, it was found that the Au NPs exhibit the excellent stability at high temperature (~180 ^{o}C) in both solution and thin-film states. Furthermore, we demonstrate that thermally stable Au NPs can be used as compatibilizers in PS/PMMA blends.

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Tailoring Core-Shell Polymer Coated Nanoparticles as Block Copolymer Surfactants

김범준

KAIST 생명화학공학과

The effect of core-shell polymer coated nanoparticles on block copolymer morphology is investigated systematically by controlling particle positioning within a block copolymer template. Our approach of varying the areal chain density of short thiol terminated polystyrene brushes on the particles is used to control the fraction of the particles adsorbed to the interface of PS-b-P2VP diblock copolymer domains. Interestingly, the addition of low volume fractions of the nanoparticle surfactants to lamellar diblock copolymers initially leads to a decrease in lamellar thickness, a consequence of decreasing interfacial tension, up to a critical value of the particle volume fraction beyond which the block copolymer adopts a bicontinuous morphology.. The relationship between domain spacing and morphology of block copolymer with the level of nanoparticle surfactants will be discussed based on a strong-segregation model. I thank my collaborators G. H. Fredrickson, J. Bang, C. J. Hawker, and E. J. Kramer.

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Increased Water Retention in Polymer Electrolyte Membranes at Elevated Temperatures Assisted by Capillary Condensation

박문정

포항공과대 화학과, 첨단재료학부

We have created microstructured membranes, composed of hydrophilic and hydrophobic domains that are more effective at extracting water from the surrounding air when the temperature of the air is increased at constant relative humidity up to temperatures as high as 90 °C. This unexpected behavior is seen when the width of the hydrophilic domains is less than 5 nm. The widths of the moist hydrophilic phases were measured by cryogenic electron microscopy experiments performed on humid membranes. Simple calculations suggest that capillary condensation is important at these length scales. The correlation between moisture content and proton conductivity of the membranes is demonstrated. Not surprisingly, the proton conductivity of these membranes also increases with increasing temperature. While this property may enable the construction of more efficient, high-temperature polymer electrolyte fuel cells, our main accomplishment is that we have uncovered a new methodology for systematically controlling the moisture content of microstructured materials.

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Long-Range Order in Block Copolymer Thin Films

박수진

울산과학기술대 에너지공학부

Controlling the orientation and ordering of the block copolymer (BCP) microdomains in thin films is essential to their use as templates and scaffolds for the fabrication of nanostructured materials. In addition, a process must be robust, simple to implement, and rapid, and should not introduce disruptive processing steps that would impede their use. Here, we describe that thin films of poly(styrene-b-4-vinylpyridine) (PS-b-P4VP) and poly(styrene-b-ethylene oxide) (PS-b-PEO) BCP films show highly oriented, cylindrical microdomains with a high degree of lateral order on a silicon substrate. In addition, the preferential solvation of the P4VP or PEO block with an ethanol caused a surface reconstruction that resulted in the formation of a nanoporous film upon drying. Highly ordered cylindrical microdomains are characterized by scanning force microscope (SFM) and grazing incidence small angle X-ray scattering (GISAXS).

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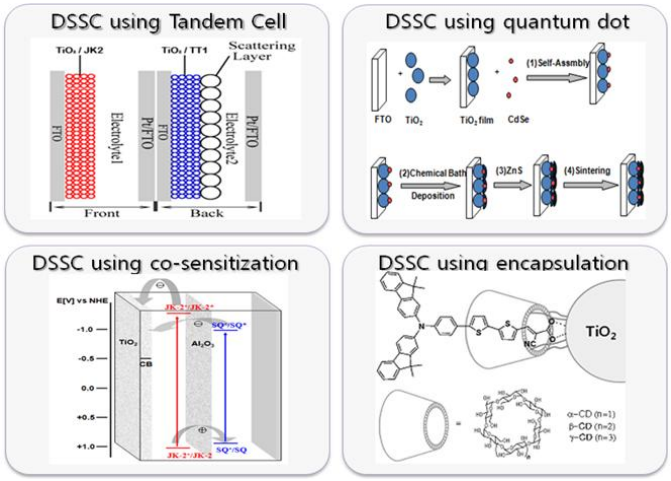
발표분야: Dye-Sensitized and Organic Solar Cells
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 진성호

New Concept of Highly Efficient Dye-Sensitized Solar Cells

고재중, 김점종, 김덕현, 최현봉, 김철우, 백상현, 조나라

고려대 소재화학과

Dye-sensitized nanocrystalline TiO2 solar cells (DSSCs) have attracted considerable interest because of their high conversion of sunlight to electricity and easy fabrication. To overcome the prohibitive cost of ruthenium metal complexes, several groups have developed metal free sensitizers and obtained efficiencies in the range of 8~9%. However, a major issue for the low photoconversion efficiency of many organic dyes in dye-sensitized solar cell is due to the formation of dye aggregates on the semiconductor surface. Therefore, for obtaining efficient photoconversion based on organic dyes, aggregation needs to be avoided through the CD(cyclodextrin). An optimal sensitizers, which combine broad visible light absorption with an excited-state directionality for favorable electron-transfer dynamics, is a key issue in the development of DSSC. So, we used a two type concept. First is the novel cosensitization based on the controlled construction of the film architecture in which a primary monolayer of dye is spatially separated from a secondary monolayer of another dye suing a layer of Al2O3, resulting in the configuration TiO2/Dye1/Al2O3/Dye2. Second concept, a tandem-structured dye sensitized solar cell composed of a front and a back sub-cells was assembled by using spectrally complementary organic dye combinations. Other issue is that The photovoltaic performance of the quantum dot-sensitized solar cells (QDSCs) was still much lower than that obtained from DSSCs. In particular, IPCE values of QDSCs were at a low level of 60%. The serious electron loss due to a charge recombination at TiO2/CdSe interface. In order to solve these issue, we proposed a new route to assemble CdSe QDs onto TiO2 films in this study. It includes four main steps: seed-sowing, seed-growing, ZnS-covering, and post-sintering. Through this route, superior electrodes with an enhanced performance of the device were achieved.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 진성호

Roles of Electrolytes for Dye-Sensitized Solar Cells

강용수

한양대 화학공학과

A main component of dye-sensitized solar cells (DSCs) is electrolyte that fills the space between dye-adsorbed nanocrystalline photoanode and counter electrode. The electrolyte contains redox couples such as I^- and I_3^- dissolved in a solvent, where electrochemical oxidation and reduction reactions can occur continuously along with diffusion of ionic species. The oxidized dyes after generating electrons from their excited states upon light absorption should be regenerated by reactions with electrons, which are provided by the oxidation reaction of the redox couples at the photoanode side. At the counter electrode, the reduction reaction of I_3^- occurs. In addition, diffusion of ions such as I^- and I_3^- also occurs, and therefore the ionic conductivity is also important in determining the performance. In this presentation, roles of electrolytes will be introduced, in particular, depending on the state such as the liquid, quasi-solid and solid states.

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High Performance Organic Solar Cells with Controlled Morphology and Interfaces

조길원

포항공과대 화학공학과

The device performance of organic photovoltaics (OPVs) is influenced much by the molecular and mesoscale structures of organic semiconductor films that determine their exciton generation and charge transport characteristics. In the operation of OPVs, charge separation from exciton and charge carrier transport are strongly dependent on the properties of two kinds of interface: interfaces between semiconductors and electrodes, where charge injection occurs from the semiconductor into the electrodes, and interfaces between donor and acceptor materials, where exciton separation takes place. Also, the molecular structure and morphology of the active layer seriously depend on the properties of the each interface. Here, several approaches for controlling interfaces and structures of semiconductor films are discussed. First, we controlled work function and surface energy of electrode (ITO) for HOMO level matching between electrode and active layer, and phase separation of active layer. Second, by using a template, we fabricated poly (3-hexylthiophene) nano rod / C60 ordered bulk heterojunction device. Increasing interfacial contact area between donor and acceptor caused the enhanced device performance. Third, by modification of end functional group of P3HT, we controlled the miscibility between P3HT/PCBM, and domain size of each material. By optimizing the phase separation and morphology of active layer, we can achieve the efficiency, ~5% with fill factor 0.68. Finally, we demonstrate bulk heterojunction solar cells based on blends of preformed P3HT nanowires and PC61BM by using marginal solvent without any post treatment, and the morphology and photovoltaic properties were studied as a function of the P3HT nanowires' aging time. Additionally, we have demonstrated an optimized morphology of the blend film using two separate steps: P3HT nanowire formation from mixed solvents and subsequent phase separation by low temperature annealing. With the help of interpenetrating

nanowire structures, carrier mobility is dramatically increased and photovoltaic performance has been improved since the subsequent light absorption with reduced recombination loss of the carriers.

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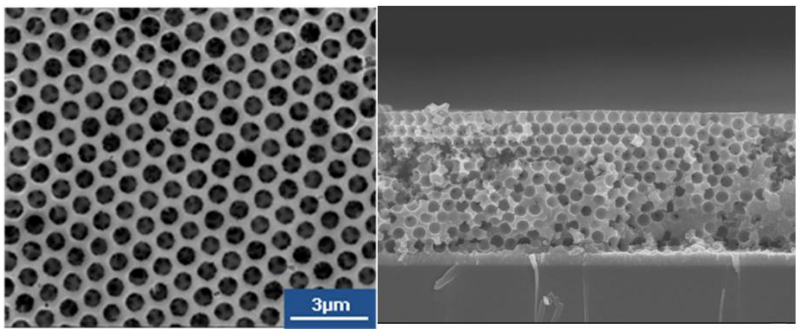
Fabrication of macroporous photoelectrodes by colloidal templating methods

이현정

KIST 고분자하이브리드센타

Dye-sensitized solar cells based on highly porous nanocrystalline TiO2 films have drawn much attention due to their high conversion efficiency and low production cost. TiO2 nanocrystalline particles have been investigated extensively as a key material. In this study, we present a new strategy to fabricate macroporous photoelectrodes using polystyrene(PS) colloidal templating methods both at high temperature (>400oC) and at low temperature (150oC>). Polymeric colloidal structures could be removed by thermal sintering or chemical treatment. This mesoporous structure provides the large empty space leading to the easy infiltration of quasi-solid state electrolytes and has additional light harvesting effect. A major advantage of this colloidal array template method is that the pore size and its distribution within TiO2 photoelectrodes are determined by those of latex beads, which can be controlled easily. These materials may have promising potentials for future applications of membrane, sensor and so on as well as solar cells.



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Study on the performance of inkjet-printed polymer solar cells

이수형

전북대 화학공학부

In this work, we fabricated hole transporting and active layers of polymer solar cells by inkjet printing. We prepared polymer solar cell devices with a hole transporting layer of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate)(PEDOT:PSS) and a photo- active layer of poly(3-hexylthiophene)(P3HT):[6,6]-phenyl C61-butyric acid methyl ester(PCBM) mixture on the ITO substrate by inkjet printing. In order to find the optimum fabrication conditions for both layers, we have investigated inkjet printing parameters such as solvent mixtures, additives and substrate temperatures of polymer inks. The controlled printing parameters and ink formulations leaded to obtain pin-hole free surface films achieving power conversion efficiency over the 3.5% for photovoltaic devices under illumination.

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발표분야: New-Trends in Inorganic Chemistry
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Beyond silicone: Wet chemical process for compound semiconductor thin films and its application to solar cells and electronic devices

한성환

한양대 화학과

지난 수십 년간 실리콘은 전자 공업과 태양전지를 이루는 가장 핵심적인 재료 중 하나이었다. 패턴닝과 도핑이 가능한 실리콘의 성질은 저가의 대량생간 공정을 이룰 수 있게 했으며 이로 인해 오늘날의 전자 문명을 가능케 한 근간을 제공하였다. 그러나 이미 실리콘의 특성은 그 한계점에 다다르고 있으며 더 나은 특성의 반도체 소자들이 요구되고 있다. 또한 최근의 화석에너지의 한계로 인해 태양에너지를 전기로 전환시키고자 실리콘 기판을 이용하여 태양전지를 생산하고 있으나 에너지적인 측면에서 아직까지는 경제성을 도저히 맞출 수 없는 수준이다. 이는 이미 실리콘을 근간으로 한 과학 기술 문명의 패러다임 전환을 요구하는 시점에 도달했음을 말해주며, 실리콘의 특성을 넘어서는 새로운 물질을 찾아내는 것이 향후 과학과 기술의 전반에 걸쳐 중요한 화두가 됨을 의미한다. 본 발표에서는 기존의 진공공정이 아닌 액상공정을 통하여 다양한 화합물 반도체 박막을 형성하는 시도를 소개하며 특별히 이러한 반도체 화합물을 이용하여 새로운 개념의 태양전지를 개발하는 노력을 함께 소개할 것이다.

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발표코드: **목7C1심**
발표분야: New-Trends in Inorganic Chemistry
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 윤성호

Bifunctional Catalyst Design by Morphology Control of Metal and Metal Oxide Nanostructures

송현준

KAIST 화학과

The synthesis of metal and metal oxide nanostructures is of considerable interest due to their intriguing physical and chemical properties dependent upon their morphologies. Metal nanoparticles are generally used as active components for heterogeneous catalytic reactions. Metal oxide nanoparticles exhibit high catalytic activity in electrochemical reactions, and are also employed for the supports of bifunctional catalysts, owing to their structural stability and electron rich character. The combination of metal and metal oxide components can maximize catalytic performances (reactivity, selectivity, stability, and so on) in various reactions. Herein, we present a rational synthesis of various metal and metal oxide nanoparticles. These nanoparticles have generally been synthesized either by a polyol process in polar solvents or by a thermal decomposition in organic solvents. The resulting particles have been treated with chemical methods in order to fit their properties for specific applications. Finally, the catalysts have been employed for various chemical reactions. This sequential nanocatalyst design from synthesis to application will provide a general methodology for developing high performance catalysts with optimal efficiency and tolerance.

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발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 윤성호

Power from the Sun using the Mesoscopic Solar Cells

Md.K.nazeeruddin

고려대&Swiss Federal Institute of Technology Zurich

The mesoscopic solar cells produce an interface with a huge area endowing these systems with intriguing optoelectronic properties. These cells are formed, for example, from nanocrystalline inorganic oxides, ionic liquids and organic hole conductor or conducting polymer devices, which offer the prospect of very low cost fabrication without expensive and energy intensive high temperature and high vacuum processes. They can feasibly be produced employing flexible substrates and are compatible with a variety of embodiments and appearances to facilitate market entry, both for use in domestic devices as well as in architectural applications. The prototype of this new PV family is the dye-sensitized solar cell (DSC), which accomplishes the separation of the optical absorption and the charge separation processes by the association of a sensitizer as light-absorbing material with a wide band gap semiconductor of nanocrystalline morphology. The DSC reaches today over 12% conversion efficiency and excellent stability rendering it a credible alternative to conventional p-n junction photovoltaic devices. One of the main components in DSC is sensitizer and in this talk I will discuss various sensitizers and their efficiencies.

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Closely Related Mono- and Di-zinc(II) and -copper(II) Schiff Base Complexes: Solution Molecular Recognition and Solid State Magnetic and Water Cluster Formation

D.G.Churchill

KAIST 화학과

I. Chiral fluorescent dinuclear zinc complexes were synthesized in a "one-pot" method in which the lysine-based Schiff base ligand was generated in situ. Under neutral aqueous conditions these species exhibit blue fluorescence (Quantum Yield = 0.17) and act in highly selective detection for certain biological phosphates, through fluorescence ON-OFF signaling. Both the fluorometric and colorimetric (indicator displacement assays) titration results have allowed for the binding preference to be established: PPi ≥ ATP > ADP. These complexes also act as highly sensitive and selective fluorescent ON-OFF probes for Cu^{2+}. Sensing can be performed in water at physiological pH. Aqueous colorimetric anion sensing and magnetic properties have also been investigated for related dicopper species. II. Analogous dinuclear acetate-bridged Cu(II) complexes, were also obtained as minor products along with their mononuclear counterparts from a “one pot” crystallization. V.T. magnetic analysis revealed weak anti-ferromagnetic coupling mediated through the phenolate- and acetate-bridged O-atoms between the two Cu(II) centers. Additionally, large numbers of solvent water molecules are present in the lattices of the mononuclear compounds. The lattice water molecules form cyclic water clusters octamer and 1-D polymeric water cluster chains, which assist the formation of 3-D hydrogen-bonded networks. The racemic D-/L-lysine used herein as a source of the Schiff base ligand led to racemic hydrogen-bonding networks containing enantiomeric complexes of D- and L-lysine Schiff base ligands in all packing structures for compounds.

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Direct observation of unstable species in porous networks by X-ray crystallography

Masaki Kawano

포항공과대 첨단재료과학부

Direct structural analysis methods, such as X-ray crystallography, are well suited for stable and crystalline compounds but in situ observation poses a significant challenge given the transient nature of unstable intermediates. Recently, we demonstrated that the pores of porous coordination networks can be used as crystalline molecular flask in which chemical reactions can occur. The robust networks maintain crystallinity and enable direct observation of the reaction products by X-ray diffraction. In this talk I would like to demonstrate that various reactive intermediates can be directly observed during crystallographic monitoring of chemical reactions within a “crystalline” flask. controlling temperature, each reaction step can be observed by X-rays. For example, we were able to directly observe, in a stepwise manner, the molecular structures of the reactant (amine), intermediate (hemiaminal), and product (imine) during the chemical transformation within the pore. These results establish crystalline flasks as a valuable tool for observing and checking structural transformations and reaction mechanisms of chemical reactions.

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발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 김진권

COORDINATION POLYMERIC GELS AND FIBERS

Jagadese J. Vittal, *Leong Wei Lee, *Sudip Kumar Batabyal

*경상대 화학과&Department of Chemistry, National University of Singapore, Singapore *Department of Chemistry, National University of Singapore, Singapore*

Metallogels and coordination polymeric gels (CP gels) are the emerging research areas and exhibit intriguing spectroscopic, catalytic and redox properties. Recently we have shown that Zn(II) and Mg(II) coordination polymers of *N*-(7-hydroxyl-4-methyl-8-coumarinyl)-amino acid ligands could be self-assembled into gel materials in the absence of long chain hydrophobic groups. The gelation process could be rationalized by the 1D CP aggregate upon complexation and further self-assemble into a 3D network structure through noncovalent interactions to entrap water molecules. The most striking finding is that the dramatic enhancement of fluorescence properties of coumarin derivative upon the formation of CP hydrogel. This could be attributed to the rigidification of the media upon gelation which slows down nonradiative decay and lead to fluorescence enhancement. Detailed mechanical studies indicate that the hydrogels are weak and thermally labile network. Further we have shown that large scale fabrication of nanofibers of CPs can be made from CP gel precursors by electrospinning method. In the absence of organic polymeric additives, viscous solution suitable for drawing fibers has been made by diluting the gel precursor which are obtained by mixing $Ni(OAc)_2$ and 4-trifluoromethylbenzoic acid with linear spacer ligands trans-1,2-bis(4-pyridyl)ethylene or 4,4'-bipyridine in organic solvents. One-dimensional CP structures have been proposed for these gels and nanofibers based on the crystal structures of compounds isolated. These fibers show some interesting field emission properties which will be discussed during the talk.

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발표분야: Materials for Biofuntional Systems
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 임용택

Quantum Dots for Bioimaging

송릿다

한국파스퇴르연구소 Nano/Bio Chemistry

Recently, CdSe/ZnS quantum dots (QDs) conjugated with molecular recognition agents such as oligonucleotides, peptides, and antibodies, have been of great interest as ultrasensitive molecular probes due to their excellent photophysical properties including high quantum yield, narrow size-tunable photoluminescence and photostability. Surface modification of QDs by various coordinating ligands has been extensively studied to gain access to biological application. The synthesis of robust amine-functionalized QDs and modification with poly(ethylene glycol) for long-term stability will be presented. These QDs showed an excellent stability over a broad pH-range and remarkable internalization efficiency into living cells. Moreover, novel QD-DNA complexes have been prepared by simple electrostatic interaction between pegylated amine-functionalized CdSe/ZnS QDs and DNA. The cationic nature of the amine functionality on the QD surface allows for the formation of an electrostatic complex with negatively charged DNA. The presence of PEG5000 molecules on the QDs lead to enhanced stability and decreased non-specific adsorption of DNA on the QDs surface. In addition, the preparation and application of QDs modified with a metal chelating nitrilotriacetate (NTA) moiety will be presented. This probe can be used for the imaging of recombinant histidine (His)-tagged proteins in vitro assay and in live cells as well. Finally, gene expression visualization approach using DNA-modified QDs will be presented. Our efforts to develop a nanoprobe for real-time sequence-specific mRNA visualization are expected to explore mRNA localization and dynamics in cells and whole organisms in correlation to specific phenotype and cellular regulation.

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Raman-Active Core-Shell Nano-Dumbbells for Highly Sensitive and Reproducible Single Molecule Detection

남좌민

서울대 화학부

Here, we developed a strategy to synthesize gold-silver core-shell dimeric nanostructures in a high yield (~80 %). We used these nanostructures in surface-enhanced Raman scattering(SERS)-based single DNA sensing applications for highly reproducible, single-molecule-sensitive DNA detection from individual nanostructures. The strategy and results paved a way of solving long-standing problems in Raman-based detection and widespread use of SERS-active nanostructures in sensing applications.

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Ordered assembly of M13 viruses on polyelectrolyte multilayers and its application to energy devices and biological sensors

유필진

성균관대 화학공학부

A novel means of incorporating ordered bio-functional viral assemblies into an electrostatic thin film nano-assembly and its application to anode material of lithium ion battery have been demonstrated. We used negatively-charged engineered M13 bacteriophage (virus) as the adsorbant species on a weak polyelectrolyte multilayer (PEM) support consisting of a cationic linear polyethylenimine (LPEI) and anionic polyacrylic acid (PAA). Due to a unique phenomenon of interdiffusion, the LPEI/PAA multilayer provides full mobility to the M13 virus, and the adsorption process drive self-assembly and entropically-driven ordering. The resulting monolayer formation of M13 virus can be tuned for its packing density and directional alignment. We also demonstrate the two-dimensional biomineralization from this monolayer template of M13 virus for nanoparticles and nanowires self-assembly. For an application, furthermore, we demonstrate the virus enabled synthesis and assembly of nanowires as negative-electrode materials for lithium ion batteries. The expression of cobalt ion binding peptides on the filamentous coat of M13 bacteriophage viruses facilitates the fabrication of homogenous Co3O4 nanowires at room temperature. Combining the virus templated synthesis at the peptide level and our methods for the control of two dimensional assembly of viruses on PEM provides a useful tool for integrating these nanomaterials to form thin, flexible Li ion batteries. Additionally, we presented that assembled virus structure can be patterned via non-conventional nano-lithographic methods and utilized as a biological sensor that can capture the specific proteins. Overall, this system represents an interface that provides a general platform for the systematic incorporation and assembly of organic, biological and inorganic materials, which can be a basis for the fabrication and integration of two-dimensional device structures.

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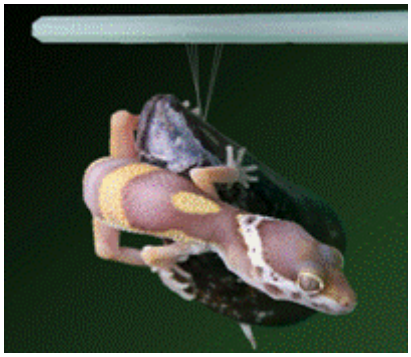
발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 전상용

Bioadhesion of Mussels and Geckos: Applications for Materials and Interfaces

이해신

KAIST 화학과

This seminar presents two examples of bioadhesions: mussels and geckos. First, the speaker will present a simple one-step aqueous surface modification method called poly(dopamine) coating. This surface chemistry is inspired by mussel adhesive proteins found in marine environment. The adhesive protein shows a repeated di-peptidyl sequence of DOPA (3,4 dihydroxylphenylalanine) and lysine that are exhaustively repeated throughout the protein. We found that dopamine, a bi-functional small molecule that has amine and catechol, which are the side chains of lysine and DOPA showed a versatile surface coating capability. We found that under oxidative conditions (pH > 7.5), dopamine surprisingly forms adherent nanofilms on virtually all natural and synthetic surfaces: metals (Au, Ag, Pt, Cu, Pd, stainless steel), oxides (TiO2, NiTi, SiO2, Quartz, Al2O3, Nb2O5), semiconductors (GaAs, Si3N4), polymers (polyethylene (PE), polystyrene (PS), polyethyletherketone (PEEK), polyurethanes, polydimethylsiloxane (PDMS), polycarbonate (PC), polytetrafluoroethylene (PTFE), polyethyleneterephthalate (PET)), and ceramics (glass and hydroxyapatite). The polydopamine-coated substrates can be utilized as versatile platform for bioconjugation, SAM formation, electroless metallization. etc. The second part of talk will discuss about a new class of hybrid adhesive called ‘Geckel’, inspired by adhesive strategies of geckos and mussels.Geckel consists of an array of nanofabricated polymer pillars as a functional mimic of gecko’s feet onto which a mussel-mimetic polymer, p(DMA-co-MEA) e.g. poly(dopaminemethacrylamide-co-methoxyethylacrylate), was coated. The geckel showed reversible adhesion in water and air environments.



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 금 16:15, 좌장: 전상용

Nanobiomaterials for The Molecular Imaging of Immunotherapeutic Cells

임용택

충남대 분석과학기술대학원

Recent advances in the design and fabrication of nanostructured materials have been providing potential applications in biomedical areas ranging from disease diagnosis to therapy. Here, we describe the design and applications of nanobiomaterials for the effective tracking of immunotherapeutic cells such as dendritic cells and natural killer cells. Our strategy in the development of nanobiomaterials for molecular imaging is the combination of magnetic resonance and optical imaging nanoprobes. In this talk, novel-types of bimodal imaging nanoprobes and their applications will be presented.

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발표분야: Chemical Approaches for Green Technology
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 최원용

Applications of Inorganic Redox Reactions to Environmental Remediation

최원용

포항공과대 환경공학부

Chemical and photochemical redox reactions are essential elements in many chemical processes including environmental remediation systems. The degradation or transformation of chemical pollutants in water and air are mainly redox chemical reactions and can be carried out under widely varying experimental conditions. This talk will introduce and discuss a variety of examples of redox-based remediation processes in both homogeneous and heterogeneous inorganic systems. The redox systems include semiconductor photocatalysis, photochemical reactions of iodides, zero valent metal reactions, and thermochemical reactions that involve the transformation of organochlorinated compounds, volatile organic compounds, arsenic, heavy metal ions, and perfluorocompounds.

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고다공성 MOF의 합성 및 기체 저장에의 응용

고낙은, 최상범, 박영관, 김자헌

숭실대 화학과

다공성 물질인 MOF 는 흥미있는 구조와 기능, 그리고 다양한 확장성 때문에, 최근 연구자들의 큰 관심을 받고 있다. MOF 는 흡착제의 일종이므로 기체의 저장과 분리에 특히 연구의 비중이 높다. 제올라이트, 카본과 비교하면 높은 표면적과 다공성을 가질 수 있다는 장점 때문인데, 실제 BET 표면적 5000 m2/g 이 넘는 MOF 도 개발되었다. 본 강의에서는 MOF 가 달성할 수 있는 현실적인 최대 표면적, 그리고 이러한 물성과 효율적인 기체저장과의 관계에 대해서 최근 연구결과를 중심으로 논의하고자 한다.

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발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 최원용

Sustainable Development for Biomass Conversion to Biofuels and Biobased Chemicals via Catalysis

장종산, 이정호, 황영규, 한요한, 김형록

한국화학연구원 바이오리파이너리연구센터

화학산업의 주요 원료로 사용되고 있는 석유자원의 점차적인 고갈은 비단 화학산업 뿐만 아니라 에너지산업을 비롯한 국가 기간산업 전체에 커다란 영향을 미치고 국가의 지속적인 발전에 심각한 장해 요인이 될 것으로 예상된다. 또한 화석연료의 사용에 의한 이산화탄소 온실가스 배출과 이로 이한 지구온난화 문제는 기후변화 협약 포스트 교토의정서 단계의 온실가스 의무감축이 가시화될 2013 년 이후 화석에너지를 사용하는 산업에 지대한 영향을 미칠 것으로 우려된다. 이에 따라 새로운 원료와 대체 에너지원 확보를 위해 식물자원을 이용하여 바이오연료 및 화학제품을 생산하는 바이오리파이너리 기술이 이산화탄소 온실기체 저감문제를 해결하는 하나의 방안으로서, 그리고 환경친화적인 지속성장 기술로서 기대를 모으고 있다. 본 발표에서는 바이오리파이너리의 특징 및 국내외 현황에 관해 간단히 살펴본 후 화학(연)에서 수행 중인 식물자원 바이오매스 유래 화합물의 촉매전환 및 공정기술 개발 현황에 관해 소개하고 토론할 기회를 갖고자 한다.

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초임계유체를 이용한 녹색기술

Green Chemistry with Supercritical Fluids

이윤우

서울대 화학생물공학부

초임계유체를 이용한 녹색기술을 소개한다. 초임계유체는 인체와 환경에 유해한 용매를 대체할 수 있는 녹색용매이다. 지금까지 초임계유체는 커피로부터 카페인을 제거하거나 호프열매로부터 쓴맛을 추출하여 맥주에 첨가하는 데 일반적으로 사용되어 왔다. 국내에서도 참기름을 생산하거나 여러 가지 천연물질을 추출하는 공정에 친환경용매인 초임계이산화탄소를 이용하고 있다. 초임계 이산화탄소는 발암물질인 퍼클로로에틸렌을 대체하는 드라이크리닝 용제로 개발되기도 하고 폐수를 획기적으로 줄일 수 있는 반도체 건식 세정, 건식염색, 고분자중합의 용매로도 활용된다. 한편 초임계 상태의 물은 폐수처리, 에너지전환, 바이오매스의 전처리, 화학공정의 중간체의 재활용, 플라스틱의 재활용에 활용도가 증대되고 있다. 본 발표에서는 서울대학교에서 수행하고 있는 최근 초임계유체 연구동향을 중신으로 지속가능한 사회를 구현하기 위한 구체적인 모델 기술로서 초임계유체기술의 전망에 대하여 분석한다.

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장소: 대전컨벤션센터

발표코드: **금9C5심**

발표분야: Chemical Approaches for Green Technology

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 강상욱

Artificial Photosynthesis for Cutting CO_2 Emission

Shunichi Fukuzumi

Department of Material and Life Science, Division of Advanced Science and Biotechnology, Graduate School of Engineering, Osaka University, SORST, JST, Suita, Osaka, Japan

The objective of this lecture is to report recent development of artificial photosynthesis for production of hydrogen using solar energy. High quantum yields and long-lived charge separation, which mimic the multi-step electron-transfer processes in the photosynthetic reaction center, have been achieved by electron donor-acceptor ensembles linked by covalent bonding.[1] During the multi-step electron-transfer processes, however, a significant amount of energy is lost to attain the final long-lived charge-separated state. Then, simple electron donor-acceptor dyads linked by covalent or non-covalent bonding have been developed to attain a long-lived and high-energy charge-separated state without significant loss of excitation energy.[2] More sophisticated supramolecular complexes composed of light harvesting and charge-separation units have been constructed by using non-covalent bonding such as p-p interaction, coordination bonds, and hydrogen bonds to attain long-lived charge-separated states with a high light harvesting efficiency.[3-5] Recent development of photocatalytic hydrogen production using artificial photosynthetic systems is also reported together with hydrogen storage by fixation of CO_2 with H_2 as a form of formic acid (HCOOH) that can be converted selectively back to H_2 in the presence of an appropriate transition metal complex catalyst.[6] Combination of photocatalytic hydrogen generation with the catalytic CO_2 fixation with H_2 and the decomposition of HCOOH back to H_2 provides excellent systems for cutting CO_2 emission.

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대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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TiO_2 Photocatalysts for Green Technology

Tetsuro Majima

The Institute of Scientific and Industrial Research (SANKEN), Osaka University, Mihogaoka 8-1, Ibaraki, Osaka 567-0047, Japan

Titanium dioxide (TiO_2) photocatalysts have been extensively studied and used for the water-splitting reaction that produces hydrogen, the degradation of organic pollutants, the surface wettability conversion, and so on. It is well-known that electron-hole pairs are generated when TiO_2 is irradiated by UV photons with energy higher than the TiO_2 band gap energy (3.2 eV) and these charge carriers can migrate to the TiO_2 surface to initiate redox reactions with adsorbates. Generation of reactive oxygen species was also detected during the TiO_2 photocatalytic reaction. In order to develop new and efficient TiO_2 photocatalysts, we have investigated the TiO_2 photocatalytic reaction mechanism with time-resolved transient absorption and emission spectroscopies, two-color two-laser flash photolysis and single-molecule fluorescence techniques. Particularly, the single-molecule fluorescence spectroscopy has been demonstrated to overcome the spatial heterogeneities of the nanoscale local environments and the inhomogeneous vibronic coupling between the adsorbed molecules and the rough surfaces of the semiconductors, involved in the interfacial electron-transfer processes.

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발표분야: Current Trends in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이진용

Conformational Structures of Isolated Biomolecules

Jean Pierre Schermann

서울대 생물물리 및 화학생물학과 & University of Paris 13, Villateneuse, France

Structures of biomolecules are crucial for their activity. They depend upon the intrinsic properties of the molecules as well as the environment. Infrared spectroscopy coupled to mass-spectrometry and quantum chemistry is a rather universal tool that allows for conformational studies of small systems such as neurotransmitters and natural or chemical substances acting as possible anti-cancer or anti-Alzheimer disease drugs.

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발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 이진용

The Role of the Fermi Surface in Adsorbate-Metal Interactions: An Energy Decomposition Analysis

Baerends Evert Jan

POSTECH & Vrije University

The interpretation of chemical bonding and reactivity has been greatly aided by the development of energy decomposition methods, which afford a quantification of concepts such as Pauli repulsion, electrostatic interaction, (frontier) orbital interaction.[1] The Kohn-Sham model of DFT uses molecular orbitals which are eminently suitable for this type of analysis. [2]We will discuss the extension of energy decomposition methods to extended systems, in particular for chemisorption of a molecule on a metal slab. This introduces a new energy component, which we call the relief of the Pauli repulsion due to the existence of the Fermi level in the metal: antibonding levels that rise above the Fermi level can be depleted by electrons falling down into the Fermi sea. We will highlight the significance of this electronic structure feature of metallic systems as the key factor that gives them their singular reactivity properties, which are so much exploited in heterogeneous catalysis.[3] The interpretation of chemical bonding and reactivity has been greatly aided by the development of energy decomposition methods, which afford a quantification of concepts such as Pauli repulsion, electrostatic interaction, (frontier) orbital interaction.[1] The Kohn-Sham model of DFT uses molecular orbitals which are eminently suitable for this type of analysis. [2]We will discuss the extension of energy decomposition methods to extended systems, in particular for chemisorption of a molecule on a metal slab. This introduces a new energy component, which we call the relief of the Pauli repulsion due to the existence of the Fermi level in the metal: antibonding levels that rise above the Fermi level can be depleted by electrons falling down into the Fermi sea. We will highlight the significance of this electronic structure feature of metallic systems as the key factor that gives them their singular reactivity properties, which are so much exploited in heterogeneous catalysis.[3] [1] F. M. Bickelhaupt, E. J. Baerends, Rev. in Comp. Chem. Vol. 15, pp1-86. [2] O. V. Gritsenko, R. R. T. Schipper, E. J. Baerends, J. Chem. Phys. 107 (1997) 5007. [3] P. H. T.

Philipsen, E. J. Baerends, J. Phys. Chem. B 110 (2006) 12470; P.H. T. Philipsen, M. Luppi, E. J. Baerends, in preparation

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 이진용

Electron Attachment to Aromatic Hydrocarbons

김성근

서울대 화학부

We studied anions of aromatic hydrocarbons and their molecular clusters as a prototypical system that contains a loosely bound electron. By using molecular beam photoelectron spectroscopy, we found a wealth of new phenomena unique to a loosely bound electron state. The size and chemical substitution of the aromatic ring were found to strongly affect the electron state. A counter-intuitive case of electron binding to bromochlorobenzenes was found that bears some resemblance to the K + ICl reaction. A particularly interesting observation was that an electron binds to the complex of CO_2 with pyridine and other azabenzene species in what appears to be "associative" electron attachment that turns a van der Waals bond between the two moieties into a covalent one. Drastic stabilization of electronic state through extended π-network is believed to be the culprit.

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Nano-electronics/spintronics and nano-optics

김광수

포항공과대 화학과

The electron transport phenomena in molecular electronics devices [1] and graphene nanoribbon spin valves are discussed based on non-equilibrium Green function theory [2]. As a highly efficient futuristic informatics device, we discuss graphene nanoribbon spin-valve devices which show the super magnetoresistance behavior [3]. The device can be used as a spin filter which selectively transmits almost 100% spin-polarized current. In addition, novel nano-optics phenomena are discussed based on nano-scale lenses which show near-field focusing and magnification beyond the diffraction limit [4]. The enhancement of micro-Raman signals for the graphene layers [5] through nanolenses is also addressed.[1] W. Y. Kim, Y. C. Choi, S. K. Min, Y. C. Cho, and K. S. Kim, Chem. Soc. Rev. 2009, 38, 2319.[2] W. Y. Kim and K. S. Kim, J. Comput. Chem. 2008, 29, 1073.[3] W. Y. Kim and K. S. Kim, Nature Nanotech. 2008, 3, 408.[4] J. Y. Lee, et al., Nature 2009, 460, 498.[5] K. S. Kim. et al., Nature 2009, 457, 706.

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Möbius Aromaticity and Antiaromaticity

김동호

연세대 화학과

Möbius aromaticity is venerable concept of almost timeless allure. Much of the fascination reflects the disparity between the intellectual simplicity, the idea a twisted [4n]annulene lying on a Möbius strip will display aromatic properties commonly with planar Hückel-type [4n + 2]annulenes, and the synthetic difficulties associated with providing for an unambiguous experimental demonstration. In fact, a single example of a Möbius aromatic hydrocarbon, a system with modest aromatic characteristics, is known, underscoring the fact that preparing Möbius-type aromatic systems remains an ongoing synthetic challenge. We have now found, and wish to report here that Möbius aromatic molecules can be obtained readily; they are formed spontaneously from meso-aryl substituted expanded porphyrins upon metallation with group 10 metals. While unexpected, this approach appears quite general with a range of expanded porphyrins, including [36]octaphyrin, [32]heptaphyrin, and [26]hexaphyrin, providing stable Möbius aromatic macrocycles via metallation and concurrent N—metal and C—metal bond formation. The presence of diatropic ring currents and characteristic absorption features in the respective proton NMR and UV/Vis absorption spectra provides important support for the proposed aromaticity, as do theoretical calculations. In addition, large two-photon absorption (TPA) cross sections are observed for the proposed Möbius aromatic complexes. The present work thus serves to validate the concept of Möbius aromaticity in an experimentally unambiguous manner, while proving a versatile entry into this potentially large, but so far quite limited, class of materials.

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Treatment of Spin-Orbit Interactions in Computational Quantum Chemistry

이윤섭

KAIST 화학과

Spin-orbit coupling is one of the most recent additions for many quantum chemical packages. General strategies available in popular packages will be compared from computational point of view, and main resulting effects of spin-orbit interactions will be qualitatively described. Spin-orbit interactions, which may be considered as part of relativistic effects, are typically ignored in electronic structure calculations of molecules in the ground state, but can be of importance for molecules containing heavy (4th to 6th row) or superheavy (7th row) elements. We have been working on ab initio molecular orbital methods that take spin-orbit terms into account utilizing two-component relativistic effective core potentials. Some of recent progress and results from this endeavor will be presented.

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Conical intersection dynamics in the chemical bond dissociation

김상규

KAIST 화학과

Nonadiabaticity of the chemical reaction is very important in understanding various ultrafast phenomena occuring among different adiabatic electronic states. In the polyatomic systems, a so-called "conical intersection" has been widely accepted as the efficient dynamical funnel for a number of nonadiabatic transitions which are ubiquitous in chemistry and biology. We investigated the photodissociation dynamics of thiophenol and thioanisole. The S-H or S-CH3 bond dissociation takes place on the repulsive potential energy surface on which two conical intersections are encountered along the reaction coordinate. These conical intersections at the planar geometry play key roles in determining the branching ratio between two distinct product channels at the asymptotic level. Using the velocity-map ion imaging method, kinetic and spatial distributions of the H or CH3 fragments have been quantitatively measured for various initial quantum states. The energy dependent behavior of the dissociation channel gives the insight into the nature of the conical intersection and its dynamic role in the whole reaction dynamics.

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발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 구현주

Unimolecular Reaction Rate Constants for Biopolymers : RRKM and Modified Beyer-Swinehart algorithm

문정희

한국생명공학연구원 단백체시스템연구단

A systematic method to automatically estimate the vibrational frequency sets of linear peptide and protein ions with any amino acid sequence, which is needed in RRKM calculations has been developed. The Beyer-Swinehart(BS) algorithm, which calculates vibrational state density and sum, was modified for simulataneous treatment of degenerate vibrations. The modified algorithm was used in the grouped-frequency mode of the RRKM unimolecular reaction rate constant calculation for proteins with molecular mass as large as 100,000. To overcome the limit of long double data type, the dual number representation - a real number for the significant coefficient and an integer for the exponent - was adopted. Meaningless add calculation was also avoided to shorten the calcuation time. Compared to the original BS method, reduction in computation time by a factor of around 3000 was achieved. The method is thought to be adequate for RRKM calculations for macromolecule in the gas phase such as the molecular ions of proteins, nucleic acid, and carbohydrates if appropriate frequency set is provided.

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Ab-initio based grand canonical Monte-Carlo simulations on hydrogen adsorption in metal-organic frameworks

한상수

한국표준과학연구원 나노소재측정센터

In this talk, I will show improved designs of metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs) for hydrogen storage. For all MOFs and COFs, the H_2 uptake was predicted from grand canonical Monte-Carlo (GCMC) simulations based on force fields developed to fit accurate quantum mechanics (QM) [second order Møller-Plesset perturbation theory using doubly-polarized quadruple-ζ (QZVPP) basis sets]. This simulation methodology was validated with reported experimental results, providing accurate hydrogen adsorption isotherms of MOFs and COFs at both of 77 and 300 K. Then strategies for the improvement of hydrogen storage in the porous materials will be discussed in detail by the ab-initio based GCMC simulations. The strategies include appropriate pore size, impregnation, catenation, open metal sites, doping of alkali elements onto organic linkers, substitution of metal oxide with lighter metals, and functionalized organic linkers. Specially I will introduce Li-doped metal-organic framework systems which meet the 2010 DOE target (6.0 wt% at room temperature and

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A striking rate phenomenon of organic reaction 'on water': A theory

정유성, *R.A. Marcus

*KAIST EEWS 대학원 *Department of Chemistry, California Institute of Technology*

Many chemical reactions can occur within a timescale that is useful for synthesis and biological processes due to catalysts. In this talk, I will describe an experimentally observed remarkable rate phenomenon where a simple molecule like water, can increase the reactivity of some organic reactions substantially in the form of emulsions. In a most dramatic case, for example, rate acceleration of more than a factor of 100 000 was observed, a catalysis that is typically seen only in enzymatic reactions. A key aspect of the latter on-water catalysis is the chemistry between water and reactants that occurs at an oil-water phase boundary. In particular, the structure of water at the oil-water interface of an oil emulsion, in which approximately one in every four interfacial water molecules has a free ("dangling") OH group that protrudes into the organic phase, plays a key role in catalyzing reactions via the formation of hydrogen bonds. To interpret the results in different media, a method is given for comparing the rate constants of different rate processes, homogeneous, neat and on-water, all of which have different units, by introducing models that reduce them to the same unit.

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Structure Prediction & Ligand Screening: Application to G Protein-Coupled Receptors

허지영

경희대 환경응용화학대학

G protein-coupled receptors (GPCRs) play an essential role in cell communications and sensory functions. Consequently, they are involved in wide variety of diseases and are targets for many drug therapies. Particularly important is the large number of orphan GPCRs, which may play important, albeit unknown, functions in various cells. To understand their respective physiological roles, it is important to identify their endogenous ligands, and to find small molecule ligands that would serve as selective agonists or antagonists. The *mas-related gene G protein-coupled receptors* (Mrg receptors) belong to the orphan GPCR family, which is expressed in a specific subset of sensory neurons known to detect painful stimuli, suggesting that they could be involved in pain sensation or modulation.The primary focus of this talk is to predict the 3D structure and the binding site of one of the Mrg receptors, mouse MrgC11 (mMrgC11) and to identify novel ligands that would be potential agonists or antagonists. We predict the 3D structure for the mMrgC11 and the binding site for the FMRF-NH_2 neuropeptide together with four singly chirally modified ligands. Subsequently, we carry out the mutagenesis experiments to validate our models and the virtual screening with the combination of QSPR and docking methods for this predicted mMrgC11 receptor.

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Photodissociation dynamics of dichlorocarbene at 193 and 248 nm

신승근, *Paul J. Dagdigian

*경희대 화학과 *The Johns Hopkins University, U.S.A.*

The dynamics of the 193 and 248 nm photodissociation of the CCl2 molecule have been investigated in a molecular beam experiment. The CCl2 parent molecule was generated in a molecular beam by pyrolysis of CHCl3, and both CCl2 and the CCl photofragment were detected by laser fluorescence excitation. The 193 and 248 nm attenuation cross section was estimated from the reduction of the CCl2 signal as a function of the photolysis laser fluence. The internal state distribution of the CCl photofragment was derived from analysis of laser fluorescence excitation spectra in the A2Δ-X2 Π band system. At 193 nm, most of the energy available to the CCl(X2Π) + Cl fragments appears as translational energy. The CCl fragment rotational energy is much less than predicted in an impulsive model. The excited electronic state appears to dissociate indirectly, through coupling with a repulsive state arising from the ground-state CCl(X2Π) + Cl asymptote. The identity of the initially excited electronic state is discussed on the basis of what is known about the CCl2 electronic states.At 248 nm, the CCl(X2 Π, v = 0) rotational state distribution was found to be bimodal, with maximum populations at N = 10 and 85, and was dependent upon the source backing pressure, and hence upon the internal state distribution of the CCl2 precursor. The 248 nm photodissociation dynamics appears to involve two separate channels, namely nearly impulsive rotational energy release and predissociation with little rotational energy imparted to the CCl fragment.

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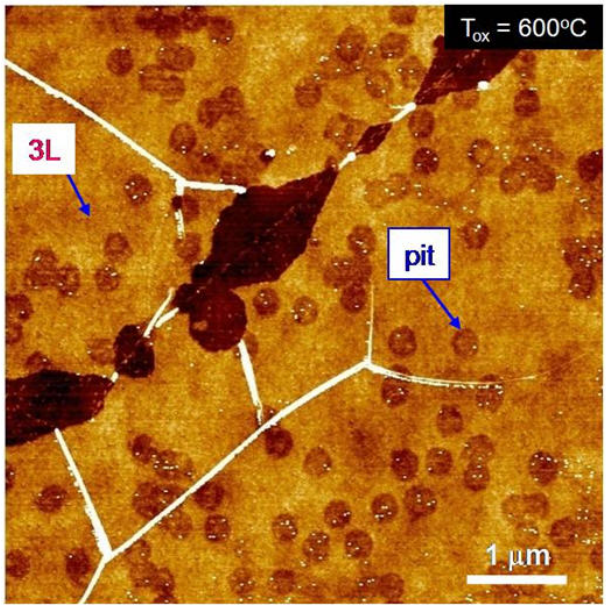
Functionalization and chemical properties of graphene

Sunmin Ryu, [*]**Li Liu**, [*]**Stephane Berciaud**, [**]**Melinda H. Han**, [*]**Michael Steigerwald**, [***]**Mark S. Hybertsen**, [****]**Philip Kim**, [****]**Tony F. Heinz**, [*]**Louis E. Brus**

Department of Applied Chemistry, Kyung Hee University [*]*Department of Chemistry, Columbia University* [**]*Department of Applied Physics and Applied Mathematics, Columbia University* [***]*Center for Functional Nanomaterials, Brookhaven National Laboratory* [****]*Department of Physics, Columbia University*

Atom-thick graphene membrane holds substantial potential for applications in future molecular-scale integrated electronics, transparent conducting membranes, nanocomposites, etc. To realize this potential, chemical properties of graphene need to be understood and functionalization toolkits are also required. To meet this need, surface chemistry of graphene has been explored by Raman spectroscopy, AFM and STM scanning probes. In the first part of the talk, two chemical reactions of graphene will be presented. Hydrogenation, the simplest basal plane functionalization, is highly reversible and strongly dependent on the thickness of graphene in the rate. Graphene sheets can be locally hydrogenated with a high spatial resolution. Thermal oxidation also proceeds at a higher rate for single layer than double layer graphene and triple layer graphene behaves like bulk graphite. The second part of the talk will illustrate the influence of underlying silicon dioxide substrates and ambient gases on properties of graphene. Raman spectroscopy shows that freestanding graphene is essentially charge-neutral implying that the “usual” hole-doping in supported graphene is mediated by oxide substrates. An STM study reveals that thermal annealing generates out-of-plane deformation of nanometer-scale wavelength and distortion in sp2 bonding on an atomic scale. Graphene deformed by annealing is found to be chemically active enough to bind molecular oxygen, which leads to a strong hole-doping. A possible form of oxides will be discussed.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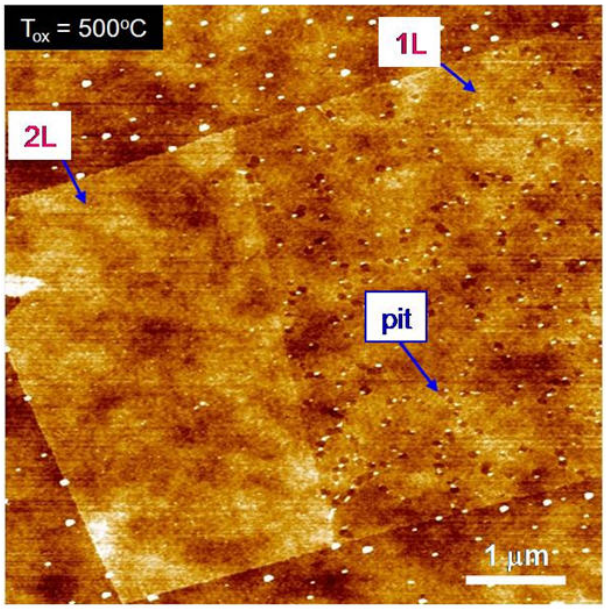
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장소: 대전컨벤션센터
발표코드: **금11G7심**
발표분야: Oral Presentation by Young Physical Chemists
발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 윤상운

Fullerenes with Diverse Structures and Their Applications

신현석

울산과학기술대 에너지공학부

Fullerene (C60), a highly conjugated organic molecule has been widely studied as one of the important organic semiconductors potentially applicable for integrated FET, superconductor, photodetector and photovoltaic device. In this talk, I will address the historical background of C60 and the recent trend of C60 structure-related research. Then, two research results on (I) C60 disks and (II) the spontaneous electron transfer from C60 to Au ions will be presented. (I) The highly selective synthesis of disk-shaped 2D single crystalline C60 was performed by using a vapor-solid process. The experimental results describe: 1) the substrate effect on the highly selective formation of C60 disks, 2) the structural characterization of the disks, 3) photoluminescence properties of the disks, and 4) the photoconductivity of a single disk. (II) The spontaneous electron transfer from C60 to Au ions readily converted the intrinsic majority charge carrier of semiconducting C60 from electron to hole by forming discrete Au nanoparticles. The resulting Au-C60 system showed a stable p-type field effect transistor (FET) characteristic even in ambient condition at room temperature. Another interesting feature of the hole-doped C60 FET device was the selective silencing of photocurrent at visible wavelength region.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이용일

소형, 경량의 휴대형 GCMS 개발

박창준, *정광우, **박한오

*한국표준과학연구원 첨단장비기술센터 *원광대 화학과 **(주)바이오니아*

대기 중 휘발성 유기물 혹은 화학전 독가스를 현장에서 실시간으로 정량 및 정성분석을 수행할 수 있는 휴대형 GCMS 질량분석기 개발현황을 소개한다. 휘발성 화합물 시료의 분리를 위하여 소형 GC 모듈 (15x15x10 cm, 3kg)과 시료농축기술을 개발하였다. 분리된 시료는 100 μm 두께의 실리콘 재질의 반투막 인터페이스를 통하여 진공도 5x10-5 torr 질량분석기 안으로 주입된다. 반투막은 고진공 유지가 가능할 뿐만 아니라, 휘발성 유기물의 경우 GC 운반기체에 비해 상대적으로 높은 투과 특성을 나타내기 때문에 100 배 이상의 시료농축효과도 얻는다. 진공펌프로는 24V DC 전원에 의하여 작동되는 소형 turbo-pump (10 L/s)와 minidiaphragm pump 를 사용한다. 반투막을 통하여 주입된 시료는 소형이온원에서 이온화되고 hyperbolic quadrupole mass filter 에 의하여 선택된 질량의 이온을 측정한다. 이온 검출기로는 최대 작동압력이 7x10-4 torr 로 높은 channel electron multiplier 를 사용한다. BTEX 시료에 대한 GC 모듈의 분리효율, 그리고 PFTBA calibration compound 와 SF6 gas 를 사용하여 얻은 질량분석부 시험결과를 기기특성과 함께 발표한다. 이 휴대형 GCMS 는 대기오염의 극미량 분석은 물론 산업현장에서의 응급사고, 화재현장의 유독가스 탐지, 그리고 군사용 화학전탐지기로도 사용될 수 있으리라 기대된다.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이용일

Laser Ablation ICP-MS for Metallomics and Microelectronic Analysis

H. B. Lim, Hansem Choi, S. K. Ma, J. Y. Chu

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In our lab, several approaches are in progress for nano scale sampling in ICP-MS, for example, nano size separation and concentration of metal ions in microchip channel with surface modified magnetic beads. For direct analysis for semiconductor or liquid bio samples with limited sample volume, surface modified PDMS array microchip was developed for accurate and fast calibration and demonstrated the determination of heavy metals for quantification using 213 nm laser coupled with ICP-MS. The microarray chip sampling technique was applied to determine metal impurites in photoresist (PR) used in semiconductor manufacturing process was performed to achieve fast analysis with high sensitivity and to reduce analytical cost. For application to not only PR but some bio samples, such as blood and urine, Al, Tl, and Pb showed excellent linearity. This developed microchip sampling was expected to provide several significant advantages, such as reliable ablation, high throughput, convenient sample preparation and loading for standard addition, and low cost due to no use of wafers.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이용일

Development of CryoSAS for the quality control of low ppts level of impurities in solar cell by LT-FT-IR

김효진

동덕여대 약학대학

Semiconductor grade silicone now widely used for the solar cell are considered the puriest material known, nevertheless contains impurities at levels of sub ppts. Therefore determination of sub-ppts level of the shallow impurities such as B and P are major concern in production of single crystal solar cell industry. Shallow impurities in single crystal silicone were determined by low temperature far mid IR transmission spectroscopy (LT-FT-IR) and Photoluminescence (PL). Detection limits of B and P as well as other shallow impurities were obtained sub ppt level with liquid He cooled bolometer by LT-FT-IR. Recently, the closed cycled cryostat (CrySAS) to reduce the consumption of liquid He has been developed for the routine quality control of the solar cell industry.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 남상호

Development of detection techniques for ultra trace nuclear materials in environmental samples

박종호, 송규석

한국원자력연구원 원자력화학연구부

As nuclear industries, such as fabrication of nuclear fuel and operation of nuclear power plants, are growing in the energy supplying system, the international society requires transparency in nuclear activities. In accordance in this matter, the analysis of environmental sample plays important role in nuclear safeguards, and monitoring nuclear activities in neighboring countries. KAERI has initiated a demanding systematic development of the analytical techniques for environmental samples and swipe samples. Bulk and particle sample analyses are two major analytical processes in determining the contents as well as isotopic information from the environmental samples. The samples for bulk analysis require chemical preparation consisting of ashing, acid digestion, and chemical separation while particle screening and transferring are necessary for particle analysis. Measurements using mass spectrometer such as induced coupled plasma mass spectrometer (ICP-MS) and thermal ionization mass spectrometer (TIMS) are followed for quantification and isotopic ratio analysis. This paper presented a discussion regarding the general procedure in systematic development of the related analytical technology along with some of the results from the bulk analysis.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 남상호

Applications of Mass Spectrometry in the Industry : Analysis of Organic Materials in Liquid Crystal Displays

조성찬

삼성전자(주) LCD 연구소

Mass spectrometry (MS) has widely accepted as one of the most important analytical techniques in the current industrial settings. Its area of application now covers analyses of synthetic chemicals, environmental hazards, and medical/biological samples to name a few. Such versatility partly comes from the inclusion of the various ways of sample introduction and the capability of hyphenation with other means, especially chromatography. Gas chromatography coupled with MS, that is, GC/MS makes possible to analyze both qualitatively and quantitatively, and that simultaneously with the help of high resolution capillary GC column. In addition, MS hyphenated with liquid chromatography, viz., LC/MS can even analyze analytes with high polarity and/or high boiling point. Such revolutionary development has positioned various industries as one of the most celebrated beneficiaries. Researchers in the field probe their products and materials more into detail hoping to get clearer conclusion with much more speedy approach. Companies that produce active matrix liquid crystal displays (AMLCD's) are not excluded from the list. AMLCD's have now become part of the many popular household appliances and the markets keep finding them with much more advanced level of technologies. Alongside, the required precision and structural complexity push the makers into using cutting-edge materials and technologies based on the most advanced chemical/physical theories. Keeping up with such trend, MS has revealed its power and beauty at the eyes of the analytical chemists. In this presentation, the useful aspects of MS are introduced as it is applied in the industry, which would reveal the value and virtue. However, it is also emphasized that MS is not so called Jack of the all trades.

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발표분야: New Frontiers in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 남상호

Current trends in laser desorption/ionization

김정권

충남대 화학과

Among various forms of laser desorption/ionization (LDI), matrix-assisted laser desorption/ionization (MALDI) is current the most common, where organic acids are used as a matrix which assists ionization of analytes by laser irradiation. On the analysis of big molecules such as proteins, polysaccharides, or nucleic acids, MALDI is the method of choice among LDIs. Recently, a great deal of interest has been focused on the analysis of small molecules such as lipids, oligosaccharides, oligonucleotide, amino acids, and small peptides. The major disadvantage of using MALDI in the analysis of small molecules is that MALDI provides interference peaks in the small m/z ranges. To overcome this disadvantage, a lot of efforts have been concentrated on developing new materials to replace the organic acids used as matrix in MALDI. In this presentation, the current trends in LDI will be overviewed and new developments in the analysis of small molecules using LDI will be introduced.

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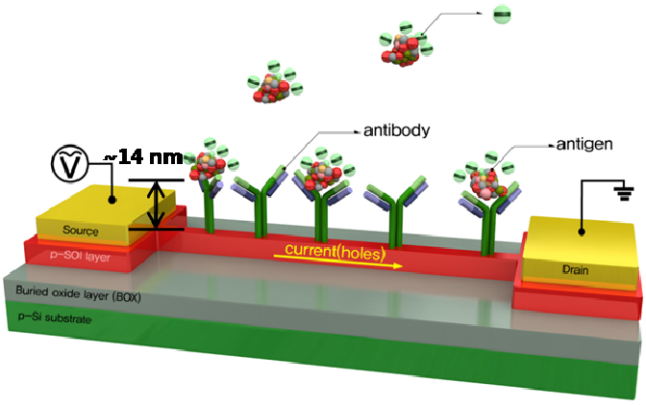
발표분야: Development and Applications of Analytical Chemistry in Bio- and Nano-Technologies
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 임용현

Direct Label-Free Electrical Immunodetection of Biomarkers in Human Serum

김안순, 아칠성

한국전자통신연구원 바이오센서연구팀

Simple and fast biomarker screens have a central role in many areas of healthcare, including disease diagnosis and drug discovery. Biologically modified field-effect transistor (BioFET) is one of the most attractive approaches because of the on-chip integration of the sensor array, fast response, high reliability and low-cost mass production. However, the BioFETs used to detect macromolecules have been operated only in buffer solution with low salt concentrations because of the Debye screening length of blood or serum. Here we report a novel detection technique for direct label-free immunodetection of cancer markers in human serum using a Si-FET that was fabricated by conventional photolithographic processes. The proposed method that is sensing in low salt buffer after immunoreaction in serum overcomes the Debye length problem of the BioFETs, and have been confirmed by using sandwich immunoassay with immunogold nanoparticles. Our results demonstrate specific label-free and real-time detection of cancer markers at a concentration of 0.2 ng/mL in human serum, and successful quantitative and multiplexed sensing.



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발표분야: Development and Applications of Analytical Chemistry in Bio- and Nano-Technologies
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 임용현

Laser Desorption/Ionization Methods for Mass Spectrometric Analyses of Organic and Biological Interfaces

한상윤

한국표준과학연구원 나노바이오융합연구단

Despite numerous researches utilizing self-assembled monolayers and nanoparticles with organically and biologically modified surfaces, appropriate analytical tools to characterize the molecular compositions of such interfaces have been rarely known. Conventional surface analysis tools are rather limited to the information of atomic level, and spectroscopic methods mainly gives the information on the functional groups of surface molecules. In an effort to develop new surface mass spectrometric methods, the laser desorption/ionization (LDI) methods are being explored. In this presentation, matrix-free LDI and MALDI methods for interface mass spectrometry will be discussed. The matrix-free nanostructure-assisted LDI methods for small molecule analyses will also be presented.

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Multifunctional Silica Nanotubes: Toxicity, Endocytosis, Imaging and Biodistribution

이상복

University of Maryland, USA

Silica nanotubes have become very attractive as multifunctional nanoparticles due to their structural attributes, such as the distinctive inner and outer surfaces, over conventional spherical nanoparticles. Inner voids can be used for capturing, concentrating, and releasing species ranging in size from large proteins to small molecules because tube dimensions can be easily controlled by the template synthesis. Distinctive outer surfaces can be differentially functionalized with environment-friendly and/or probe molecules to a specific target. These multifunctional silica nanotubes (SNTs) have shown enormous potential in biomedical application including therapeutic tools, bio-imaging, drug delivery, bioseparations, and biocatalysis, and also provided a model system to study wetting /diffusion problems and reactions in nanoscale containers. In this presentation, the recent results on the endocytosis mechnism and biodistribution of SNTs will be mainly descibed.

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발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 김성환

Synthetic Lipid Bilayer Platform for Bioanalytical Applications

남좌민

서울대 화학부

The development of sophisticated diagnostic technologies to tailor appropriate combinations of therapeutic methods to individual patients is of paramount importance for the early treatment and eradication of numerous devastating and infectious diseases. Current techniques for genetic screening and protein expression profiling, while fortuitously successful in some cases, are indirect and cannot be expected to comprehensively cover the disease space. In many cases, however, early, fast, and accurate diagnosis is not possible with current methods. The overall objective of our research effort is the development of new, hybrid technologies that use a model cell membrane platform, supported lipid bilayer (SLB), to detect molecular interactions between cell membrane and molecules of interest and to interface live cells with non-living materials that are useful for biological and medical applications. This work involves deciphering the molecular language by which cells communicate, developing new methodologies for the manipulation and control of biological molecules, and the integration of these developments into functional systems. The core scientific strategy is based on reassembly of lipids and proteins into membrane structures supported on inorganic scaffolds. These so-called supported membranes recapitulate many of the properties of live cell membranes that diffuse freely and engage their cognate receptors on the cell in a life-like manner. Here, we propose supported membrane-based methods that provide a uniquely powerful solution to the growing demand for molecular and cellular diagnostic tools. Applications include electrophoretic detection of membrane-binding targets using fluid lipids and optical imaging of lipid-tethered gold nanoparticle for the detection of membrane receptor-ligand interactions.

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발표종류: 심포지엄, 발표일시: 금 10:55, 좌장: 김성환

Microfluidic Separation Technologies for Analytical Chemistry

박제균

KAIST 바이오및뇌공학과

The development of microfluidic separation technologies is one of the major issues in the area of lab-on-a-chip and micro total analysis system. However, previously reported passive methods for particle separation cannot separate microparticles without the aids of sheath flows and complex channel networks. In this presentation, separation and sorting of microspheres, including DNAs, blood cells, and mammalian cells, were demonstrated by using a novel microfluidic mechanism, "hydrophoresis", which uses slanted or anisotropic obstacles to induce hydrodynamic interaction between the obstacles and the particles subjected to rotational flows induced by the obstacles. The equilibrium positions of the particles by the hydrodynamic interactions depend on their size. Continuous separation and focusing of micro- and nano-particles were also achieved using a contraction-expansion array microchannel, demonstrating the potential of microfluidic techniques in a biochemical, clinical, and environmental field with high-throughput, low-cost and continuous separation.

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Chemical Approach for Specific Enrichment and Mass Analysis of Nitrated Peptides

Kwang Pyo Kim, Woon-Seok Yeo

Department of Molecular Biotechnology, Konkuk University, Seoul 143-701, Korea

The analysis and detection of 3-nitrotyrosine are biologically and clinically important because protein tyrosine nitration is known to be involved in a number of biological phenomena such as cellular signal transduction, pathogenesis of inflammatory responses, and age-related disorders. However, the main obstacles in the study are low abundance of nitrated species and lack of efficient enrichment methods. Here in, we introduce new chemical approaches to analyze nitrated peptides using mass spectrometry by incorporating specific tagging groups in the peptides through simple chemical transformations. We further demonstrated the utility of our approaches by detection of nitrated peptides in complex samples such as tryptic peptide mixtures of bovine serum albumin (BSA), Huh7 cell lysate and HeLa cell lysate.

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발표분야: Biochemistry of Protein Structures and Functions
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 허용석

Dynamic structural changes of nuclear receptors and its application for FRET biosensor development

우의전

한국생명공학연구원 단백체의학연구센터

Nuclear receptors regulate gene expression in multicellular organisms in response to a wide range of developmental, physiological, and environmental cues. Rev-erbβ is a nuclear receptor that plays an important role in circadian clock, lipid homeostasis and inflammation. Reverb, once known to be orphane receptor, binds Heme at the ligand binding pocket sensing diatomic gas such as NO or CO. The structural comparision of the apo form (Woo et al, 373, 735-744, J Mol Biol, 2007) with the recently determined ligand bound form (Pardee et al, 7,384-398, PLoS Bio, 2009) shows significant conformational change at the ligand binding pocket. The ligand binding pocket of the apo form is filled with bulky hydrophobic residues resulting in a small residual cavity size and the significant conformational change of the Helix 11. Lacking the ligand and the helix 12, Rev-erbβ appears to stabilizes the hydrophobic cluster in the LBP by adopting the unique geometry of Helix H11. The dynamic conformational change observed in nuclear receptors can be utilized to develop FRET biosensor. Recently, we have applied FRET to various hormone receptors including ER (estrogen receptor). The in vitro analysis performed with FRET Estrogen Receptor can discriminate the agonists and the antagonists indicating the different conformational change of the receptor. Nuclear Receptor FRET can be utilized to identify and to screen for various useful bioactive compounds.

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발표분야: Biochemistry of Protein Structures and Functions
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 허용석

Structural basis for substrate recognition and reaction mechanism of a bacterial aminopeptidase

이상호

성균관대 생명과학과

The substrate specificities of aminopeptidases must be tightly regulated to prevent unwanted peptide cleavage otherwise damaging essential cellular functions. Bacterial aminopeptidase PepS shows substrate specificity towards small peptides possessing arginine or aromatic residues at the N-terminus, but mechanisms underlying this specificity remain elusive. Here we report the crystal structures of PepS from Streptococcus pneumoniae in two conformations and its complexes with a substrate or inhibitors. PepS exists as an elongated dimer where each monomer consists of N- and C-terminal domains. The relative orientation of the two domains permits PepS to adopt at least two distinct conformations: closed and open. The closed, active conformation of PepS limits the substrate entry, while the open, inactive conformation accommodates the substrates into its binding pocket with the catalytic residues positioned away from the active configuration. The closed dimer features face-to-face, eclipsed arrangement and the open dimer have two monomers in staggered position. Substrate recognition is achieved by two kinds of filters: S1 substrate binding pocket determining the identity of the cleaving residue ("specificity filter") and internal cavity and elongated dimeric arrangement limiting the length of the substrate ("length filter"). We propose that PepS alternates between open and closed conformations by domain movements during each catalytic cycle: opening for swallowing in the substrate, closing for the hydrolysis of the bound substrate, and re-opening for the release of the products.

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장소: 대전컨벤션센터
발표코드: **목14H3심**
발표분야: Biochemistry of Protein Structures and Functions
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 허용석

Type I restriction-modification system

김정선

전남대 화학과

DNA imported into microorganisms is removed by restriction-modification (RM) systems (restriction enzymes) in host cells. Of these, type I RM systems are specific in their DNA translocation and restriction mechanisms as well as their DNA recognition and are composed of hetero-oligomeric proteins encoded by three closely linked genes: a specificity subunit (HsdS or S) for recognizing a DNA sequence, a methylation subunit (HsdM or M) for methylating recognized target bases, and a restriction subunit (HsdR or R) for the translocation and random cleavage of non-methylated DNA. We elucidated crystal structures of a specific subunit from Methanococcus jannaschii and a restriction subunit from Vibrio vulnificus CMCP6, which provide several interesting features to understand its unique mechanism. The detailed structural features will be discussed.

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발표분야: Biochemistry of Protein Structures and Functions
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 허용석

Variable lymphocyte receptors; antigen recognition and application

한병우, *Brantley R. Herrin, *Max D. Cooper, **Ian A. Wilson

*서울대 약학대학 약학과 *Emory University **The Scripps Research Institute*

Variable lymphocyte receptors (VLRs) rather than antibodies play the primary role in recognition of antigens in the adaptive immune system of jawless vertebrates. Combinatorial assembly of leucine-rich repeat (LRR) gene segments achieves the required repertoire for antigen recognition. We have determined a crystal structure for a VLR-antigen complex, VLR RBC36 in complex with the H-antigen trisaccharide from human blood type O erythrocytes, at 1.67 angstrom resolution. RBC36 binds the H-trisaccharide on the concave surface of the LRR modules of the solenoid structure where three key hydrophilic residues, multiple van der Waals interactions, and the highly variable insert of the carboxyl-terminal LRR module determine antigen recognition and specificity. The concave surface assembled from the most highly variable regions of the LRRs, along with diversity in the sequence and length of the highly variable insert, can account for the recognition of diverse antigens by VLRs. VLRs have a good possibility for antibody substitutes in diverse biotechnology fields.

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발표분야: Biochemistry of Protein Structures and Functions
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 허용석

The Secret Life of Slicer - Argonaute

송지준

KAIST 생명과학과

Argonaute proteins and small interfering RNAs (siRNAs) are the known signature components of the RNA interference effector complex RNA-induced silencing complex (RISC). However, the identity of "Slicer," the enzyme that cleaves the messenger RNA (mRNA) as directed by the siRNA, has not been resolved. Here, we report the crystal structure of the Argonaute protein from Pyrococcus furiosus at 2.25 angstrom resolution. The structure reveals a crescent-shaped base made up of the amino-terminal, middle, and PIWI domains. The Piwi Argonaute Zwille (PAZ) domain is held above the base by a "stalk"-like region. The PIWI domain (named for the protein piwi) is similar to ribonuclease H, with a conserved active site aspartate-aspartate-glutamate motif, strongly implicating Argonaute as "Slicer." The architecture of the molecule and the placement of the PAZ and PIWI domains define a groove for substrate binding and suggest a mechanism for siRNA-guided mRNA cleavage.

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발표분야: Nanomaterials and Nucleic Acids for Molecular Therapy
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Shell-crosslinked Magnetic Nanoparticles for Targeted Labeling and Imaging

이해신

KAIST 화학과

We prepared highly stable and functionalized magnetic nanoparticles for targeted labeling and imaging applications. A library of functionalized PEGs was screened to transfer and stabilize organic synthesized iron oxide nanoparticles (IONPs) in aqueous solution by a vacuum-drying method. For preparing highly stable nanoparticles and their specific targeting, the coated PEG on IONPs were crosslinked using hyaluronic acid. The shell-crosslinked magnetic nanoparticles exhibited high stability in aqueous solutions with various pH and high salt concentrations for over a month, compared to IONPs coated only with 6PEG-NH2. The shell-crosslinked magnetic nanoparticles also showed enhanced internalization into cells expressing CD44 receptor, such as mesenchymal stem cells, by specific uptake. The shell-crosslinked magnetic nanoparticles showed high application potentials for stem cells and trafficking, or targeted cancer imaging.

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발표분야: Nanomaterials and Nucleic Acids for Molecular Therapy
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 민달희

Oligopeptide/drug-derived cationic nanoparticles for in vivo delivery of siRNAs

오유경

School of Pharmacy, Seoul National University, Seoul, South Korea

Recently, small interfering RNAs (siRNAs) have been emerging as a potential anticancer therapeutics (1) with several candidates in preclinical trials. The limited delivery of naked siRNAs to cancer cells and the polygenic nature of cancer, however, hampered the development of siRNA monotherapy as potent anticancer strategy. Substantial progress has been made in siRNA delivery technologies using cationic lipid or polymer-based systems (2-4). Moreover, the combination therapy of siRNAs and anticancer drugs has been attempted to enhance the therapeutic outcome (5). In this study, we tested the use of oligopeptide or cationic anticancer drug-derived nanoparticles as a delivery system of siRNAs. Cationic nanoparticles composed of oligopeptide or anticancer drug-derived cationic lipids could form electrostatic complexes with negatively charged siRNAs. When compared with Lipofectamine 2000 (L2K), the cationic nanoparticles provided increased cellular delivery of siRNAs in various cell lines such as KB, A549, HeLa, and Hep3B tumor cells. Unlike L2K showing confluency-dependent transfection efficiency, the cationic nanoparticles exhibited the confluency-independent delivery of siRNA with high efficiency. More than 95% of the cells were positive for siRNA following its delivery with the cationic nanoparticles at 90% of cell confluency. A survivin-specific siRNA delivered using the cationic nanoparticles effectively reduced the mRNA expression of the target genes in the cell lines tested. siMcl complexed to the cationic nanoparticles provided significantly higher anticancer activity than did the cationic nanoparticle alone or luciferase-specific siRNA complexed to the cationic nanoparticles. In vivo study revealed the enhanced antitumor effects by delivery of siRNA using the cationic anticancer drug-derived nanoparticles. Compared to the untreated control group, the cationic nanoparticle-treated group exhibited signficantly reduced tumor growth. The highest tumor growth inhibition in nude mice was observed in the group treated with siMcl delivered with the cationic nanoparticles. These results suggest the potential of

dual function cationic nanoparticles which can deliver therapeutic siRNAs while exerting anticancer activity per se. The combined treatment of anticancer siRNAs with anticancer cationic nanoparticles may potentiate the efficacy of cancer therapy.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 민달희

Combinatorial method to screen RNA-cleaving oligodeoxyribozyme and inhibitory RNA aptamer for therapeutic application

김동은, 박꽃한아름

건국대 생명공학과

Nucleic acids provide an enormous potential as a therapeutic reagent against viral diseases and cancers. Especially, RNA-cleaving oligodeoxyribozyme and RNA aptamer against pathogenic proteins are promising tools as therapeutic nucleic acids. A class of antisense oligodeoxyribozymes, known as the 10-23 DNAzyme, has been shown to efficiently cleave target RNA at purine-pyrimidine junctions in vitro. A screening strategy was performed to identify accessible cleavage sites for DNAzyme in the target RNA, Hepatitis C virus nonstructural gene 3 (HCV NS3) that encodes viral helicase and protease, starting from a pool of random DNAzyme library. The screened DNAzymes, when transfected to the human hepatoma cells harboring the HCV subgenomic replicon RNA, efficiently inhibited HCV RNA replication in cells by reducing expression of HCV NS3 RNA and protein. Thus, the selected oligonucleotides as well as the selection strategy can be applicable for a new class of anti-HCV drugs as antisense oligonucleotides-based therapy. The same approach with the DNAzyme screening has been executed to inhibit beta-catenin expression in the colon cancer cells. The selected DNAzymes have shown effective degradation of beta-catenin RNA and subsequent expression of the gene in colon cancer cells. Another example of oligonucleotide-based molecular therapy is RNA aptamers that specifically bind and inhibit the activity of certain pathogenic protein. RNA aptamers have been isolated against SARS coronavirus (SCV) NTPase/Helicase from RNA library containing random sequences of 40 nt using in vitro selection technique (SELEX). The isolated RNAs were observed to efficiently inhibit double-stranded DNA unwinding activity of the helicase. These results suggest that the pool of selected aptamers might be potentially useful as anti-SCV reagents.

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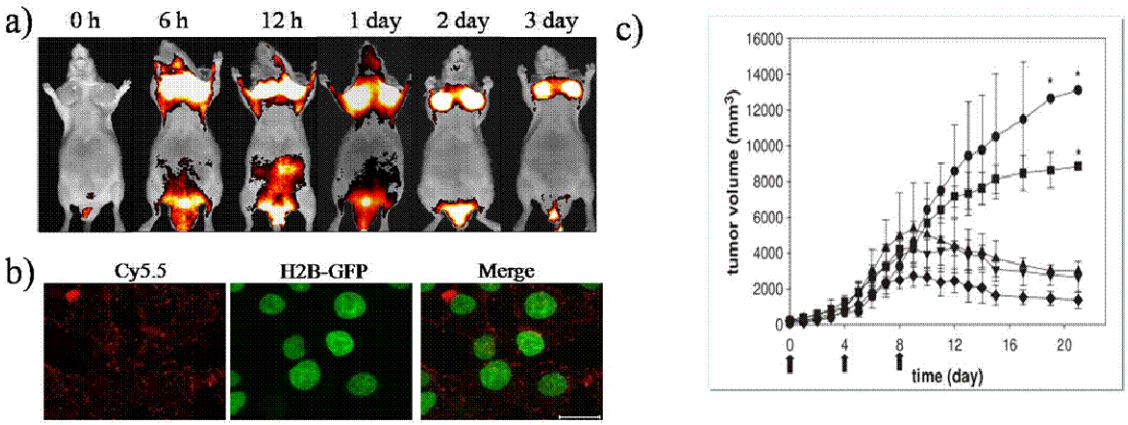
발표분야: Nanomaterials and Nucleic Acids for Molecular Therapy
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 김동은

Tumor Homing Nanoparticles for Cancer Imaging and Therapy

김광명

KIST 의과학연구센터

This presentation proposes a new polymeric nanoparticle-based technology that offers unprecedented paradigm shift opportunity to cancer theragnosis (therapy and diagnosis). Interdisciplinary research in the interface of polymer chemistry and the biomedical sciences has produced various nano-sized drug carriers and imaging probes for both therapy and diagnosis. With the help of polymer chemistry, we propose novel polymeric nanoparticles for the development of smart probes and new drug carriers for the treatment and imaging various cancers. For example, chitosan-based nanoparticles were labeled or loaded of various imaging agents and therapeutic drugs which demonstrated specific cancer imaging and therapy. Nanoparticles based cancer theragnosis holds great promise for a myriad of cancer treatment. Fig. (a) Time-dependent biodistribution of Cy5.5 labeled HGC nanoparticles in tumor-bearing mice. (b) Fluorescence images of Cy5.5 labeled HGC nanoparticles treated cells showing cellular uptake. (c) in vivo anti-tumor activity of PTX loaded HGC nanoparticles. The symbols are as follows: saline (●), HGC (■), cremophore EL-based PTX (▲), PTX-HGC 20 mg/kg (▼), and PTX-HGC 50 mg/kg (◆).



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장소: 대전컨벤션센터
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발표분야: Nanomaterials and Nucleic Acids for Molecular Therapy
발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 김동은

Novel Nanoplatforms for Targeted Imaging of and Drug Delivery to the Cancer

허용민

연세대 의료원

Key challenge of medical applications of nanomaterials lies in how unique nanoproperties of nanoplatform such as ultrasensitivity and multifunctionality can be translated into medical area by integrating various biological contents. In this seminar I want to describe our group contribution to this great scientific movement of integrating nanotechnology and medical technology. Specifically, the convergence of ultrasensitivity (as contrast agent) and targeting contents has led to target-specific detection of early stage cancer. Furthermore, when target specific smart contrast agent was combined with various therapeutic contents, target specific delivery of therapeutic contents and monitoring their efficacy could be realized.

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발표분야: Nanomaterials and Nucleic Acids for Molecular Therapy
발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: 김동은

Ultrasensitive tracking of oxidized guanine incorporation into DNA and RNA via nucleotide salvage with accelerator mass spectrometry

하상수

경희대 화학과

Growing evidence suggests that oxidative damage to cells generates mutagenic 7,8-dihydro-8-oxo-2'-deoxyguanosine (8-oxodG), which initiates diseases related to aging and carcinogenesis. Insufficient detection sensitivity, however, has hampered measurement of these putative mutagenic products in cells or animals. I report use of a sensitive and precise accelerator mass spectrometry (AMS) assay to track the fate of [14C]8-oxodG incorporation into DNA and RNA of MCF-7 human breast cancer cells. MCF-7 cells were grown in the presence of [14C]8-oxodG and radiocarbon was found to be partitioned into both DNA and RNA, indicating that 8-oxoguanine was detached from the deoxyribose ring and attached covalently to a ribosyl species to form an appropriate nucleotide for incorporation into RNA. I also observed evidence for phosphorylated 8-oxodG derivatives and 8-oxoG derivatives in the nucleotide pool. Moreover, oxidative stressing of the cells by exposure to 17ß-estradiol reduced the rate of 8-oxodG incorporation, indicating induction of a mechanism to limit the triphosphate derivative of 8-oxodG required for incorporation by DNA polymerases. These data suggest that 8-oxodG in the nucleotide pool is an unexpected source of 8-oxoguanine forDNA and RNA incorporation, which may have important consequences for understanding diseases resulting from mutagenesis and altered protein function.

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발표분야: New Development in Organic Chemistry (Reaction, Methodology, and Synthesis)
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김건철

Organic Syntheses and Properties of Novel Conjugated Polymers for AMOLEDs

Youngeup Jin, Suhee Song, *Sun Hee Kim, **Sung Heum Park, *Kwanghee Lee, **Alan J. Heeger, Honsguk Suh

Dept. of Chemistry & Chemistry Institute for Functional Materials, Pusan National University
**Department of Material Science and Engineering, Gwangju Institute of Science and Technology*
***Center for Polymers and Organic Solids, University of California at Santa Barbara*

Conjugated polymers with a stabilized blue emission are of importance for the realization of large flat panel AMOLED displays using polymer light-emitting diodes. Several novel conjugated polymers using newly developed templates for the stabilized EL emission are reported. Poly(2,6-(4,4-bis(2-ethylhexyl)-4H-cyclopenta[*def*]phenanthrene)) (PCPP) is a new class of blue-emitting polymers utilizing a new back-bone. This material emits a efficient blue EL without exhibiting any unwanted peak in the long wavelength region (green region) even after prolonged annealing at an elevated temperature of 150°C in air, or operation of the device. In addition to this, poly(5,5,10,10-tetrakis(2-ethylhexyl)-5,10-dihydroindeno[2,1-*a*]indene-2,7-diyl) (PININE) was synthesized. In PININE, the vinylene group was cyclized using two 5-membered rings to prevent the oxidation of the vinylene group. PININE shows stable spectra of UV-vis, and PL, and EL even after harsh irradiation with white light in air, or after operation of the device.

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발표분야: New Development in Organic Chemistry (Reaction, Methodology, and Synthesis)
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 구상호

고 윤능민 선생님을 추모하면서

(In Memory of the Decedent Professor Nung Min Yoon)

차진순

영남대 화학과

고 윤능민 선생님의 서거를 추모하기 위해, 고인의 학술활동(학력, 경력, 연구업적 등) 및 사회활동을 정리함으로써 기초과학에 기여한 공로를 되새겨 보며, 아울러 생전의 모습을 조명해 봄으로써 후학으로서의 학문자세를 가다듬고자 하는 내용을 담고 있음.

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발표분야: New Development in Organic Chemistry (Reaction, Methodology, and Synthesis)
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 구상호

Cross-Coupling Reactions of Organoboron Compounds

Akira Suzuki

Professor Emeritus, Hokkaido University, Sapporo, Japan

The palladium-catalyzed cross-coupling reaction between different types of organoboron compounds and various organic electrophiles including halides or triflates in the presence of base provides a powerful and general methodology for the formation of carbon-carbon bonds. The (sp2)C-B compounds (such as aryl- and 1-alkenylboron derivatives) and (sp3)C-B compounds (alkylboron compounds) readily cross-couple with organic electrophiles to give coupled products selectively in high yields. Recently, the (sp)C-B compounds (1-alkynylboron derivatives) have been also observed to react with organic electrophiles to produce expected cross-coupled products.

Such coupling reactions offer several advantages: (1) ready availability of reactants; (2) mild reaction conditions: (3) water stability; (4) easy use of the reaction both in aqueous and heterogeneous conditions; (5) toleration of a broad range of functional groups; (6) high regio- and stereoselectivity of the reaction; (7) insignificant effect of steric hindrance; (8) use of a small amount of catalysts; (9) application in one-pot synthesis; (10) nontoxic reaction; and (11) easy separation of inorganic boron compound.

These coupling reactions have been actively utilized not only in academic fields but also in industrial processes.

In this lecture, the overview of the coupling reaction will be discussed to understand the outlines.

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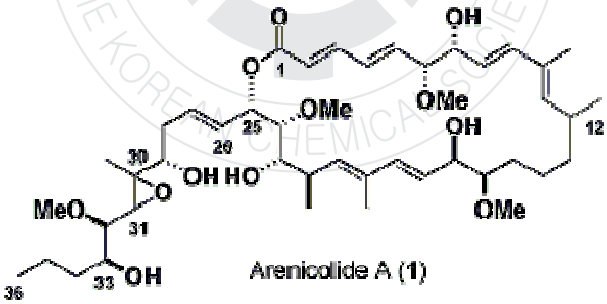
발표분야: New Development in Organic Chemistry (Reaction, Methodology, and Synthesis)
발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 이원구

Synthesis of C20-C26 and C27-C36 Fragments of Arenicolide A

이덕형

서강대 화학과

Arenicolides A was isolated from the large-scale fermentation of the S. arenicola strain CNR-005 in 2007 and the relative stereochemical relationships except C-12, C-30, and C-31 chiral centers were proposed by 1H NMR, 13C NMR, Mass, IR, UV, CD, and chemical degradation methods. Arenicolides A is 26-membered macrolide with three conjugated dienes and nine chiral centers in the ring. There is one side chain which comprises the C27-C36 carbon chain with five consecutive chiral centers.



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장소: 대전컨벤션센터
발표코드: **목16J4심**
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발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 이원구

Diversity of Boron Hydride Reduction

조병태

한림대 화학과

Sodium borohydride and borane are well-known and very important selective reducing agents for organic synthesis. Many applications with these reagents have been published. Recently we reported solvent-free reduction and reductive amination of aldehdyes and ketones using solid acid-activated sodium borohydride. On the other hand, a large number of boron hydride-based catalytic and non-catalytic asymmetric reduction have been extensively studied over the past three decades. Among them, oxazaborolidine-catalyzed borane reduction provides an impetus for asymmetric reduction. This method proves to be very effective and convenient for the catalytic asymmetric reduction of a variety of ketones including most of aryl alkyl ketones and various aromatic functionalized ketones, giving high enantioselectivity with predictable configurations. In recent years, significant advances for developing a wide range of new chiral catalysts and improvement studies toward enhancing the enantioselectivity and practicability of boron hydride-based catalytic asymmetric reduction of ketones and ketimines have been accomplished. In this symposium, recent advances for such reductions will be presented.

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발표분야: New Development in Organic Chemistry (Reaction, Methodology, and Synthesis)
발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 이원구

Synergistic effect in nucleophilic substitution reactions

지대윤

서강대 화학과

Our continuing interest in the development of fluorination led us to use various ionic liquids (ILs) as both reaction media and phase transfer catalysts, and we found that nucleophilic fluorination is accelerated in ILs. We also reported that tert-alcohol solvents show good performance in nucleophilic fluorination, thereby allowing side reactions to be remarkably suppressed via a weak F-H hydrogen bond, which maintains the inherent nucleophilicity and reduces the basicity of the fluoride anion. The synergistic effect in nucleophilic fluorination was found when we combined two solvents - IL and tert-alcohol – into one molecule. Consequently, these functionalized ILs not only increase the nucleophilic reactivities of the fluoride anion but also remarkably reduce the olefin by-product. Encouraged by a synergistic effect on nucleophilic fluorination, an imidazolium mesylate salt possessing two different solvent properties in one molecule was utilized in various nucleophilic substitution reactions. By a comparison study with 1-n-butyl-3-methylimidazolium ionic liquids, this functionalized IL has proved to be better phase transfer catalyst even under room temperature conditions. It was successfully applied to other nucleophilic substitution reactions such as fluorination, chlorination, bromination, iodination, acetoxylation, azidation, and cyanation.

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장소: 대전컨벤션센터

발표코드: **금17J1심**

발표분야: New Development in Organic Chemistry (Function, Recognition, and Device)

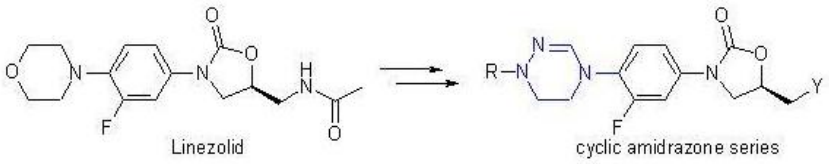
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 안세창

Discovery of LCB01-0371: New Oxazolidinone Antibiotics with Cyclic Amidrazone Function

박태교

레코켐바이오사이언스 신약연구소

수 많은 항생제의 발견에도 불구하고, 내성균주의 창궐로 인해 새로운 항생제에 대한 연구-개발 노력은 중단되지 않고 있다. 리네졸리드(Linezolid)로 대표되는 옥사졸리디논 계열 항생제는 다제약제내성(multi-drug resistance)균을 포함하는 그람양성균에 우수한 효능을 보여왔다. 이에 레고켐은 옥사졸리디논을 포함하는 신규 약물을 연구-개발하기로 하고, 다양한 구조변경을 시도하였다. 이와 같은 시도에는 리바록사반(Rivaroxaban)이라는 Factor Xa 저해제 또한 옥사졸리디논 기본골격을 공유하고 있어서, 새로운 아이디어가 있으면 두 가지 프로젝트에 공히 접목해 볼 수 있다는 현실적인 이유도 작용하였다. 연구과정에서 발견한 cyclic amidrazone 그룹은 약효(in vitro & in vivo) 뿐만 아니라, 약물유사성(druglikeness) 관점에서도 약물로서 갖추어야 할 훌륭한 성질을 고루 갖추고 있음이 밝혀 졌다. 이번 심포지움에서는 cyclic amidrazone function 을 가진 옥사졸리디논 계열 항생제 개발후보물질인 LCB01-0371 의 발굴과정과, 이물질이 가지고 있는 여러가지 특성을 발표하게 될 예정이다.



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Structure-Based Drug Design of Protein Kinase Inhibitors

김경희

LG생명과학 의약연구소

Protein Kinase 는 단백질의 Tyr, Thr, Ser 에 phosphate group 을 붙여주는 enzyme 이다. human 은 516 종 이상의 protein kinase 를 가지고 있고, 이를 총칭하여 kinome 이라고 부른다. protein kinase 는 metabolism, gene expression, cell growth, cell motility, cell division 등 다양한 cellular function 에 중요한 역할을 하고 있다. Protein kinase 의 over-expression, mutation, activation 등이 cancer, diabetes, hypertension 과 같은 질환과 연관성이 있다는 것이 알려져 있다. 이로인해 protein kinase 는 druggable genome 의 20~25%를 차지하고 있고, 제약회사의 drug discovery program 의 20~30%가 protein kinase inhibitor 연구에 투입되고 있다. 현재 8 종의 protein kinase inhibitor 들이 FDA 승인을 받아 항암제로 이용되고 있고, 140 여종 이상의 화합물들이 임상실험 중이다. Protein kinase inhibitor 들은 binding 구조에 따라, type I 과 type II inhibitor 로 구분된다. 다양한 protein kinase 와 inhibitor 의 complex 구조들을 분석하고, 이 자료들을 새로운 inhibitor design 에 적용하는 방법에 대해 소개하고자 한다.

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Air Stable Novel OTFT Materials

권순기

경상대 나노신소재공학부

Organic thin film transistors (OTFTs) have attracted much attention as alternatives with low-cost and simple fabrication methods to conventional silicon-based one. A number of p-type organic transistors have been reported so far, OTFT fabricated from a few materials show a comparable mobility to amorphous silicon. The most well-known OTFT materials is pentacene which has a mobility and on/off ratio of about 1 cm^2/V.sec and 10^7, respectively.In this presentation, we report the syntheses and characterization of new vacuum deposition and solution process p-type OTFT materials. OTFT devices of alkoxynaphthalene end-capped OTFT material show a charge carrier mobility of 0.64 cm^2/Vs and on/off ratio of above 10^5 by vacuum deposition.OTFT devices of phenylacetylene containing anthracene derivative show a charge carrier mobility of 0.4 cm^2/Vs and on/off ratio of above 10^4 by vacuum deposition.OTFT devices of 9,10-bis(trialkylpropylsilylethynyl)anthracene derivatives show a charge carrier mobility of 0.1 cm^2/Vs and on/off ratio of above 10^7 and some morphology will be discussed.OTFT devices of polymeric organic semiconductors containing naphthalene show a charge carrier mobility of 1.7 x 10^{-2} cm^2/Vs, on/off ratio of 4.8 x 10^4.OTFT devices of polymeric material with high aromatic density ahow a charge carrier mobility of 0.12 cm^2/Vs, on/off ratio of about 10^5.OTFT devices of polymeric amorphous OTFT material show a charge carrier mobility of 2 x 10^{-2} cm^2/Vs, on/off ratio of about 10^6.

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차세대 Display OLED의 핵심 소재 개발

이재철

LG화학기술 연구원 정보 전자 소재 연구소

OLED (Organic Light Emitting Diode)는 유기 재료에 전류를 가하여 전기 에너지를 빛으로 바꾸어주는 소자로서 자체 발광, 고속 응답속도, 광시야각, 경량, 초박형, 고화질, 내구성, 내구성, 넓은 구동 온도 범위 등 디스플레이로서 필요한 모든 요소를 갖추고 있어 이상적인 차세대 Display 로 주목 받고 있다. OLED 에 대한 연구는 1960 년대 초에 시작되었으며, 1987 년 Eastman Kodak 에 의해 고효율 다층 박막 형태의 구조가 개발되면서 본격적인 연구 개발이 시작되었으며, 발표 당시 소자 효율은 1.5 ln/W, 소자의 수명은 200 시간 정도였으나 현재는 녹색 소자의 경우 110 ln/W, 소자의 수명은 30,000 시간 이상이 발표되고 있어 단시간에 빠른 속도로 개발이 진행되어 왔다. AM 방식의 OLED 는 20”급 및 40”급의 시제품이 발표되었고 2 ~3” 급의 소형 제품은 2007 년 말에 양산을 시작하여 현재는 본격 양산을 진행하고 있으며 주요 평판 디스플레이 산업으로 자리잡고 있다. OLED 디스플레이 산업은 타 디스플레이에 비해 핵심 소재 및 장비의 의존성이 매우 큰 산업이며, 그중에서 OLED 핵심 소재는 OLED 디스플레이의 소비 전력, 효율, 수명 등을 결정하여 제품의 경쟁력을 부여하는 아주 중요한 품목으로 LCD 등의 타 디스플레이 품목에 비해 소재의 중요성이 더욱 강조되고 있다. 이번 세미나에서는 OLED 의 개념 및 작동 원리, 타 디스플레이와의 특성 비교, OLED 소재가 갖추어야 할 특성과 소재 개발 및 기술 동향을 소개할 예정이다.

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Dye-Sensitized Solar Cell: Light Management for High Light Harvesting Efficiency

박남규

성균관대 화학공학부

Dye-sensitized solar cell (DSSC) utilizing nanotechnology and photosynthesis attracts much attention due to its high solar-to-electricity conversion efficiency, low cost and colorful appearance. Basic components in DSSC are the nanocrystalline TiO_2 film, the dye and the redox electrolyte, where charge is generated by dye and TiO_2 film acts as both charge separation and electron transport. In DSSC, high conversion efficiency depends on photocurrent density, photovoltage and fill factor. Photocurrent density is related to external quantum efficiency that is the collective measure of three key efficiencies of light harvesting, charge separation and charge collection. Although three efficiencies are equally important, light harvesting efficiency is crucial. In this talk, technologies based on nano-engineering will be introduced to have high light harvesting efficiency in DSSC

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항생제 내성 현황과 대책

김양수

울산의대 서울아산병원 감염내과

전세계적으로 항생제 내성이 심각한 문제로 대두되었다. 최근 그람양성균 치료의 최후 보루인 vancomycin 에 내성을 보이는 황색 포도구균 (VRSA, vancomycin-resistant Staphylococcus aureus)과 장구균 (VRE, vancomycin-resistant enterococci)이 출현하였고, 그람음성균 치료의 최후 보루인 carbapenem (imipenem, meropenem 등)에 내성인 녹농균 (Pseudomonas aeruginosa)과 아시네토박터균 (Acinetobacter baumanii) 등 그람음성균이 자주 분리되고 있어 큰 충격을 던지고 있다. "기적의 약물"인 항생제가 스스로 만들어낸 기적을 파괴하고 있는 "파라독스"가 벌어지고 있는 것이다. 최후의 보루인 vancomycin 이나 carbapenem 이외의 항생제 내성도 매우 심각한 상태이다. MRSA (methicillin-resistant Staphylococcus aureus), 3 세대 cephalosporin 에 듣지 않는 E. coli 와 K. pneumoniae, fluoroquinolone 내성 그람음성균, 다제내성 폐구균, 다제내성 살모넬라균, 다제내성 결핵균 등도 심각한 내성을 보이는 균들로서 인류에게 커다란 위협을 가하고 있다. 장기이식, 항암치료, 여러가지 침습적 모니터링 기구들의 사용 등 현대의학은 대체로 면역저하와 그에 동반된 감염증을 필연적으로 수반하기 마련이며, 항생제 사용에 따른 감염증의 조절에 의지하여 발달된 측면이 강하다. 항생제 내성이 심각한 현재의 상황에서는 현대의학의 기반 자체가 흔들릴 수도 있다. 사실 5 억년 세균의 역사에서, 세균에게 항생제 만큼이나 위협적인 존재는 없었다. 세균의 입장에서 보면 항생제 내성은 살아남기 위한 당연한 몸부림으로 보아야 할 것이며, 따라서 항생제를 사용하는 한 항생제 내성은 지속될 것이다. 항생제를 사용했기 때문에 나타나기 시작한 항생제 내성은, 지금까지는, 인류가 이를 극복할 수 있는 더욱 좋은 항생제를 개발함으로써 해결해 왔다. 그러나 인류의 항생제 개발에 맞서, 세균은 나름대로 유전학적 진화를 거듭하였고 급기야 최근에는 새로운 항생제를 개발하는 인류의 능력을 앞지르게 되었다. 그 결과 항생제 내성은 핵폭발 직전의 심각한 상황에

이르게 된 반면, 인류는 새로운 항생제 개발 라인에 아무 것도 보유하고 있지 못하는 지경에 이르렀다. 이러한 당면한 과제를 해결하기 위해서는 항생제가 사회적인 약물이라는 인식하게 항생제를 적절하게 상용해야 한다. 항생제 내성을 억제하기 위한 노력은 정부와 의약계 종사자 뿐 아니라 화학회, 수의학계, 미생물학계, 소비자단체, 교육계 언론계 등 사회의 여러 분야에서 일하는 분들이 함께 노력해야 할 문제이다. 항생제를 잘 쓰기 위해서는 1) 항생제가 어디에 얼마나 사용되고 있는지에 대한 파악 2) 공공부문 (보건복지부, 농림부, 해양수산부, 행정자치부 등), 사적부문 (병원, 소비자단체, 학술단체, 언론기관 등) 사회 각 분야에서의 항생제를 잘 쓰기 위한 공동의 노력 3) 환자, 일반인, 의료인에 대한 교육과 홍보 4) 새로운 항생제 개발을 위한 투자 등 종합적인 대책이 필요하다.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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Recent Trends in the Development of New Antibiotics against Superbugs

곽진환

한동대 생명과학부

Recently, the use of antibiotics has been hampered by the continuous emergence of resistant bacteria. Therefore, the constant development of new antibiotics is necessary to overcome the emerging resistance. The new families of antibiotics were discovered traditionally by random screening of natural products and chemical libraries. For the last 3 decades most research has been dedicated to the improvement of existing classes of molecules rather than on the development new families of antibacterial agents. However, the recent aim of the pharmaceutical industries is obviously to be one step ahead rather than behind bacteria in this continuous race by developing new antibiotics acting on new targets against which no specific resistance preexists. Choosing new targets for which no natural product inhibitors are known markedly decrease the emergence of specific resistance mechanisms. Rationally selected bacterial targets should lead to more powerful new agents with well defined behavior. New technologies such as bacterial genomics are becoming available for more efficient target selection. Some pharmaceutical companies seek to identify bacterial genomes that are essential to bacterial viability in vitro or to bacterial growth and virulence in vivo. Inhibition of virulence factors rather than bacterial death could provide an alternative and more ecological therapy. In this presentation, new targets for new antibiotics, which are under development by several pharmaceutical venture capitals, will be discussed

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새로운 옥사졸리디논 항생제의 개발

김용주

(주)레고켐바이오사이언스 신약연구소

기존 항생제에 내성을 가진 슈퍼박테리아(MRSA)의 출현은 인류의 건강을 위협하는 심각한 사회문제이며 이를 치료할 수 있는 슈퍼항생제의 개발이 시급히 요구되고 있다. 그러나 현재까지 이의 치료에 가장 효과적인 항생제는 Pfizer 에서 개발한 Linezolid (상품명 Zybox) 밖에 없으며, Linezolid 의 부작용과 내성균에 좀 더 효과적인 2 세대 옥사졸리디논 항생제의 개발이 절실히 요구되고 있다. 최근 개발중인 옥사졸리디논 계열의 항생제와 레고켐 바이오사이언스에서 개발중인 항생제 LCB01-0371 의 profile 과 이의 유사 화합물들의 Structure Activity Relationship 을 소개한다.

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Development of novel types of small molecule inhibitors against HIV

유지창

가톨릭대 성의교정 병리학교실

The Human Immunodeficiency virus(HIV), a causative agent of AIDS(Acquired Immune Deficiency Syndrome), is a lentivirus containing about a 10Kb RNA genome. The viral genomic RNA packaging, or alternatively known as encapsidation, into viral particles from its host cells is a formidable task for the sake of viruses. It is especially important for RNA viruses as they have to discriminate the viral RNA from a pool of numerous cellular RNAs.The components involved in the packaging of the HIV viral genomic RNA during virion assembly is believed to be mediated by a specific interaction between the Nucleocapsid(NC) in the gag polyprotein and a packaging sequence, so-called psi(ψ), located near the 5'-end of LTR(long terminal repeat) region of the viral genome. In addition to having this essential role, the NC protein has been known to be involved in many other important steps in the viral life cycle such as the viral reverse transcription, translocation of PIC (pre-integration complex) into host nucleus, integration, and gene expression stages.Moreover, as being "mutation non-permissive" in its nature, the NC protein has been emerged as a highly promising target for the development of new types of anti-HIV inhibitor.Yet, the identification and development of such molecules has been hampered in part due to a lack of a functional assay for the NC protein.By exploiting a novel functional cell-based assay that probes the specific protein-RNA interaction between the NC protein and psi(ψ) RNA, we are able to not only to decipher and dissect the specific interaction of the HIV NC-psi(ψ) RNA in vivo, but also to identify for the first time a novel types of anti-HIV small molecules targeting the NC and NC-Psi interaction. The significance of the results and usefulness of our system for developing other antiviral agents will be presented

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비핵산계열의 역전사 효소 저해제(NNRTI) 연구

손종찬

한국화학연구원 신물질연구단

FDA 의 승인을 얻은 에이즈 치료제는 현재까지 23 가지에 이른다. 이들은 모두 HIV 의 life cycle 의 한 부분을 단절시키는 화합물들로서, entry 저해제가 2 종(Enfuvirtide, Maraviroc), 핵산계열의 역전사효소 저해제가 8 종(Zidovudine, Didanosine, Zalcitabine, Stavudine, Lamivudine, Abacavir, Tenofovir, Emtricitabine), 비핵산계열의 역전사효소 저해제가 4 종(Nevirapine, Efavirenz, Delavirdine, Etravirine), protease 저해제가 8 종(Saquinavir, Ritonavir, Nelfinavir, Amprenavir, Lopinavir, Atazanavir, Tipranavir, Darunavir), integrase 저해제가 1 종(Isentress)이다. HIV 에 감염되었다 하여도 이러한 치료제들을 combination 으로 사용하면 수명연장에 큰 효과가 있는 것으로 알려져 있다. 그러나, HIV 는 이러한 화학요법제에 대항하여 끊임없이 내성을 발현하고 있고 기존 치료제들이 부작용이나 독성면에서 완벽하지는 못하기 때문에 더 좋은 치료제의 개발은 지속적으로 요구되고 있다. 이러한 노력의 일환으로, 한국화학연구원은 Gilead 사와 공동연구를 수행하여 비핵산계열의 역전사효소 저해제로서 전임상을 마친 에이즈 치료제 후보물질을 창출한 바 있다. 본 발표에서는 후보물질을 창출하기까지의 과정을 간략히 소개하고자 한다

일시: 2009년 10월 28~30일(수~금) 3일간

장소: 대전컨벤션센터

발표코드: **목18F6심**

발표분야: Current Struggles against Infectious Diseases

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 금교창

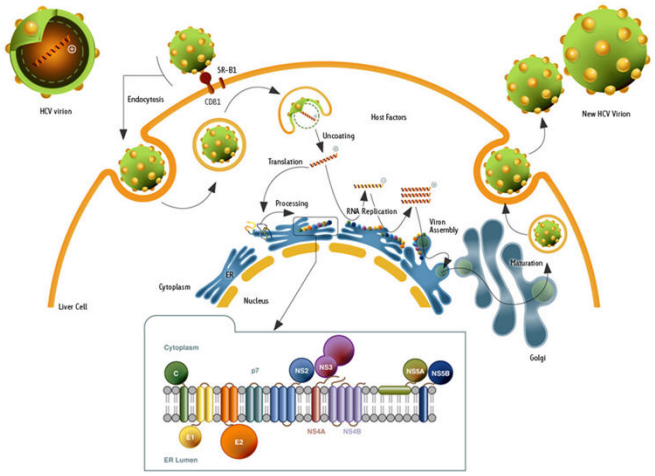
The face of future hepatitis C antiviral drug development

장승기

포항공과대 생명과학과

Chronic hepatitis C virus (HCV) infection is a worldwide health problem. More than 170 million people are estimated to be infected by HCV, and HCV infections results in hepatitis, liver cirrhosis, and hepatocellular carcinoma. Response rates to current standard of treatment (pegylated IFNs and ribavirin) are low in patients with the prevailing genotype 1. Therefore, development of new drugs for HCV infection is urgently needed. Potential therapeutic targets for new drugs, current status of anti-HCV drug development, and new approaches to develop new anti-HCV drugs will be discussed. Moreover, our efforts to find a cellular protein (GRP94) required for HCV proliferation and the effects of chemicals inhibiting GRP94 in HCV proliferation will be discussed. Moreover, the effects of aptamers against HCV E2 on viral infection will be presented.

Life Cycle of Hepatitis C Virus (HCV)



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발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 금교창

Substituted Flavone; A Novel Antiviral Scaffold

정유훈

건국대 생명공학과

With 170 million people infected worldwide and lack of the specific antiviral treatment option, hepatitis C virus (HCV) infection represents a major global health threat. In addition, because of the error-prone nature of HCV RNA replication, drug-resistance mutants will develop that is associated with reduction in the effectiveness of the antiviral drugs. Thus, current active pursuit of the specific antiviral agents against HCV has to be concerned about the possible drug resistance issue against the antiviral agent under development. In general, combination therapy for treatment of drug resistant virus combines three or more drugs from at least two different classes to suppress the viral replication in at least two different ways. Combination therapy, however, remains an expensive option and increases life-threatening toxicities. In this study, in order for more efficient and safe combat against the drug-resistant virus, we attempted to design a dual enzyme inhibitor which inhibits two key viral enzymes at the same time. In this context, we envisaged that a natural nucleic acid mimic flavone scaffold might competitively bind at the substrate binding sites of both HCV polymerase and helicase which use nucleic acids as the common substrate. Design, synthesis, and antiviral activity of novel flavone analogues against HCV polymerase as well as helicase will be presented.

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발표코드: **목19B1심**
발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이기라

Assembly of Nanoparticles for New Supra-structures and Memristic Switching Devices

천진우

연세대 화학과

나노입자를 이용한 어셈블리는 다양한 초격자 구조를 창조할 수 있다. 단일 나노입자를 이용한 1-3 차원 구조가 모두 가능하고, 두가지 다른 종류의 나노입자를 이용한 경우 binary supra structure 를 얻게 되며, 이러한 경우 나노 입자간의 화학반응을 통해서 기존의 특성을 획기적으로 증가시키는 물성을 얻을수 있다. 또한 3 차원구조의 구현을 통하여 새로운 전자소자를 구현할 수 있으며, 특별히 멤리스터 (Memory-Resistor 의 결합어)를 구현가능하였다. Ref: 1. Cheon et al. Proc. Natl. Acad. Sci. USA 2006, 103(9), pp3023-3027.

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발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이기라

Metal-free Elementary Semiconductor Nanowires: Synthesis, Assembly and Device Applications

황동목

성균관대 신소재공학부

Semiconductor nanowires are the focus of great scientific interest, due to their wide array of potential applications in various nanoscale devices. In particular, silicon nanowires are a natural choice for the building blocks of future functional nanoscale device applications because of their compatibility with existing silicon technology. So far, metal-catalyzed chemical vapor deposition methods have proven to be the most successful in producing silicon nanowires and their related heterostructures, as the structures and electrical properties can be tailored to various device applications. However, a metal-free approach for controlled nanowire growth is highly desired since unavoidable metal impurities in metal-catalyzed nanowires are detrimental to commercial device applications. Here, I will present (1) metal-free large-scale synthesis of single-crystal silicon and germanium nanowires with controlled dimension, morphology, and electrical properties and (2) approaches for controlled assembly of the wires on large area.

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발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이기라

Large-Area Block Copolymer Nanopatterning Integrated with Conventional Lithography

김상욱

KAIST 신소재공학과

고분자의 분자조립 현상을 이용한 나노패턴기술은 그 패턴 형태나 크기를 다양하게 조절할 수 있고, 패턴의 형성이 병렬적으로 진행되어 대면적 공정이 가능하다는 장점을 가지고 있어, 주로 직렬식 공정에 의존하고 있는 기존 나노패턴기술들의 단점들을 극복할 수 있는 중요한 기술로서 관심을 모으고 있다. 본 발표에서는 고분자의 분자조립현상을 365 nm i-Line lithography, 193 nm ArF lithography 그리고 마이크로임프린트공정등다양한 기존 리소그라피공정들과 융합하여 대면적에서 잘 정렬된 고분자 나노패턴을 형성시키는 공정들을 소개할 것이다.

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발표코드: **목19B4심**
발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 이기라

Self-Assembled Nanostructured Materials for Energy Conversion and Biosensing

이진우

포항공과대 화학공학과

Self-assembled nanostructured materials have attracted much attention owing to their application to catalyst supports, hosts for biomolcules, and sensors. The first synthesis of ordered mesoporous materials stimulated research on the self-assembly of block copolymers with inorganic materials. Herein, we present functional nanostructured materials synthesized by the self-assembly of block copolymers with inorganic materials. Highly crystalline mesoporous transition metal oxides were fabricated through 'one-pot' assembly method employing PI-b-PEO block copolymers. We developed intermetallic nanoparticle loaded highly ordered mesoporous carbon and transition metal oxides by the assembly of PI-b-PEO block copolymer. Formic acid oxidation with the resulting catalyst shows higher mass activity and lower onset potential compared with commercial Pt based catalyst. Highly crystalline mesoporous TiO2 was employed as self-cleaning sensors with higher sensitivity compared with commercial TiO2 pastes. Large cellular porous silica materials were synthesized by the self-assembly of commercially available block copolymers, P123. One-pot multi-catalyst system, so called "nanofactory", was developed entrapping magnetic nanoparticles and oxidases in large cellular mesoporous silica with high loadings of simultaneously above 40 wt% MNPs and 20 wt% enzymes. Our approach provided highly loaded MNP system and any highly loaded enzymes with superior activity, stability, and reusability, thereby making further applications as versatile sensors for detecting DNA, protein, and cell highly promising.

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발표코드: **목19B5심**
발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 이진우

Self-Assembled Polymeric Photonic Crystals : Synthesis, Fabrication, and Applications

이원목

세종대 화학과

Due to their potential as technologically useful materials such as sensor platforms, variable-wavelength lasers, and reflective color displays, tunable band gap photonic crystals have been intensively investigated. Optical characteristics of photonic crystals can be manipulated over a desired wavelength range by tailoring either one or a combination of their characteristic parameters: domain refractive index, domain periodicity, and domain orientation. Fabrication method of photonic crystal can be classified to top-down (eg. Lithography) and bottom-up (eg. Self-assembly) approach. Among a number of clever ideas to construct a large area, defect-free photonic crystal platform based on self-assembly techniques, colloidal crystals from spherical microspheres and microphase-separated block copolymers (BCPs) have attracted attention as a promising material platform for creating photonic crystals. In this presentation, syntheses of polymer microspheres by emulsion polymerization and million molar mass BCPs by anionic polymerization will be introduced, and some of interesting photonic crystal applications (eg. sensors, laser reflectors) using them will be discussed.

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발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 이진우

Ultraviolet nanoimprint lithography processes for optical device applications

정준호

한국기계연구원 나노융합기계연구본부

A new high-efficiency polymer based multi-layer photonic crystal organic light emitting diode (PoMPC)-OLED has fabricated using a low pressure and room temperature ultraviolet nanoimprint lithography (UV-NIL) process. The anode, organic layers and metallic layers are deposited directly onto the PC structures. The PC effect on the substrate, anode and organic layers and the Bragg diffraction on the patterned metal mirror results in a high efficiency even with a sub-100 nm pillar height. A patterned anode structure resulted in a decrease of the operating voltage. A PoMPC-OLED with a pillar height of 50 nm was fabricated showing a power efficiency 93% higher than a reference OLED without a PC structure. In a PoMPC-OLED, when the pillar height is below a certain value, deposition of the anode and the organic layers can be achieved without sharp edges which are the source of electrical leakage. In addition, as no additional planarization process is necessary before the deposition of the anode, it is much easier to control the particle contamination problem. Much better OLED performance can be obtained by optimizing the pillar height of the PC structure.A novel UV-NIL that employs photosensitive titanium (IV) di-n-butoxide bis(2-ethylhexanoate) is presented for the fabrication of well-ordered titanium dioxide (TiO2) nanostructures at room temperature. This approach allows direct fabrication of TiO2 nanopatterns with lines down to sub-50 nm in width and three-dimensional TiO2 hybrid micro/nano-patterns without observable defects for use in applications where ordered surface nanostructures are required, such as photovoltaics, photonics, and optical waveguides.

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발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 이진우

Self-organizing process in aluminum anodization and template-based nanofabrications

이우

Korea Research Institute of Standards and Science (KRISS)

During recent years, the anodization of aluminum, due to its great industrial importance, represents one of the most popular methods employed for the synthesis of ordered porous structures consisting of close-packed cells in a hexagonal arrangement with cylindrical nanopores at their centers. Over the past decades, this process has raised substantial scientific and technological interest due to its diverse applications that include formation of electrically insulating layer, anti-corrosion and wear resistance coating, and decorative coloration of surfaces by incorporation of pigments during the sealing of anodized materials. Recently, a self-organizing process that occurs during the anodization of aluminum in acidic electrolytes has attracted a vast amount of research attentions, coupled with the ever-increasing demand for the development of effective, inexpensive and technologically simple methods for the synthesis of low-dimensional nanostructures over a macroscopic area overcoming many of the drawbacks of conventional lithographic techniques.In this contribution, recent progress in the state-of-the-art fabrication of ordered nanoporous alumina will be discussed, including a newly developed pulse anodization, hard anodization, and generic approaches to three-dimensional pore structures with periodically modulated diameters. Nanoimprint lithography for long-range ordered pore arrays in wafer-scales will be presented. Stencil-based nanofabrications of vertically aligned semiconducting nanowires and extended arrays of ferroelectric nandots will be touched upon. Discussion will also cover electrochemical methods for the preparation of various functional nanostructures, which are potentially useful in advanced optoelectronic devices, biological assays, sensors, and catalysts.

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발표분야: Large-Scale Nanopatterns by Self-Assembly
발표종류: 심포지엄, 발표일시: 목 17:10, 좌장: 이진우

R2R Printing of Silver Oxide Pastes and Their Conversion to Silver Patterns

전상기, 이동욱, *황인석, **이기라

*LG화학기술연구원 정보전자소재연구소 *LG화학 기술연구원*
***한국기초과학지원연구원 물성과학연구부*

This is to report a continuous roll-to-roll printing of mesh patterns of silver oxide pastes on flexible polymer films and subsequent process for the patterned pastes to convert to silver patterns. The pastes consist of silver(I) oxide particles, silver salt of tertiary fatty acid, AgOCO-C(CH3)2-(CH2)n-CH3 and a-terpineol as the solvent. During the thermal process at 150˚C for 30 min., nano-sized silver particles were formed by the thermal reduction of silver oxide particles and the salt, followed by spontaneous condensation and further fusing, resulting in conductive silver films. The linear chain length n of silver salt, AgOCO-C(CH3)2-(CH2)n-CH3, in the pastes, affects the electrical conductivity of resulting silver films significantly. [1]The mild thermal treatment (10 min at 150˚C) followed by chemical treatment is effective for the enhancement of both electrical conductivity and blackness. Chemical treatment with acidic metal chloride solution were performed on printed silver patterns for 30 sec, which induced the dissolution of silver ion and re-crystallization forming larger silver crystalline particles. Sintered larger silver crystalline particles in those line patterns have shown much higher electrical conductivity. In case of ferric chloride (FeCl3), silver chloride layer (~300nm) was spontaneously formed on conductive silver surface, which is called blackened layer because they can reduce metallic reflection by silver patterns, which is critical for EMI shielding film in display devices. Ref. 1. Chun, S. et al., Chem. Mat. 2009, 21, 343-350

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발표코드: **금20B1심**
발표분야: Identifying the Material Characteristics for Medical Applications
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 허용민

나노입자 이용 복합(multiplex) 다중(multimodal) 생체 영상

이동수

서울대

영상용 나노입자 또는 신규재료는 결국 인체에 사용하려면 임상응용 가능성과 유효성을 검증하겠다는 전망아래 개발하는 것이 좋다. 인체응용은 생체적용 가능성을 평가할 전임상시험을 동반하는데, 나노입자로 전임상시험을 수행할 때 비침습적으로 추적할 방법이 필요하다. 분자영상방법으로 이런 전임상시험에 기여할 수 있고 이 때 다중(multimodal) 생체영상법을 이용한다. Cobalt ferrite 입자에 rhodamine 을 넣은 실리카를 덮고, 그 위에 luciferase 와 NOTA 링커 Ga-68 을 표지하여 생물발광(Bioluminescence), MRI, 양전자단층(PET)영상을 순차적으로 한 개체에 대하여 얻을 수 있었다(Chemistry; a European J, 2009). 실제 신재료 개발에 응용할 때는 형광과 양전자단층영상, 또는 MRI 와 생물발광, 형광을 조합하여 사용한다. 나노실리카와 Ga-68 을 표지한 것으로 감시(sentinel)림프절 영상을 얻은 예(Mol Imag Biol, 2009), 누드마우스에 이식한 세포지지체복합체에서 마우스 P19 세포를 retinoic acid 로 분화할 때 특정 microRNA 의 발현여부를 형광으로 감지하면서, 생물발광으로는 대조군과 같은 양의 세포가 그 자리에 있다는 것을 확인하고, MRI 로는 지지체 내의 세포위치까지 검색하며, 결국 떼어낸 조직의 형광을 확인하여 분화와 관련한 형광의 증강이 있다는 것을 보인 예가 있다(Hwang et al, submitted). 세포의 표면마커와 세포내 생물학적프로세스가 특정질환에 대표적인 단일 이상소견이 있는 경우 드물고, 적어도 몇 가지 배합하여야 특성을 찾을 수 있으므로 다중 탐지가 필요한 경우가 대부분이다. microRNA 의 생성과 작동을 보려면 두 가지 luciferase 를 리포터유전자로 사용하여 가능한데(J Nucl Med 2008, FEBS J 2009), 여러 종양표지자(c-Met, Her2, MAGE-A)나 여러 microRNA 를 동시에 탐지하려면 복합(multiplex)영상이 가능한 quantum dot 나 SERS (Surface-Enhanced Raman Scattering) dot 을 이용할 수 있다. 나노입자가 생체에 적합하고 독성이 없는지는 꼭 입증하여야 한다.

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장소: 대전컨벤션센터
발표코드: **금20B2심**
발표분야: Identifying the Material Characteristics for Medical Applications
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 허용민

Aptamer-Mediated Combined Cancer Imaging and Therapy

전상용

광주과학기술원 생명과학과

Aptamers are a novel class of ligands that are small, non-immunogenic, easily synthesized amd modified, and exhibit high specificity and affinity for their target antigen. Considering the many favorable characteristics of aptamers, which have resulted in their rapid progress into clinical practice, we began to exploit this class of molecules for targeted drug delivery. Recently we described the first proof-of-concept drug delivery vehicles utilizing aptamers for targeted delivery of drug encapsulated nanoparticles. In the first part of this seminar, I will discuss the fabrication of the aptamer-nanoparticle conjugate with rational design concepts and its efficacy as a targeted delivery vehicle to prostate cancer in vivo as well as in vitro. We have recently developed a novel strategy for generating an aptamer-drug conjugate by intercalating a drug between nucleic acid bases of the aptamer. Using doxorubicin as a model drug and the A10 PSMA aptamer as model aptamer, we have developed a stable aptamer-dox conjugate through physical interactions. The resulting physical conjugate demonstrated the following characteristics: 1) high discrimination between cancer cells expressing target antigen and cells lacking target antigen and 2) efficient delivery of anticancer drug to target cancer cells. This work will be discussed in the second part of this seminar.

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발표코드: **금20B3심**
발표분야: Identifying the Material Characteristics for Medical Applications
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 이광렬

다양한 나노구조 표면의 제작 및 이에 대한 세포반응 양태와 세포내 신호전달기전

이규백

고려대 보건과학대학 생체의공학과

암세포 또는 혈액세포를 제외한 일반적인 동물세포는 표면에 부착하여 자라야 하는 부착의존성을 가진다. 따라서 세포의 표면 부착 상태에 따라 세포가 증식, 분화, 사멸의 과정이 진행된다. 최근 나노기술이 발달하면서 세포가 부착하는 표면의 상태를 정밀하게 조절함으로써 세포의 거동을 제어하고자 하는 시도가 활발히 이루어지고 있으며, 다양한 연구를 통하여, 심지어 10 nm 미만 크기의 나노구조물도 세포가 인식할 수 있음이 밝혀졌다. 그러나 세포가 어떤 기전을 통하여 나노구조물을 인식하며 어떤 나노구조물이 세포의 특정 반응을 유발하는지에 대해서는 아직 명확히 밝혀지지 않았다. 본 발표에서는 양극산화알루미늄, 레이저 간섭 리소그래피 등을 이용하여 나노임프린트용 마스터 스탬프를 만들고 이를 이용하여 세포배양이 용이한 고분자 표면에 다양한 나노구조를 저비용으로 대량 제작하는 방법과 그 표면에 대한 골아세포, 줄기세포, 수지상 세포 등의 반응하는 양태 및 본 연구를 통하여 현재까지 밝혀진 세포내 신호전달 기전에 대하여 소개하고자 한다. 특히 양극산화알루미늄을 이용한 나노임프린트 방법은 저비용으로 나노구조물의 중심 간격이 65 nm ~ 500 nm 의 범위를 갖는 다양한 나노구조 표면을 제작할 수 있게 하며 또한 나노구조물의 크기가 순차적으로 다른 gradient 형태의 나노구조 표면도 가능하게 한다. 이러한 특성은 어떤 크기와 간격의 나노구조물이 세포반응을 유발하는 지에 대한 정보 스크리닝에 매우 유용하다. 나노구조물에 대한 반응 양태는 나노구조물의 크기 및 간격이 세포의 반응에 크게 영향을 미치는 것으로 관찰되었으며 동일한 나노구조물에 대해서도 세포의 종류가 다를 경우 반응이 다르게 나타났다. 나노구조물에 의하여 영향을 받는

세포내 신호 전달기전은 integrin related signaling pathway 와 밀접한 연관이 있었으며 특히 Rho family small GTPase 중 Cdc42 의 활성이 크게 변화하였다.

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발표분야: Identifying the Material Characteristics for Medical Applications
발표종류: 심포지엄, 발표일시: 금 10:50, 좌장: 이광렬

Nanomedical Technology in Personalized Cancer Medicine

허용민

연세대 의료원

In designing the personalized cancer therapies (PCT), target contents are most important in cataloguing patient subgroups and evaluating targeted anticancer drug efficacy as well as its resistance. In vitro measurement of target contents can be used in optimizing personalized cancer medicine. Furthermore, in vivo understanding of target molecules via molecular imaging with nanoprobe is crucial to assessment of indication for targeted drug and monitoring its efficacy in patients, which are the key factors in planning PCT. Thus it is very important to develop useful in vivo and in vitro diagnostic tools to detect multiple targets and/or signaling pathways of cancer for realization of effective PCT. In this seminar, I will describe our recent efforts in establishing the necessary in vivo and in vitro diagnostic tools for powerful PCT.

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At the Interface of Nanomaterials and Mammalian Cells

민달희

KAIST 화학과

Various nanomaterials are currently under development for applications in diverse research fields ranging from material science to medicine. Currently, some nanomaterials such as silver nanoparticle, titanium oxide and fullerene are routinely used as a part of industrial products or cosmetics. Many researchers expect that more and more nanomaterials will be actively used as ingredients of the goods used by the public in the future. Therefore, concerns on toxicity and biocompatibility of nanomaterials are growing. In this talk, I will describe cellular responses to certain nanomaterial, in specific, carbon based nanomaterials in this talk. Particularly, cytotoxicity, cell shape change, cell spreading, and focal adhesion change of mammalian cells will be discussed in response to nanomaterials of interest.

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발표분야: Electrochemical Microchip Devices
발표종류: 분과기념강연, 발표일시: 금 13:30, 좌장: 여운석

Electrochemical Detection of Metal Ions and Biomolecules

곽주현

KAIST 화학과

The amperometric detection methods of chemical species, especially metal ions and biomolecules, using various elelectrodes will be broadly discussed. First, for the amperometric detection of the heavy metal ions, the anodic stripping volammetric technique can be selected as a very sensitive tool. For example, this traditional electrochemical technique was implemented to make a miniaturized low-power wireless remote environmental monitoring system with the help of modern semiconductor technique. Secondly, the enzyme-amplified electrochemical detection method was recently developed for the sensitive detection of biomolecules such as DNA and protein. We will discuss how to generate the enzyme-amplified amperometric signal caused by the DNA hybridization reaction or antigen-antibody interaction. For the enhanced detection of biomolecules, we developed a method combining the old and new techniques, namely anodic stripping voltammetry and enzyme-amplified electrochemical detection method. In brief, the silver metal was deposited by the immobilized enzyme with specific interaction of biomolecules at the modified electrode. When the accumulated silver metal is stripped out with anodic potential scan, the anodic current signal allows us the ultrasenstitive detection of biomolecules.

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발표분야: Electrochemical Microchip Devices
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 박종만

Electrochemistry for Biochips and Biosensors

여운석

건국대 생명공학과

The surfaces with biological activities are currently widely used for biochip microarrays, lab-on-a-chip devices, and for basic researches in biology. The arising issue in this area is the surface-engineering at the molecular level for incorporating dynamic properties and maintaining biological activities of surfaces. In this talk, I will discuss several classes of dynamic interfaces which can manipulate the activities of immobilized ligands in real-time with electrochemical controls. Further, a new electrochemical method of microscale patterning for the development of microarray and cell chip will be discussed. The strategy relies on the electroactive moieties on the surfaces which reveal organic functional groups or undergo electrochemical reactions upon an electrochemical treatment. The electrochemically activated substrates are then subsequently used for cell adhesion, protein immobilization, or preparation of microarrays. Finally, an electrochemical analysis tool to detect hybridized oligonucleotides will be introduced. The hybridization of oligonucleotides on biochips induces electrochemical signals which are utilized for enzymatic assays and small molecule detections.

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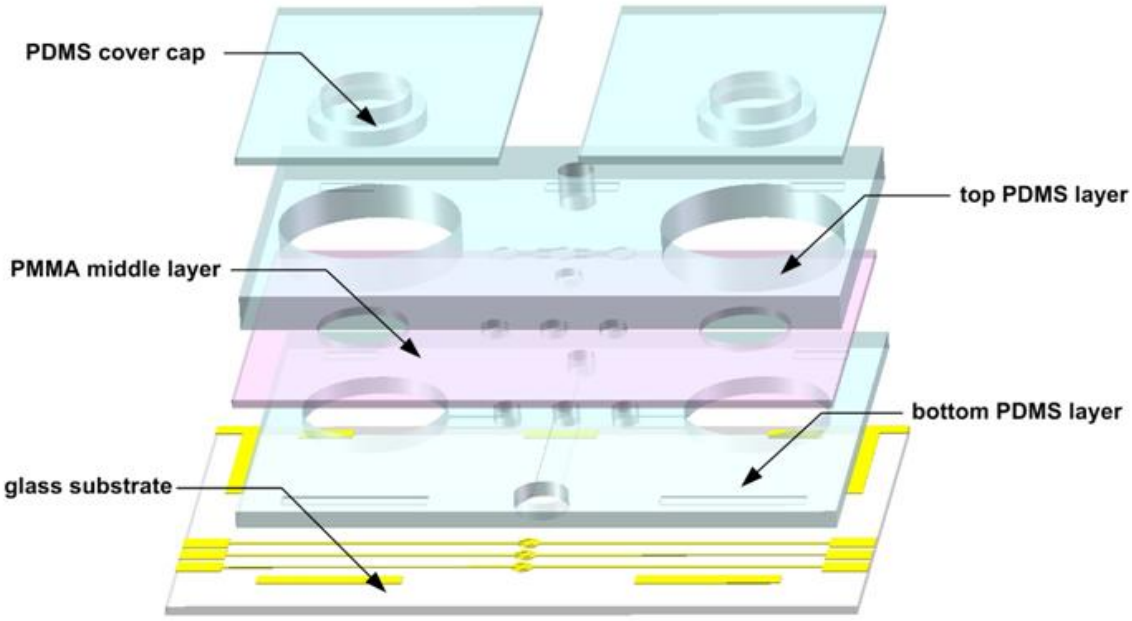
Bioelectrocatalytic Sensing of Protein Affinity Interactions on MEMS (microelectromechanical systems)

윤현철

아주대 분자과학기술

Our group has been addressing two important issues of affinity biosensors, including the construction of biofunctionalized surfaces for efficient affinity reactions and the development of signal registration strategies from protein affinity interactions that converts reactions into highly quantifiable electrochemical signals. The employed electrochemical signaling reactions are modified versions of enzyme-catalyzed immunoassays, adopted from histochemical fields. A comparative study was performed to evaluate the signal amplification strategies in electrochemical affinity sensing, including the direct electron transfer and diffusible-group mediated electron transfer between label enzymes that were specifically bound to target proteins and chemically modified electrode surfaces. For biosensing devices, a number of microscale systems (MEMS) combining microfabrication and microfluidic technologies were employed, including a PDMS multi-stacked hand-operated chip, a chip integrated with latch mechanism for hand-operation, a silicon chip containing temperature-controllable microelectrodes and a self-contained fluid maneuvering microfluidic chip. Design and fabrication of these devices, integration of biochemical parts with the MEMS, and bioanalytical applications will be covered.



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POCT용 혈액 자동분석기를 위한 평면형 소형 전기화학 센서

남학현, *신정원, *강태영, *하정한, *김현숙, *허혁, 차근식

*광운대 화학과 *(주)아이센스 부설연구소*

혈액내 생체시료 분석은 현대 의료진단에서 중요한 부분을 차지하고 있으며 따라서 보다 쉽고 정확하며 경제적으로 검출하기 위한 화학센서 개발에 관한 연구가 활발히 진행되고 있다. 최근 혈액센서의 연구개발은 측정시 환자 곁에서 극소량의 혈액을 채취하여 바로 검사결과를 볼 수 있으며 경제적인 측정 산출가를 가진 현장현시검사(point-of-care testing; POCT)용 검사장비를 개발하는 추세에 있다.본 연구에서는 혈액내에 여러 가지의 화학종을 동시에 자동으로 분석하기 위한 전기화학 센서(electrochemical sensor)들을 평면의 작은 플라스틱(polyethylene terephthalate; PET) 위에 스크린 프린팅 방법으로 제작하였다. 스크린 프린팅 방법은 제조시 항상 모든 전극이 균일하게 형성되므로 센서의 성능을 일정하게 유지시킬 수 있으며 대량생산이 용이하다는 장점을 가진다. 기본적으로 스크린 프린팅 방법으로 Ag 전극들을 형성하였고, 전위차법(potentiometry)의 작동전극은 분석하고자 하는 이온종에 따라 최적화된 내부겔과 외부막을 형성된 전극 위에 분주하고 건조함으로써 각각 이온센서를 구성하였다. 전류법(amperometry)의 작동전극과 보조전극은 백금흑(platinum black) 전극을 형성하여 사용하였다. 기준전극은 내부 기준용액과 시료가 일정하게 흐를 수 있는 흐름계(flow system)를 구성하여 액간 접촉전위(liquid junction potential)가 일정하게 유지되도록 하였다. 또한 혈액내의 적혈구 용적율(hematocrit)을 측정하기 위하여 2 개의 백금흑으로 전도도(conductivity) 측정 전극을 구성하였다.이와 같이 제작된 전기화학 센서는 혈액 자동분석기의 주요 소모품인 교정용액 및 폐기용기 등과 함께 한번에 쉽고 간편하게 교체되도록 카트리지화하였다. 또한 최신의 IT 기술과 Window XP Embedded OS(operating system)를 기반으로 사용자 친화적인 UI(user interface) 소프트웨어를 탑재하여 쉽게 조작할 수 있으며 신호 처리에서부터 자동 분석 시퀀스 구동에 이르기까지 정확한 분석이 가능하도록 개발된 소형 혈액 자동 분석장비를 제작하였다. 카트리지와 자동 분석장비로

구성된 POCT 용 혈액 분석기를 평가한 결과 2 주 이상의 우수한 감응성, 직선성 및 재현성을 유지하였으며, 특히 Na+, K+ 및 Cl- 분석의 경우 3 가지의 control level 에 대하여 모두 3.0%CV(n=60)이내의 정밀도를 나타냈다. 전혈(whool bood) 시료에 대한 비교평가는 기준장비로 널리 사용되는 Radiometer 사 ABL835 와 측정값을 비교하였으며 매우 높은 상관관계를 보여주었다.

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AFM Cantilevers Integrated with Ring Microelectrodes for Extending Applications of SECM

신흥주

울산과학기술대 기계신소재공학부

SECM(Scanning Electrochemical Microscope) is a powerful analytical tool providing surface topological data as well as the electrochemical information by collecting redox current through a microelectrode integrated at the end of a long glass tube. In spite of the variety of the applications, the functionality of the SECM as a spatial scanning tool is limited by the poor repositioning capability and difficulty of the manipulation. To overcome these limitations, combined SECM-AFM (scanning electrochemical microscope-atomic force microscope) was introduced capable of collecting spatially resolved electrochemical data with high resolution. This talk introduces the development and applications of batch processed multifunctional SECM-AFM cantilevers capable of collecting the information of surface electrochemical activity as well as surface morphology without effect of the surface morphology. Each cantilever tip is integrated with a ring microelectrode at a pre-determined position from the tip apex so that electrode-to-surface distance affecting the size of redox current is maintained constant during sample surface scanning resulting in geometry-effect-free electrochemical data collection while imaging surface topology of stationary sample as well as moving sample such as a live cells. The high yield and reproducible batch processed cantilevers satisfy the needs for low cost reproducible electrochemical scanning tools that is necessary for the research areas such as biology, chemistry, and corrosion study where meaningful data requires many of experiments and electrodes which become easily degraded. The applications of the combined SECM-AFM can be extended to sensing electrochemical/biological properties and surface modifications by using various type of materials as the electrode material or integrating bio/chemical acceptors onto the electrode surface.

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Creation of Lab-on-a-Chip Devices in Polymer Substrates Utilizing Electrochemistry at Micro-ITIES, Marangoni Effects and Pressure Pinched Injection Methods

이혜진, *Hubert H. Girault

*경북대 화학과 *Ecole Polytechnique Federale de Lausanne*

Miniaturization of analytical systems (lab-on-a-chip) into a single fully integrated device is important for the development of fast sensing platforms with the advantages of requiring very small amounts of samples, high precision, shortened analysis times and good reproducibility. During the last decade, intensive efforts have been devoted to the design of integrated microfluidic platforms for applications such as genetic and clinical analysis, trace-metal detection, portable instrumentation and industrial process control. In this talk we will first demonstrate the fabrication of micro-capillary electrophoresis integrating "Ionodes" detectors on a poly(ethylene terephthalate) (PET) substrate. An Ionode is an amperometric sensing platform that measures the current associated with the transfer of ions across a polarized micro-interface between two immiscible electrolyte solutions (micro-ITIES); in this case, the interface between an aqueous sample solution and a 2-nitrophenyloctylether-polyvinyl chloride (NPOE-PVC) gel phase. A simple electrokinetic injection and separation procedure by means of a floating high voltage (HV) source was developed to improve the electrical decoupling between the HV source and electrochemical detection currents. In addition, a novel electrochemical method for driving fluids in micro-channels will be presented whose underlying principle is the onset of Marangoni flow along the interface between an aqueous solution (mobile phase) and an organic electrolyte polymer gel coated on the inner walls of the microchannel. Another simple approach to drive fluids in a micro-channel network which utilize a pressure pinch method combining a multi-port injection valve and syringe pumps will also be discussed.

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발표분야: Electrochemical Microchip Devices
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Voltammetric and Microgravimetric Studies on the Interaction between Carbohydrates and Proteins using Carbobydrate-Modified Gold Nanoparticles

이원용

연세대 화학과

The Quartz Crystal Microbalance(QCM), as a simple and powerful technique, has been widely employed in chemical and biological sensing. It has been explored as alternatives to biosensors in order to study on the interactions between carbohydrates and proteins. In this work, self-assembled monolayer of thiol-modified carbohydrates have been prepared and used for the interaction studies as well as the quatitation of toxin compounds. A protein, concanavalian A(Con A), from Canavalia ensilformis, which binds specifically to mannoside and glucoside, was used as a model system to study the interactions between carbohydrates and proteins. The binding constants of the carbohydrates self-assembled on a gold of quartz-crystal and proteins has been determined by this approach. In order to amplify the QCM signal, carbohydrate-modified gold nanoparticles have been employed. Since the Con A has four binding sites, the carbohydrate-modified gold nanoparticles can be binded to the Con A, which is already binded to the carbohydrates self-assembled on the gold electrode of quartz crystal, thus increasing the QCM signal. Voltammetric methods along with gold nanoparticles also have been employed to study on the interactions between carbohydrates and proteins. In this work, stripping voltammetry of gold nanoparticles have been used to determine the concentration of Con A and cholera toxin.

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발표분야: Emerging Pollutants in the Environment
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 장윤석

잔류성유기오염물질의 전지구 모니터링 및 모델링 연구동향

최성득, *장윤석

*울산과학기술대 도시환경공학부 *포항공과대 환경공학부*

잔류성유기오염물질(POPs)은 다이옥신을 비롯한 다양한 유기오염물질로서 환경 중에 오래 지속되고 대기와 해양을 통해 장거리 이동을 거치므로, 국경이 없는 전 지구적 환경문제이다. 그러나 실시간으로 측정할 수 있는 고농도의 오염물질과는 달리, POPs 분석에는 비용과 시간이 많이 들기 때문에 전지구 규모에서 고해상도 분석결과를 얻기 힘들다. 대부분의 POPs 는 대기 중으로 배출되므로, POPs 의 전지구적 오염원과 이동을 파악하기 위해서는 대기 모니터링의 역할이 중요하다. 따라서 최근에는 기존의 능동대기채취기를 대체할 수 있는 수동대기채취기(PAS: passive air sampler)를 개발하고 있다. 특히, 캐나다 환경부와 토론토대학교에서는 Global Atmospheric Passive Sampling (GAPS) study 를 통해 전 세계에 PAS 를 설치하여 POPs 오염수준을 연구하고 있다. 본 연구진도 이 연구에 참여하고 있으며, 북극/남극과학기지와 국내 다수의 지점에서 관련연구를 수행하고 있다.그러나 이와 같은 노력에도 불구하고, 시료 개수의 한계로 인해, POPs 모니터링 결과에만 전적으로 의존할 수 없는 상황이다. 따라서 전지구 규모를 포함한 다양한 공간규모의 환경거동모델들이 개발되고 있다.본 발표에서는 최근의 전지구 POPs 모니터링 및 모델링 연구동향에 대해 소개하고, 앞으로 국내에서 동북아시아 중심의 연구를 활성화하는 방안을 모색하고자 한다.

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발표분야: Emerging Pollutants in the Environment
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 장윤석

Analysis & Management of Environmental Emerging Pollutants

송기봉, 신선경, 황승률, 강영렬, 구소현

국립환경과학원 환경건강위해성연구부 화학물질거동연구과

As of August 2007, more than 32 million substances were registered with the American Chemical Society's Chemical Abstract Service, with over 15 million of them being commercially available. Unfortunately, regulatory controls only exist for approximately 250,000 (1.6%) of these substances. Therefore, around 98% of the commercially available compounds are not inventoried and are essentially unregulated substances, some having a high degree of uncertainty associated with their environmental fate, transport, and toxicological effects. For convenience, Emerging pollutants are categorized as follows: global organic contaminants (POPs), pharmaceuticals and personal care products (PPCPs), endocrine disruptor compounds (EDCs), nanoparticles, industrial chemicals and biological metabolites and toxin. It should be recognized that these categories are not exclusive and that many compounds fit into multiple categories.This paper introduced the analytical methods and management status of the emerging pollutant such as new candidate POPs and PPCPs in environments.

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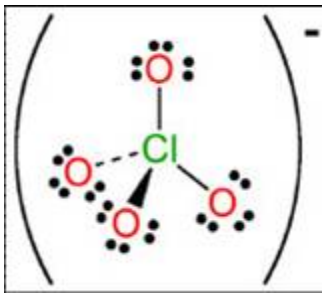
Overview of Environmental Perchlorate: A Current Understanding and Chemistry Issues

강남구

한국표준과학연구원 삶의질표준본부

Perchlorate anion is an emerging, widespread, environmentally persistent, inorganic pollutant. This chemical is naturally occurring and manmade anion in the acid or salt forms. In addition to its well-known use as an oxidizer in propellants and explosives, perchlorate has a wide variety of applications in areas ranging from electronics manufacturing to pharmaceuticals. As an endocrine disrupting compound, the perchlorate anion has a unique and profound ability to inhibit iodine uptake by the human thyroid, with potential adverse effects on the growth and development of fetuses, infants, and children. As its occurrence is virtually ubiquitous over the Earth and in the atmosphere, perchlorate contamination is of growing concern. Thus, its occurrence, fate, metabolism, transport and toxicity have been subjects of intensive study for more than a decade, but almost exclusively in the United States and very recently in Japan. This presentation will be the first-ever, brief introduction to provide the chemists and environmental scientists in Korea with the comprehensive and current understanding of environmental perchlorate. Key questions and debating issues especially concerning the origins and environmental fates of perchlorate will be addressed with a chemist's perspective.



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Monitoring and transport of estrogenic compounds in surface water

김상돈

광주과학기술원 환경공학과

The occurrence of estrogenic compounds in Yeongsan and Seomjin rivers in Korea was monitored during 2005-2008. Target compounds were 4-nonylphenol (NP), 4-tert octylphenol (OP), bisphenol A (BPA), estrone (E1), 17β-estradiol (E2), 17α-ethynylestradiol (EE2) and genistein (Gen). Water samples were pretreated and analyzed by liquid-liquid extraction (LLE) and gas chromatography/mass spectrometry (GC/MS), respectively. The effects of treatment processes on estrogenicity were evaluated by examining estradiol equivalent (EEQ) concentrations in influents and effluents of sewage treatment plants (STPs) located along the rivers. The results showed that phenolic groups of estrogenic compounds (i.e., NP, OP and BPA) were frequently found in surface water. The concentrations, followed the order of NP >> BPA > OP, were smaller than those reported by previous studies in Korea. Natural hormones (E2, E1) were also determined at several ng/L levels in water samples. Synthetic hormone (EE2) was rarely found in surface water although it was detected in the influents of the monitored STPs. Meanwhile, the phytoestrogen (i.e., Gen) were smaller than limit of detection in most samples. This study provided a general view of the distribution and transport of estrogenic compounds in Korean surface water.

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Integrated Approach towards Environmental Assessment of Trace Organic Pollutants

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An integrated approach looking for biological effects in addition to chemical detection becomes of great concern in environmental assessment of trace organic pollutants worldwide, however, such approach has not been well adopted in Korea yet. Until mid-1990s, very few studies reported trace organic contamination in coastal area of Korea and most of them focused sorely on analytical determination. The concept of biological effects together with chemical identification was first employed in our pollution study in late 1990s and I hereby summarize the major findings we obtained. The present abstract will highlight toxicity identification and evaluation (TIE) and mass balance approach (MBA), which are the keys in determining biologically effective chemicals present in environmental mixture samples. Overall, the instrumental data suggested that concentrations of target trace organic pollutants were relatively low to moderate but showed widespread distribution. The compositional pattern and spatial distribution indicated that their sources were independent of each other though. There were also some localized zones with extremely high concentrations of certain chemicals indicating point sources. To address biological effects, in vitro bioassays using H4IIE-luc (dioxin-like) and MVLN cells (estrogenic) exposed to organic extracts and TIE and MBA are performed. Most of the dioxin-like activities were observed in the fractions containing dioxins, furans, and certain polycyclic aromatic hydrocarbons (PAHs) and about half of the samples showed significant estrogenic activities in PAHs and alkylphenols fractions. A direct relationship between instrumental data and in other bioassays such as amphipod and sea urchin test will be further analyzed cross the full data set. Overall, we found that the combined approach of chemistry and toxicology was useful but it should be noted that the known composition and concentrations of target chemicals could not fully account for overall biological responses. Therefore, we expect more elaborate

characterization of chemicals and their composition associated with some fractions should improve further understanding.Keywords: POPs, biological effect, pollution, coastal environment, Korea

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Environmental Metabolomics for Health Impact Assessment

이정애, *정봉철

*KIST 생체대사연구센타 *KIST 생체대사연구센터*

Environmental metabolomics is an emerging technology for examining metabolic profiles in biological systems exposed to environmental stress using mass spectrometry, which provides a blend of sensitive, rapid, and selective qualitative and quantitative analyses with the ability to metabolites. It involves the application of advanced analytical and statistical tools to profile changes in levels of endo- and exogenous metabolites in tissues and biofluids result from disease onset, stress, or chemical exposure. It is applying to distinguish between sites and mechanisms of toxicity as well as to develop biomarkers of exposure. After collecting mass spectra from a statistically-relevant number of organisms, the number of metabolites changing in response to a given toxic insult from a large sample population can be analyzed by various computational methods (PCA or PLS-DA) to simplify large amounts of data. This provides the ability to quickly determine metabolic changes as opposed to assessing changes simply by eye. It offers considerable potential for rapid assessment of the metabolic status of organisms and can provide molecular information that is closely related to whole-organism physiology and function. Ultimately, we should strive towards the integration of omics data sets because this will enable us to exploit the advantages of each approach and will provide the most comprehensive molecular description of organisms in the environment.

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Understanding of Dye-Sensitized Solar Cell Technology

박남규

성균관대 화학공학부

Dye-sensitized solar cell (DSSC) utilizing nanotechnology and photosynthesis attracts much attention due to its high solar-to-electricity conversion efficiency, low cost and colorful appearance. DSSC is composed of the high surface area nanoparticle oxide semiconductor film that is sensitized with dye molecules, the redox electrolyte (or hole transport material) and the metal counter electrode. Unlike the conventional pn junction solid state diode, charge generation and charge transport occur in different material for the case of DSSC. In addition, electrolyte-semiconductor interface is 3-4 orders of magnitude higher than that in the solid-solid pn junction. Performance of DSSC are therefore dependent on constituent materials and interface as well as device structure. In this seminar, material, interfacial and device engineering for high efficiency dye-sensitized solar cell will be presented and discussed about future technology to hurdle the current limitation.

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연료전지 개발 현황 및 전망

조은애

KIST-연료전지연구단

21 세기 인류가 당면하고 있는 가장 큰 문제 중 하나가 에너지 자원의 한계성과 지구의 환경오염임은 누구도 부인할 수 없을 것이다. 수소에너지는 에너지와 환경문제를 동시에 해결할 수 있는 꿈의 에너지원으로 평가되고 있으며, 현재 인류가 안고 있는 화석연료의 한계인 부존자원의 고갈과 지구온난화 및 환경오염 문제를 극복할 수 있는 유일한 대안이라 할 수 있다. 특히, 연료전지는 이러한 수소에너지를 이용하는 전력변환 장치로 기존의 화석연료-내연기관 조합보다 에너지 효율을 극대화시킬 수 있는 차세대 고효율 청정 발전 기술로 각광을 받고 있다. 최근에는 저탄소 녹색 성장을 이끌 신성장동력, 그린에너지 중점기술에 선정되어 더욱 활발한 연구개발이 이루어질 것으로 기대된다. 본 강좌에서는 연료전지의 기술개요와 함께 응용분야별 현황 및 전망에 대해 소개하고자 한다.

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Recent Issues in Rechargeable Batteries

조원일

KIST 이차전지연구센터

A battery has been regarded as a simple power source to operate remote controllers, cellular phones, and notebook pc. But today's concerns with a battery technology are focused on its energy storage applications such as HEV, PHEV, EV and power grids. Practically rechargeable batteries have been used as electric energy storage devices for ups (un-interruptible power source), driving golf cars and forklifts. Electric energy storage is one of the most important technologies to increase the energy efficiency and it is inseparably related to renewable energy such as wind power and solar cells, smart grids, and distributed generation. Now rechargeable lithium battery is the most advanced battery, but there are endless requests for improving its performances like capacity, cycle life, safety, and even price. Those issues in rechargeable lithium batteries will be treated in accordance with major parts of batteries in this talk. And also large scale batteries

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Materials in lithium ion battery, the here and the hereafter

최상훈

LG화학 기술원 Battery연구소

A historical introduction is given to previous research & understanding of materials in Li ion battery. Mobile IT devices usually have used layered lithium metal hydroxides that has larger theoretical capacity than 3D oxide materials. Today, new regions of energy generation and consumption appear. Many automobile company approach to electrification. For the mid-term, they will increase its use of hybrid technology, and introduce plug-in hybrid electric (PHEV). For the long-term, they will focus on the battery electric vehicles (BEV) on the market. Above all, high power and safety are the most important requirements in their electric vehicle system. One of new worlds is energy storage system (ESS). This technology and market also will grow up with renewable energy generations. This technology also need safer batteries and materials than commodity products. In this lecture, I will introduce the new material in lithium ion battery. Nano-sized Lithium Iron (II) Phosphate (LFP) was prepared as Li ion battery cathode material and extensively studied from 1996 when Dr Goodenough introduces at first. LFP has been celebrated in many publications as being more environment-benign than layered lithium metal oxides. This was despite use of sophisticated techniques such as carbo-reducing and carbo-thermal methods.

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Biorefinery and Biomass-Based Chemistry as a Sustainable Solution in Chemical Industry

장종산

한국화학연구원 바이오리파이너리연구센터

석유자원의 점차적인 고갈은 화학산업 뿐만 아니라 국가 기간산업 전체에 커다란 영향을 미치고 국가의 지속적인 발전에 장해 요인이 될 것으로 예상된다. 또한 화석연료의 사용에 의한 이산화탄소 온실가스 배출과 이로 이한 지구온난화 문제는 기후변화 협약 포스트 교토의정서 단계의 온실가스 의무감축이 가시화될 2013 년 이후 화석에너지를 사용하는 산업에 지대한 영향을 미칠 것으로 우려된다. 이에 따라 새로운 원료와 대체 에너지원 확보를 위해 식물자원을 이용하여 바이오연료 및 화학제품을 생산하는 바이오리파이너리 기술이 이산화탄소 온실기체 저감문제를 해결하는 하나의 방안으로서, 그리고 환경친화적인 지속성장 기술로서 기대를 모으고 있다. 최근에 우리나라 정부부처 차원에서도 식물자원을 이용한 신화학 산업으로서 바이오화학 산업을 재정의하고 R&D 및 투자전략을 수립 중에 있다. 「바이오리파이너리(Biorefinery)」는 오로지 바이오매스로부터 생물학적인 전환 및 화학적 전환과정을 거쳐 바이오연료 및 화학제품을 제조하는 새로운 개념이다. 기존의 석유화학산업에서 원유를 정제한다는 의미의 리파이너리(Refinery)란 용어에 기원을 두고 탄생하기는 했지만 실제로는 바이오매스 원료로부터 생물학적 및 화학적 전환과정을 거쳐 바이오연료를 포함한 모든 바이오 화학제품을 생산하는 과정으로서 산업바이오의 실현을 위한 전주기적 핵심 기술을 의미한다. 특히 바이오리파이너리에서는 미생물에 의한 발효공정과 발효산물의 촉매 전환공정이 결합된 “Syncretic Process(융합공정)”를 통해 기존의 석유화학제품의 신공정 또는 새로운 화학제품의 생산이 가능하게 하는 특징을 갖는다. 이때 바이오 촉매와 화학 촉매는 식물자원으로부터 바이오 연료 및 화학제품 생산을 가능하게 하는 가장 핵심적인 요소로 작용한다. 본 발표에서는 바이오리파이너리의 중요한 분야인 바이오매스 유래 화학적 전환기술의 특징과 문제점, 한국화학연구원을 비롯한 국내외 기술개발 현황 및 개발 방향 등을 소개하고 토론할 기회를 갖고자 한다.

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The Molecular Simulations and a Percolation Study of the Effects of Chain Stiffness and Polymer Segmental Dynamics on the Tracer Diffusion

정현태, 성봉준

서강대 화학과

The diffusion of tracer molecules in polymeric materials has been an issue of great importance because the tracer diffusion has been an important factor to improve the performance of fuel cells and separation membranes. The tracer diffusion is determined not only by the intermolecular interaction between a tracer and a polymer, but also by the polymer structure. Recently, it was reported that as one changed the polymer structure by stiffening polymers, the diffusion of tracers was significantly changed. (J. Phys. Chem. B 113, 2247 (2009)) However, the effects of the chain stiffness and the polymer structure have not been understood clearly yet. For example, it is still not clear whether the pore space in polymeric materials, which is considered a dominant factor to determine the tracer diffusion, should be changed upon stiffening chains. Therefore, we investigate the effect of the chain stiffness on the diffusion of tracer molecules using molecular simulations and a percolation theory. Using the equilibrated configuration of polymers, which is quenched in space, the diffusion coefficients of tracers are calculated via molecular simulations. And we locate a pore percolation threshold by carrying out Voronoi tessellation and calculating the mean cluster sizes of pores. We found that the diffusion coefficients of tracer molecules are decreased significantly, as polymers become stiffer and extended. However, the pore percolation threshold concentrations do not vary much with an increase in chain stiffness. We found by comparing to a previous simulation study (Polymer 45, 3923 (2004)) that the decrease in the tracer diffusion is attributed mainly not to a change in pore structure but to the segmental dynamics of polymers that slows down as one stiffens the polymer chains.

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Order-Order Transition in Thin Films of a Diblock Copolymer Composed of a Linear Polymer Block and a Brush Polymer Block with Mesogenic Oligothiophenyl Bristles

안병철, *윤진환, 진상우, 노예철, **Tomoyasu Hirai, **Rina Maeda, 박삼대, 김진철, 권원상, 김동민, 정정운, 김미희, 김경태, **Teruaki Hayakawa, 이문호

*포항공과대 화학과 *University of Massachusetts, USA **Tokyo Institute of Technology, Japan*

In this study, we quantitatively investigated the temperature-dependent phase transition behaviors in thin films of an interesting semi-rod-coil diblock copolymer, poly(styrene)-*b*-poly(oligothiophene side chain modified isoprene) (PS-*b*-POTI), and the resulting morphological structures using synchrotron grazing incidence X-ray scattering combined with differential scanning calorimetry. These analyses provided detailed information about the morphologies of the phase-separated domains and the molecular structures formed in each domain. At room temperature, the diblock copolymer molecules in thin films were found to form an alternately stacked structure comprised of amorphous PS and smectic-A POTI microdomains whose stacking direction is parallel to the film plane. On heating, the films underwent a phase transformation to a hexagonal cylinder structure with cylindrical POTI domains in the PS matrix oriented normal to the film plane. This phase conversion is induced by the transformation of the POTI domains from a smectic-A phase to an isotropic phase, where the smectic-A phase is composed of a laterally ordered structure of interdigitated bristles in the POTI blocks. On the basis of these structural analysis results, we propose models for the molecular structures of the diblock polymer thin films at various temperatures.

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Molecular design of novel stimuli-responsive polymers and gels based on amphiphilic functional polyaspartamides for drug delivery

문종록, 김지홍

성균관대 화학공학과

Recently, the interest in stimuli-responsive materials has increased during the last decades. Among them, polymer systems that undergo nano-aggregations (or micelle formation) and hydrogel in response to biological temperature and pH have been widely investigated for tissue engineering, gene and tumor targeting delivery. Here, we report recent work on the characterization and application of smart biomaterial based on the polyaspartamide(PASAM)-based biodegradable copolymers. A series of amphiphilic polyaspartamide derivatives with the combination of different amines including N-isopropylethylenediamine (NIPEDA), 2-diisopropylaminoethylamine (DIPAEA), ethanolamine (EA), O-(2-aminoethyl)-O`-methylpolyethylene glycol (MPEG), alkylamines (hexyl HA, octyl OA, and lauryl LA), were synthesized from polysuccinimide (PSI) via successive nucleophilic ring-opening reaction. The composition of the prepared amphiphilic copolymers was analyzed by H-NMR. Molecular design of novel copolymers and hydrogels (chemical or physical) based on amphiphilic polyaspartamide derivatives containing cationic pendants were investigated to identify materials as double-responsive (temperature and pH) polymers and gels potentially useful for biomedical applications including controlled and targeted drug delivery system.

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pH-Dependent Structures of an i-Motif DNA in Solution

노예철, 안병철, 진상우, 이택준, 박삼대, 김진철, 김동민, 정정운, 권원상, 김미희, 고용기, 이문호

포항공과대 화학과

We have investigated for the first time the structure of i-motif DNA in solution at various pH conditions by using synchrotron small-angle X-ray scattering technique. To facilitate direct structural comparison between solution structures of i-motif DNA at various pH values, we created atomic coordinates of i-motif DNA from a fully folded to unfolded atomic model. Under mild acidic conditions, the conformations for i-motif DNA appeared to be similar to that of the partially unfolded i-motif atomic model in overall shape, rather than the fully folded i-motif atomic model. Collectively, our observations indicate that i-motif DNA molecule is structurally dynamic over a wide pH range, adopting multiple conformations ranging from the folded i-motif structure to a random coil conformation. As the i-motif structure has been used as an important component in nanomachines, we can therefore believe that the structural evidence presented herein will promote the development of future DNA-based molecular-actuator devices.

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Nafion films : Excellent Candidate for Biomaterial.

김진철, 김가희, 이택준, 박삼대, 진상우, 김동민, 정정운, 노예철, 안병철, 권원상, 김경태, 김미희, 고용기, 이문호

포항공과대 화학과

We investigated bioadhesion (bacterial and cell adhesion) and biocompatibility of Nafion and compared the results with those of poly(vinylidene fluoride-co-hexafluoropropylene) (PVFHFP). When incubated with bacteria for 4 h to 7 days, Nafion film exhibited scarce bacterial adhesion at 6 h, after which the adhesion was gradually increasing to relatively low levels. In contrast, significant bacterial adhesion to PVFHFP film was observed at 4 h, and much higher adhesion levels were shown after then. Although HEp-2 human cells adhered normally to both films reaching confluence in 7 – 8 days, the cells adhered to Nafion appeared more lively and stable than those to PVFHFP. Subcutaneous implantation in mice revealed that Nafion elicited a mild acute inflammatory reaction without chronic inflammation or tissue necrosis, indicating excellent biocompatibility in mice. PVFHFP, however, provoked a moderate and prolonged acute inflammatory response. These differences in the biological characteristics of Nafion and PVFHFP films may be attributable to the differences in the chemical and physical natures of these polymer films. Nafion film provided a sufficiently solid support, expressing a high surface charge density and good water-wettability. In summary, Nafion is suitable for use in biomedical applications that require biocompatibility with a reduced possibility of post-operative infections.

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Gradient Surfaces for the Index of Cellular Adhesion Properties

김현정, KHATUA DIBYENDU, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

The interaction between cells and a solid substrate are very important in tissue engineering and biomedical applications. Many surface properties such as charge, wettability, chemical structure, roughness, and rigidity influence adhesion of cells. To evaluate a favorable cellular response in a specific application, testing of all combinations of various screening factors are a highly time-consuming process. Furthermore the using different substrates at different conditions may complicate the conditions for cell-to-cell comparision. The problem can be minimized by using gradient surfaces, wherein two or more properties vary independently across the specimen. The use of gradients allows cell behavior to be directly compared over a range of different surface properties on a single sample and under identical conditions. In this talk, I would like to present our recent research for preparing charge density/ wettability orthogonal gradient surface and the cell adhesion properties of different types of cells on the surface. Then, we will introduce a simple indexing method to evaluate the cellular adhesion properties to each cells quantitatively, which will be benefit to sort them out depending on their adhesion properties.

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New Approach for Preparation Cylindrical Microdomains in PS-b-P4VP Thin Films Using Solvent Annealing & Its Applications

김성남, 김승빈

포항공과대 화학과

Many scientists have been attracted to block copolymers (BCPs) which form various ordered nanostructures, like spheres, cylinders, lamellae and bicontinuous gyroids, depending on the number of different blocks and their compositions. Especially, the cylindrical microstructures oriented normal to the surface of BCPs films are very useful for fabricating nano-devices. Many efforts and strategies have been devoted to this topic. This work involves new simple method to make perpendicular cylindrical microstructures in PS-b-P4VP thin films from its micelle stacks by solvent annealing process. These BCPs templates have been applied to manufacture various nanostructures of inorganic materials, Au, Ag and so on, because the inorganic salts can stick to P4VP microdomains selectively.

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Analysis of PS-Br synthesized by ATRP using MALDI-MS TOF

김기현, 장태현, *백현종

*포항공과대 화학과 *부산대 고분자공학과*

The polymer synthesized by conventional radical polymerization is difficult to control the molecular characteristics such as molecular weight distribution (MWD), chain end functionalities, chain architectures or compositions. In this regard, recently developed controlled radical polymerization (CRP) technique can do a far better job. For example, polymerization of styrene by atom transfer radical polymerization (ATRP), which is one of the CRP, yield PS-Br with a relatively narrow MWD, which in turn can be used as a macroinitiator to synthesize a block copolymer. Despite the importance of the end-functional macroinitiator, its characterization cannot be said to be done rigorously.Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) is a powerful tool to characterize the molecular characteristics of polymers. A few research groups have tried to analyze the PS-Br by MALDI MS, but the reactivity of the end group of PS-Br resulted complex spectra to make the interpretation difficult. In this work, we analyzed MALDI MS spectra to successfully elucidate the by-products from reaction of the end-group during the MALDI process.

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Organic Conductors for Regenerative Medical Bionics

Gordon G. Wallace

ARC Centre of Excellence for Electromaterials Science, Intelligent Polymer Research Institute, University of Wollongong, Wollongong, NSW 2522, Australia.

Bionic implants aimed at restoring some element of human function will likely consist of a three dimensional structure comprising a scaffold with appropriate, physical and mechanical properties, a means of delivering electrical stimulation, and a supply of bioactive molecules, perhaps even stem cells, to facilitate repair.Some degree of control over each of these properties and the accessibility to the bioactive components will ensure performance can be optimised. This control may be “programmed” into the material structure or achieved via electrical stimulation or both. Either way dynamic materials whose behaviour can be modified to assist repair of the biological system are needed.Organic conducting polymers have recently emerged as excellent candidates capable of performing many of the functions required of regenerative bionic implants. Here we will discuss our most recent findings in the quest to develop implants for nerve and muscle repair.Many challenges remain and a significant multidiscipline multi-national approach is required for efficient progress.

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Hybrid organic-inorganic diode devices

송명훈

울산과학기술대 기계신소재공학부

We present an investigation of high brightness, efficient, and encapsulation-free, high brightness encapsulation-free composite metal-oxide-polymer light emitting diodes (LEDs). In these diodes, mesoporous and/or compact form of metal-oxide layers have been used for electron injection and a MoO_3 layer for hole injection. We demonstrate that compact ZnO operates phenomenally well and significantly better than compact or mesoporous TiO_2. We make also use of the high refractive index of ZnO to confine these modes away from the absorbing electrodes, and include a nano-imprinted grating in the polymer layer to introduce distributed feedback and enhance optical out-coupling. Further to improved LED operation, we demonstrate optically-pumped lasing in devices that also function as LEDs. This demonstrates the scope to use such architectures to improve the external efficiency of organic semiconductor LEDs, and opens new possibilities for the realisation of polymer injection lasers.

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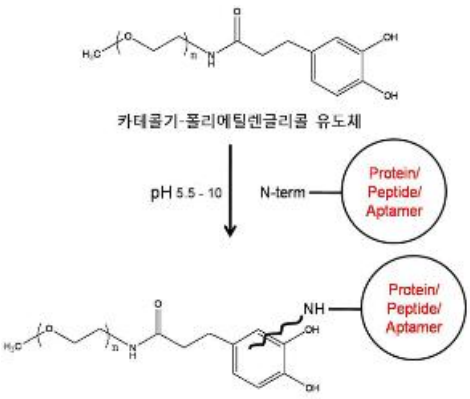
Site-specific mono-PEGylation of proteins using catechol modified polyethylene-glycol

이혁진

KAIST 화학과

Funtional PEGylation has been widely appied to many of the biological and physical sciences, including cell and molecular biology, medical diagnosis and imaing, tissue egineering and bioprocess engineering. In this study, we report a novel site specific PEGylation approach for proteins and peptides by employing the mussel inspired bio-adhesive molecules (catechol). Catechol modified polyethylene-glycol (catechol-PEG) was synthesized and utilized to react specifically to the N-terminal amine of proteins and peptides. Compared to aldehyde modified poylethylene-glycol, catechol-PEG allow stable conjugation under aqueous condition for prolonged time. To evaluate site specific PEGylation, granulocyte-colony stimulating factor (G-CSF) and basic fibroblast growth factor (bFGF) were PEGylated using catechol-PEG under physiological condition. PEGylated proteins were analyzed by SDS-PAGE, SEC-HPLC, RP-HPLC, and MALDI-TOF. The detailed chemistry of N-terminal amine and catechol-PEG was also studied using H-NMR.



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Polymers for Nanostructure Fabrications

이승우

영남대 디스플레이화학공학부

In the field of nanoscience and nanotechnology, the development of lithographic methods for fabricating submicrometer and more recently sub-100 nm features is of great interest for both fundamental and technological purposes. Many structures, when miniaturized to the sub-100 nm length scale,possess architecture dependent chemical and physical properties. The ability to print such structures and interface them with larger architectures is opening applications in electronics, optics, catalysis, and biosensing. Examples of lithographic methods for making micro and/or nano scale patterns include photolithography, microcontact printing, e-beam lithography, nanoimprint lithography, and dip-pen nanolithography (DPN). However, most DPN methods have employed patterning of alkanethiol molecules and alkanesilane molecules on a gold surface and silicone oxide surface, respectively. Recently, Crook reported DPN on a modified poly(acrylic acid) surface. In here, we synthesized a polymer containing NHS (N-hydroxy succinimide) ester moiety as side groups and characterized their abilities for DPN.

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Stimui-responsive dendritic polymers

장우동, 이은영, 김주호

연세대 화학과

Dendrimers are nanoscopic hyperbranched macromolecules with well-predictable three-dimensional shapes and potential building blocks for the construction of organized functional materials. Various applications of dendrimers have been proposed using their unique structures as well as functional varieties. Recently, we have designed several dendritic materials with stimuli-responsibility against light, temperature, and pH. In this symposium, we are going to introduce several stimuli-responsive dendritic materials, and discuss about their application.

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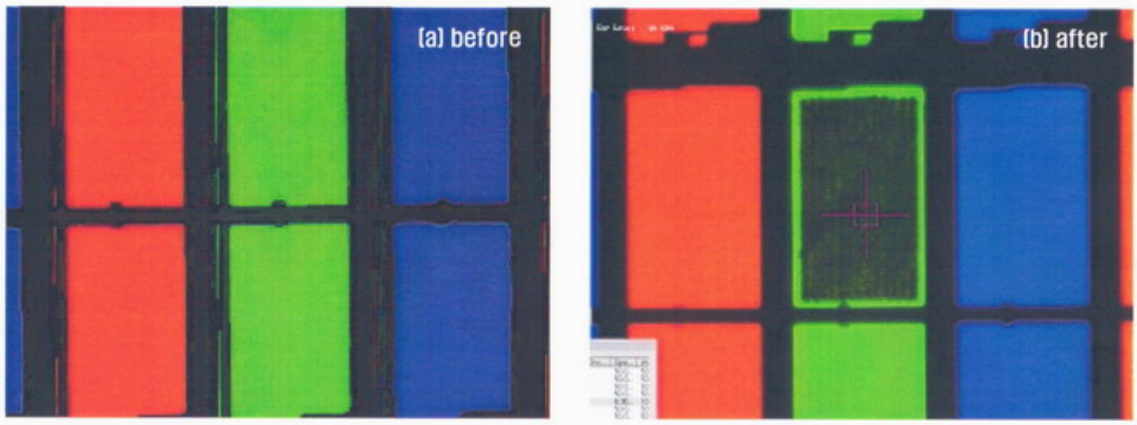
Novel repairing technology of TFT-LCD panel by LASER ablation

이영범

삼성전자(주) DS총괄 LCD사업부

We report a novel repairing technology of thin film transistor-liquid crystal display (TFT-LCD) panel using a laser system. It was demonstrated the direct darkling repair of RGB filters on TFT-LCD panel attached with/without a polarizer film using a laser ablation assisted technique. The repair method has been developed by applying laser pulses on color filter substrate attached with/without a polarizer film.



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Light Harvesting with Nanostructured Porphyrins: Towards Artificial Photosynthesis

David L. Officer

ARC Centre of Excellence for Electromaterials Science,Intelligent Polymer Research Institute, AIIM Facility,University of Wollongong, Squires Way, Wollongong NSW 2519, Australia.

Replicating photosynthetic processes in devices could provide a new generation of economical photovoltaic devices and lay the foundation for sustainable hydrogen production through water splitting. In the dye-sensitised solar cell (DSSC) or Grätzel photoelectrochemical cell, light is harvested using a large surface area of dye (that may be a chlorophyll-like molecule) bound to a mesoporous thin film of nanostructured titanium dioxide and, following charge separation and injection of an electron into the semiconductor, the oxidised dye is reduced by a redox mediator. This has often been likened to the light harvesting component of photosynthesis. However, in the exquisitely structured photosynthetic light harvesting process, light is absorbed by a 3-dimensional non-covalent array of up to three hundred chlorophyll "dyes" that make up the light harvesting antenna, and the energy transferred to the "special pair" of bacteriochlorins in the Reaction Centre, within which charge separation occurs. In other words, in photosynthesis, the energy absorption and transfer, and charge separation processes are somewhat isolated from each other. Emulating this in the titanium dioxide solar cell would offer the potential to improve cell efficiency both through enhanced light harvesting as well as control of the energy and electron transfer processes.In this lecture, we will discuss our progress in understanding the action of porphyrins ("artificial chlorophyll") in the DSSC with a view to developing structures on nanostructured titanium dioxide that emulate photosynthesis.

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Theoretical studies on ethylene polymerization processes catalyzed by half-metalocene complexes of titanium

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Density Functional Theory based computational methods have been applied in the mechanistic studies of the ethylene polymerization processes catalyzed by the half-metalocene titanium (IV) complexes with different ligands. In particular, a special attention has been paid to the catalysts with aryloxo ligands due to their activity in the high-temerature polymerization and co-polymerization experiments. The main goal was to rationalize the changes in activity for the systems with different substituents on the phenoxo ligand. For comparison, a well-known constrained-geometry-catalyst (CGC) was also included in the investigated set of complexes. The results reproduce the experimental trends: it has been found that the activity of systems with a single substituent in the ortho position of the phenyl ring (*asymmetric systems*) is comparable to that of CGC, while the complexes with two substituents at both ortho-carbon atoms (*symmetric systems)* are substantially less active. Further, it has been shown that an unique feature of the asymmetric complexes is a preference of the back-side pathway of the ethylene insertion. In contrast, a preference of front-side insertion is observed for the symmetric complexes as well as for CGC. It has been also demonstrated that a rotation of the aryloxo ligand around the Ti-O-C bonds is feasible; it allows for an easy transformation between the non-reactive and reactive isomers/pathways. Results of the static DFT calculations were supported by Molecular Dynamics (MD) simulations, performed at the semiempirical (MSINDO) and the *ab initio* (CP-MD) level.

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In Search for Single-Component Selective and Switchable Catalysts for Ethylene Oligo- and Polymerization.

Sandro Gambarotta

Dept of Chemistry, University of Ottawa, Ottawa, Ont. Canada

The processes of ethylene polymerization and selective tri- and tetramerization may be regarded as belonging to the same family of C-C bond forming processes. Yet, the reaction mechanisms followed by these reactions (respectively chain growth and metallacycle ring expansion) are conceptually very different. This is furthermore in contrast to the fact that both processes employ identical Ziegler-Natta type of conditions (use of a mixture of catalyst and activator). During this presentation, we will describe the results of our efforts to isolate catalytically active species. This was aiming at extracting critical information about reaction mechanism, metal oxidation state and factors responsible for the type of catalytic activity (poly- and oligomerization) and selectivity. A few catalytically active, hetero-dimetallic systems have been isolated, characterized and tested. The role of their geometry and structure within the catalytic cycle will be examined.A new simple and yet effective hemilabile ligand system has been designed while searching for mono-metallic single component catalysts. The results of the catalytic testing of these novel species will be described alongside with their chemical behavior and mechanistic significance.The use of this information to assist future design of novel catalytic systems will be also discussed.

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Fast and hybrid methods and their applications

최철호

경북대 화학과

The objective of our research is to establish new theoretical methods in the study of intermediate size and extended systems. Specifically, the research includes developments of new *ab initio* theories and their applications. Intermediate means a system that is sufficiently large to have intermediate chemical and physical properties between small molecules and extended systems. An example might be a significant portion of a nanostructural material.

With the help of ever improving computer hardware and new theories, computational chemistry, and electronic structure theory in particular, is evolving into an essential tool in exploring and understanding the nature of chemical systems. At the same time, it is quite clear that conventional electronic structure theories may not be able to keep pace with the growth of demands due to the fact that even in the simplest method, the Hartree-Fock (HF) theory, the amount of computations needed increases roughly as $O(N^4)$, where N is the number of basis functions.

In talk, we present our on-going theoretical developments and proposals to overcome the bottlenecks of current quantum mechanical methods, and their applications to extended systems, in which new methods could bring us new chemical insights.

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The Conversion of the CdTe Nanoparticles into Nanoribbons shapy by Self-Assembly

이광원, 김상현, 김기섭

충주대 화공생물공학과

The electrical and optical properties of nanoparticles (NPs) and nanowires (NWs) have been extensively studied for use in electronics, photonics, and sensors. Recently, one of the most active areas of research in nanoscience is to develop novel structures of nanomaterials such as nanohelices (NHs), nanosheets (NSs), and hollow nanocrystalls, which open up the possibility of a new generation of advanced materials.Given that the properties of materials largely depend on their unique structure, identification of the key factors in synthesis can be helpful in reaching specific desired shapes. The study on synthesis of NRIs started on the basis of simple hypotheses and modifications of the procedures described. First, the aqueous redissolution step of NPs obtained after precipitation of the original stable dispersion by methanol treatment proceeds under ambient light, because light might cause some defect such as truncation. Second, the ratio of thioglycolic acid (TGA) to Cd2+ is reduced at the synthesis step of CdTe NPs, because we can readily predict that highly photoluminescent (PL) CdTe nanocrystals (NCs) will be obtained at reduced ratios.Furthermore, the excess stabilizers in the CdTe solutions and the stabilizers on the NP surface can be efficiently removed at reduced ratios.

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Silver nanorods in ultrathin porous anodic alumina for surface-enhanced Raman scattering(SERS)

구근회, *서정쌍

*서울대 화학과 *서울대 화학부*

We have calculated the minimum enhancement factor for single molecule detections from the SERS data measured from well defined silver nanorod arrays. Silver nanorods were fabricated by electrodepositing them evenly near the mouth of the pores of anodic aluminum oxide templates with a very shallow depth. The SERS intensity increased almost linearly with increasing the concentration of the mother solution. From the data of the enhancement and the number of molecules irradiated by the laser beam at the detection limit, the minimum SERS enhancement factor for non-resonant single molecule detections was calculated to be approximately 10^{11}.

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Viscosity-dependent rebinding kinetics of CO to microperoxidase-8 in water-glycerol mixture

박재홍, 임만호, 김주영, 이태곤, 김혜림

부산대 화학과

Microperoxidase-8 (Mp), a fragment of cytochrome c consisting of a heme with an 8 amino acid peptide that covalently linked to a heme through a histidine and mimicking the heme protein structure in the absence of a specifically organized distal pocket, is an excellent model system for obtaining the reaction characteristics of the heme free from conformational change and protein structure. Femtosecond vibrational spectroscopy was used to study the rebinding dynamics of CO to the heme after photolysis of MpCO in glycerol/water mixtures. Significant fraction (30-75 %) of CO rebinds nonexponentially within 1 ns at room temperature solution. The geminate yield of CO rebinding increases and its rate accelerates as the viscosity of the solution increases either by increasing glycerol content in glycerol/water mixtures at room temperature or by decreasing temperature of solution. The nonexponential rebinding kinetics can be described by the theory of diffusion-controlled reaction and the data are well reproduced by the pair survival probability function in the absence of any interaction potential between pair. The rebinding kinetics was also modeled by the SRC model, a distributed linear coupling model for the CO binding. The SRC model reproduces data very well, too. The nonexponential rebinding of CO to Mp will be discussed based on the fitted parameters from both models.

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The contrast characteristics of iMQCs MR imaging

조지현, *안상두, 전성란, 이철현

*KBSI 자기공명영상팀 *중앙대 화학과*

Recently, a new method for contrast enhancement in magnetic resonance imaging based on the detection of relatively strong signals from intermolecular multiple quantum coherences (iMQCs) both in vitro and in vivo has been reported. These signals are strongly depending on the local magnetic properties of samples which can be modified by appropriate contrasting agents. In this study, several metal salts have been tested as contrast agents affecting the iMQCs signals at 14.1 T μMRI on the purpose of observing the characteristics of iMQCs signals and looking for a good contrasting condition fitting to this new method. These results showed that the iMQCs microscopic images were readily observable and had unique contrast depending on the micro-structures of samples. The detailed contrast characteristics of iMQCs MR images with these metal salts for several phantoms and model cell systems will be discussed.

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Signature of coherent energy transfer in IR and Raman spectra of water

양민오, *J. L. Skinner

*충북대 화학과 *Department of Chemistry, University of Wisconsin-Madison*

A mixed quantum /classical approach has been developed to calculate the IR absorption and Raman spectra of water in the spectral range of the OH stretching mode. Excellent agreement between the theoretical and experimental line shapes has been achieved without introducing any adjustable parameters and the line shapes are interpreted in time domain. It has been shown that extremely fast coherent vibrational energy transfer prevails collectively over many chromophores in neat water and is responsible for the appearance of the characteristic band located at 3250 cm^{-1} in the IR absorption, isotropic, and parallel polarized Raman spectra. It is discussed that major features of the IR and Raman line shapes of neat water are determined by how the effect of coherent energy transfer is manifested by the field-matter interactions, which are distinct in the respective experiment.

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Reaction dynamics of a fluctuating single enzyme molecule

정원, 성재영, 양성은, 박보정

중앙대 화학과

Enzymes as a biological catalyst have been studied extensively. We propose a simple kinetic model controlled by a fluctuating bottleneck where the rate of product formation is proportional to enzyme's cross-sectional area. We introduce a decaying parameter λ that indicates the fluctuating rate of an enzyme. We obtain an approximate analytic expression for waiting time distribution dependent on λ and compare with simulation data. We find that λ's effect is fairly significant and suggest that previous studies modeling simple Poisson process and slow fluctuating limit process should be revised.

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The Extraordinary Behaviors of 2-, 3-, 4-Bromochlorobenzene Monomers and Dimers upon Electron Attachment

김남두, 손태일, 이상학, *김성근

*서울대 화학부 *서울대 화학부, 서울대 생물물리 및 화학생물학과*

The extraordinary behaviors of 2-, 3-, 4-bromochlorobenzene (BCB) cluster anions upon electron attachment were investigated by using TOF-MS, photoelectron spectroscopy (532 nm, 2.329 eV and 355 nm, 3.496 eV) and *ab initio* calculations. In the mass spectrum, Br^- shows a distinctly more intense peak than any other moieties, indicating dissociative attachment of electron to bromine. In photoelectron spectra, the vertical detachment energies (VDEs) of all three isomers were determined to be ~2.5 eV, which agrees well with the calculated values. Dissociated bromine atom was found to form a van der Waals complex with its parent molecule. In contrast to the monomeric cases, the VDE of 4-BCB dimer is extremely small at ~0.3 eV, while that of 2-BCB and 3-BCB are 1.1 eV, 2.69 eV, respectively. We calculated several possible structures and found that a parallel-staggered structure and a T-shaped one are the most likely structures for 4-BCB dimer anion, with a VDE value of 0.36 and 0.30 eV, respectively. For 3-BCB dimer, second 3-BCB molecule stabilize monomer anion by solvation effect to form T-shape.

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Refractive Index Control in Methylene-Biphenyl Bridged Silsesquioxane Thin Films

최진규, 정현담

전남대 화학과

A series of methylene-biphenyl bridged silsesquioxane thin films was fabricated from 4,4'-bis(trimethoxysilylmethyl)biphenyl (MBP) and methyltrimethoxysilane (MTMS) monomers with different molar ratios. Sol-gel process which contains hydrolysis and condensation reactions was used to synthesize precursors for thin films followed by spin-coating on silicon wafer (Si-wafer). Optical properties of the thin films were investigated by ultraviolet-visible (UV-Vis) spectroscopy and spectroscopic ellipsometry (SE). Refractive index values of the thin films decrease from MBP 100 % of 1.60 to MBP 0 % of 1.40. The thin films' complex dielectric function which consists of real part and imaginary part relating to refractive index and extinction coefficient was also investigated. Thin films of MBP 100 and 75 % show differences in and compared to those of MBP 50, 25, and 0% ones due to the planarization of biphenyl rings.

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An Experimental Study of OH Heterogeneous Reaction on the Surfaces of Atmospheric Importance under Dry and Wet Conditions

박종호, *Andrey V. Ivanov, *Mario J. Molina

*한국원자력연구원 원자력화학연구부 *University of California, San Diego*

An experimental study of the dependence of the OH uptake coefficient over a relative humidity of 0-48 % was carried out at 100 Torr and room temperature, using a differential bead-filled flow tube coupled to a high-pressure chemical ionization mass spectrometer. Various organic (paraffin wax, pyrene, glutaric acid, and soot) and inorganic (NaCl, KCl, $MgCl_2$, $CaCl_2$, Na_2SO_4, and sea salt) surfaces served as proxies for tropospheric aerosols. A virtual cylindrical flow tube approximation and a surface coating dilution technique were successfully employed in the study, which included measurements of high radical uptake with an initial probability of near unity. For inorganic salts, the effect of water vapor, enhancement or inhibition of the OH uptake coefficient, was found to be dependent on the blocking of anions and changes in surface pH. Although OH uptake by NaCl, the major component of sea-salt aerosols, is weakly dependent on water vapor, it is enhanced by a factor of 2 for $MgCl_2$ and determines the net relative humidity dependence of the radical uptake on sea salt, which is enhanced by a factor of 4. For the organic surfaces studied, the enhancement effect of a factor 4 was also observed only for a hydrophilic organic surface, namely, glutaric acid. Results of the uptake studies suggest that the effect of relative humidity is important and should be accounted for in atmospheric modeling of tropospheric aerosol chemistry.

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2-Dimensional Organic Half Metal

이은철, *김광수

*한국과학기술정보연구원 슈퍼컴퓨팅본부/응용지원실 *포항공과대 화학과*

In half metals which have the metallic nature for one electron's spin and the non-metallic nature for the other, the current can be completely spin polarized. However most half metals are inorganic systems and 3-dimensional systems. There have been some reports on 1-dimensional and 2-dimensional organic (or organometallic) half metals: graphene nanoribbon (GNR) under strong electric field, edge-modified zigzag GNR, hybrid BCN nanoribbons, and 1D organometallic half metals. The advantage of using organic materials as spin-based electronic (spintronic) devices is that the spin relaxation length and spin lifetime are considerably long because of weak spin-orbit and hyperfine interactions. In addition, organic materials are usually inexpensive light materials and would be candidates for flexible devices. Here, we discuss 2-dimensional organic half metal, 2,4,6-tri-(1,3,5-triazinyl)methyl radical polymer, which is a candidate of complete spin polarized carrier sources. It would be possible to achieve spontaneous magnetic ordering.

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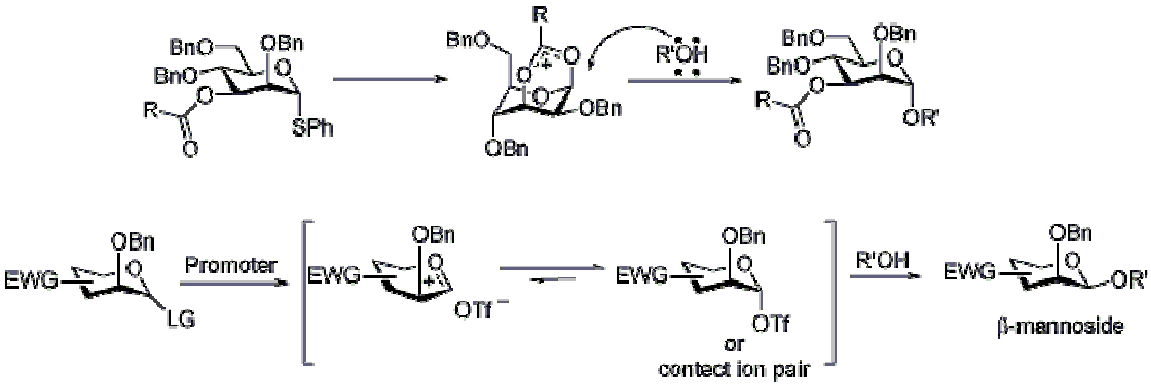
Effect of Electron-Withdrawing Group at O-3, O-4 and O-6 of Glycosyl Donors on the Mannosylation Stereochemistry

백주열, 이보영, 김관수

연세대 화학과

Mannosylations of various acceptors with donors possessing an electron-withdrawing o-trifluoromethylbenzenesulfonyl, benzylsulfonyl, p-nitrobenzoyl, benzoyl, or acetyl group at one of O-3, O-4, and O-6 positions were found to be β-selective except those with donors having 3-O-acyl and 6-O-acetyl groups, which afforded α-mannosides as major products. The counter anion, namely the triflate anion, of the mannosyl oxocarbenium ion was found to be crucial for the β-selectivity of the present mannosylation. Covalent α-mannosyl triflates having an electron-withdrawing group at O-3, O-4, and O-6 were detected by the low temperature NMR. The strongly electron-withdrawing sulfonyl groups, which exhibited the higher β-directing effect in the mannosylation, made the α-mannosyl triflates more stable than the weakly electron-withdrawing acyl groups. The mechanism for the α-selective mannosylation, therefore, was proposed by assuming the stabilization of the α-mannosyl triflate by the electron-withdrawing groups and the subsequent reaction of the α-triflate (or its contact ion pair) with the acceptor.



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Development of a Novel Benzopyran-containing Androgen Receptor Antagonist to Treat Antiandrogen-resistant Prostate Cancer

오상미, 박승범

서울대 화학부

Bioactive ligands with specific alteration of biological events are powerful research tools in chemical biology. Furthermore, those bioactive ligands have a high potential to be developed as novel therapeutic agents. For the identification of novel bioactive ligands for androgen receptor (AR), our library containing 2,500 unique compounds was subjected toward the cell-based reporter gene assay in LNCaP cells measuring antagonistic effect in competition with dihydrotestosterone (DHT) to identify novel antagonists. AR is androgen inducible nuclear receptor superfamily which has been focused on key molecular target in growth and progression of prostate cancer. Despite of few side effects and relatively good oral bioavailability of nonsteroidal anti-androgens, such as bicalutamide, anti-androgen resistance has been discovered after long-term drug usage and often progressed into anti-androgen withdrawal syndrome. Therefore, developing new small molecule anti-androgen is very urgent to treat anti-androgen resistant prostate cancer.The compound library was constructed in our laboratory using Diversity-oriented Synthesis, which is the synthetic algorithm to generate combinatorial libraries of small molecules using forward synthetic analysis. We found a novel antagonistic compound on AR with benzopyran-fused hydroxyisoindoledione moiety. Based on structure activity relationship (SAR) using medicinal chemistry approach, we constructed focused library with 19 members of compounds to improve antagonistic effect of initial hit compound. Among them, the lead compound 6f was identified with good antagonistic activity, confirmed by western blot analysis, RT-PCR, and cellular proliferation assay. We also demonstrated that compound 6f has a therapeutic efficacy toward not only normal AR but also mutant AR such as T877A or W741L (bicalutamide-resistant AR mutant), which cause the antagonists to act as agonists. AR mutations are one of proposed mechanisms to explain anti-androgen resistance. Therefore, compound 6f has an excellent potential to address the anti-androgen resistant prostate cancer.

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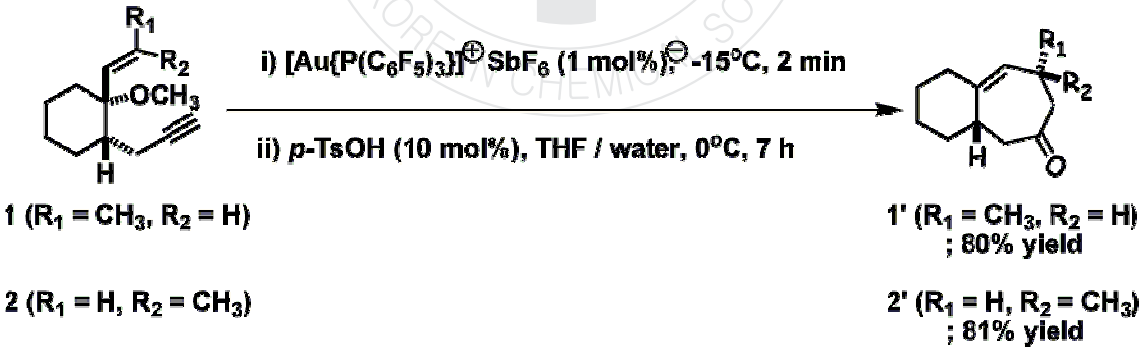
Studies on the Structural Effects in the Gold(I)-Catalyzed Cycloisomerization of 3-Methoxy-1,6-enynes

배효진, 이영호

포항공과대 화학과

Recently, we developed a new gold(I)-catalyzed cycloisomerization of 3-methoxy-1,6-enynes via tandem heterocyclization and [3,3]-sigmatropic rearrangement to access highly substituted cycloheptene moiety. Interestingly, the efficiency of the gold(I)-catalyzed cycloisomerization using 3-methoxy-1,6-enynes was highly dependent upon the structure of the substrate. In this presentation, a mechanistic rationale for these results will be discussed.



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Selective Sulfate Binding Induces Helical Folding of an Indolocarbazole Oligomer in Solution and Solid State

김준일, **juwarker,** 정규성

연세대 화학과

We have synthesized oligoindolocarbazoles that fold into helical structures and function as novel synthetic receptors for anions. A foldamer consisting of three indolocarbazoles units was prepared by sequentially connecting three indolocarbazoles by ethynyl linkers. Upon folding, the oligoindolocarbazole forms a tubular cavity where anion binding can occur through hydrogen bonding to the indole NHs and aliphatic OHs. The anion is hydrogen bonded to six indole NHs and to two aliphatic OHs resulting in selectivity towards the tetrahedral, dianionic sulfate anion. The folding properties of the oligoindolocarbazoles were characterized by ^{1}H NMR, 2D ^{1}H-^{1}H NMR and fluorescence spectroscopy. Characteristic upfield shifts of the aromatic protons, indicative of anion binding induced π-stacking was observed in the ^{1}H NMR spectrum. Similar correlation peaks were detected by ^{1}H-^{1}H NOESY. Fluorescence experiments display batho- and hypochromic shifts of the emission wavelength, owing to the aromatic π-stacking of the turns. These spectral changes are induced by anion complexation and allow us to evaluate and compare the anion binding affinities of these novel foldamers in 10% CH_3OH/CH_3CN. The binding of anion with a helical cavity was confirmed by a crystal structure of the indolocarbazole trimer with sulfate. Physical measurements detailing the folding and anion binding are reported here.

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In-Situ FTIR Study of Atomic Layer Deposition of Ruthenium.

Sun Kyung Park, Yves J. Chabal, *Jeff Anthis, *R.Kanjolia

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Ruthenium is attractive for a number of reasons: 1) high chemical and thermal stability with high-k materials; 2) no detrimental interface reactions or interdiffusion at the ruthenium-dielectric interface (i.e. most suitable noble metal electrode material); 3) potential capacitor electrode material for DRAMs and FRAMs, and potential gate metal in future metal-oxide-semiconductor field effect transistors (MOSFETs) due to is relatively high work function (4.7eV); 4) barrier and seed layer for copper, the interconnection metal in microelectronics. Since atomic layer deposition (ALD) is a technique of choice for deposition of thin, uniform, and conformal film growth even on structured surfaces such as trenches and via holes, there is an active search for ruthenium ALD precursors possessing appropriate physical and chemical properties, which are important for the development of a proper deposition process. There is also the need to understand the chemical interaction of these new precursors with various surfaces and the mechanism of ALD growth, requiring *in-situ* characterization.

In this study, we present *in-situ* Fourier transmission infrared (FTIR) studies of ALD growth of cyclopentadienyl ethylruthenium dicarbonyl [$CpRuEt(CO)_2$] and O_2. There is no measurable ALD of RuEt below 200°C. At higher temperatures, the RuEt begin to react with both SiO_2/Si(100) and H-terminated Si(111) surfaces. The reaction is complete at 300°C. Since the precursor decomposes at 350°C leading to CVD growth, the ALD window is very narrow. The IR spectra give clear evidence for ligand exchange and adsorption of surface species, making it possible to identify and quantify surface chemical reactions during the ALD process. IR absorption measurements also make it possible to observe the electronic absorption associated with the growth of Ru and RuO_2 films, with a transition from isolated, nucleated film to a continuous film. At that point, the absorbance is higher at lower frequencies, indicative of Drude absorption.

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Facile One-pot Synthesis of Multi-functional Hybrid Silica (MHS) Particles and Their Self-assembly to 3-Dimensional Structure

정찬윤, 구상만

한양대 화학공학과

Multifunctional hybrid particles have recently emerged as a new approach for smart materials in nano, bio, and material sciences. Various types of preparation methods for multi-functional hybrid particles have been developed and including by core shell synthesis, layer-by-layer technique, multi-block copolymer emulsification method, surface modification, and etc. As compared with single functional particles, multi-functional particles could be used for not only multiplex tasking such as multi-color imaging, selective binding, and targeting, but also 3-dimensional building block for photonic crystals and integrated circuits. Therefore, the development of a simple and efficient preparation method for particles with various types of functionalities is of great importance in order to be used in wider application.In this work, we introduce a facile preparation method for multi-functional hybrid silica (MHS) particles by self emulsion process without using any surfactant. Droplets of mixed orgno-silane monomers with phenyl, amine, and thiol functionalities were initially formed under a strong acidic condition and then homogenous MHS particles were obtained after condensation reaction in a basic condition. Two different reactive dyes, fluroescamine for amine functionality and rhodamine red for thiol functionality, were tagged to MHS particles so that the distribution of functionalities on particles was investigated. In addition, amine functionality was converted to carboxyl acid group by chemical reaction with glutaric anhydride so as to give another functional group on MHS particles. Self-assembly to 3-dimentional structure demonstrated a potential ability of MHS particles for building block through acid-base reaction between two MHS particles with different size and functionalities (one with -COOH (1.4 μm) and another with $-NH_2$ (200 nm)). We also applied self-assembly of MHS particles to patterning on amine functionalized substrate. The acid-base reaction between amine groups on the glass surface and carboxylic groups on the surface of MHS particles leads to the formation of the patterned assembly of MHS particles on the glass.

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Synthesis of one-dimensional Te nanostructure and transformation into Metal chalcogenides (MxTey)

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One-dimenstional nanostructures have been a main focus in many fields, such as electronics, photonics, and nanomechanics since they can give high potential with their use. Although a large number of solution-based methods have been suggested and demonstrated to synthesize 1D nanostructures, anisotropic growhth of semiconductor 1D nanostrucures via solution process is not easy because most solution-phase processes tend to limit the growth to zero-dimensional nanostructures in the form of spherical nanocrystallites or colloids. In this talk, we will provide synthetic routes to fabricate one-dimensional tellurium structure in aqueous and organic medium. Furthermore, the as-synthesized Te nanostructures can be a great template for the formation of various metal chalcogenide semiconductor (Ag2Te, CdTe, ZnTe, and PbTe) through cation exchange reaction. The final product transformed from the initial Te nanostructures keep their single crystallinity due to the small regime of reaction involved in this transformation.

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Synthesis and ^{129}Xe NMR Characterization of LTA Zeolite with Controlled Mesoporosity

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KAIST 화학과

A series of mesoporous LTA zeolite samples was hydrothermally synthesized by using various amounts of 3-(trimethoxysilyl)propyl hexadecyl dimethylammonium chloride as the mesopore-generating agent. The LTA zeolite exhibited a fairly narrow distribution of mesopore diameter, as indicated by N_2 adsorption isotherms. The pore diameter at the maximum of distribution shifted gradually from 6 to 10 nm with increasing the amount of the organosilane surfactant. The mesopore diameters were somewhat larger than the values that could be expected from the size of the surfactant molecules. Successive analyses of the pore diameters as synthesized, after solvent washing, and also after calcination in air revealed that the large mesopores were templated by surfactant micelles which were expanded by the excessive surfactants. The mesopores were disordered and 3-dimensionally interconnected as shown in transmission electron micrographs taken after generation of Pt nanowires. Molecular diffusion into the LTA zeolite was characterized by ^{129}Xe NMR spectroscopy after xenon was put in contact for 12 h under 1 atm at 297 K. In the case of the most highly mesoporous zeolite, the ^{129}Xe NMR spectrum clearly showed six peaks corresponding to xenon atoms located in the zeolite micropores. On the other hand, the solely microporous LTA zeolite showed no conspicuous ^{129}Xe NMR signals. This ^{129}Xe NMR experiment provided direct evidence for rapid transport of xenon into the zeolitic micropores via mesopores. The adsorption analysis revealed that the xenon diffusion into the mesoporous LTA zeolite occurred 200 times more rapidly than diffusion into solely microporous zeolite.

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Spherical nanoporous TiO_2 structure as scattering layer for high-efficiency dye-sensitized solar cells

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In recent years, dye-sensitized solar cells (DSSC) have attracted great attention due to their low cost, easy fabrication, high energy conversion efficiency and flexible device is available. In general, the bilayer structure with light scattering particle over the nanocrystalline TiO_2 film in the DSSC has been adopted widely, because it enhances the photocurrent density and the overall conversion efficiency. Herein, we developed and optimized new type bi-functional scattering materials for light scattering and charge generation. For this purpose, controlling the size of monodispersed nanoporous spherical TiO_2 structures ranging from 200 nm to 800 nm have been synthesized by altering the concentration of water in the sol-gel reaction with titanium alkoxide and modified solvothermal treatment. The prepared nanoporous TiO_2 sphere structures with high surface area were applied to scattering layer in DSSC. By introducing this scattering layer, the achieved the photovoltaic conversion efficiency was higher than that of the DSSC with commercial scattering materials such as 300 nm-sized single-crystalline anatase TiO_2 particles. By using the this bi-functional scattering materials, we achieved optimum conversion efficiency over the 10 % under AM-1.5G one sun light intensity. The correlation between scattering efficiency depend on the size of TiO_2 sphere and photovoltaic conversion efficiency were also discussed.

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Synthesis of mesoporous silica microspheres using phosphate surfactants or polymeric surfactants as a cosurfactant

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Synthesis of mesoporous sililca microspheres have drawn special interest from many researchers because the micron-sized uniform silica particles rather than the nanoparticles are more suitable in a packed-bed reactor system and a fluidized-bed reactor system. In addition, the very small nanoparticles also have the potential environmental and biological effects, and therefore the nanostructured microparticles are becoming more and more attractive to many chemist and chemical engineers. However, the synthesis of mesoporous silica microspheres via the surfactant template synthesis normally requires an expensive silica precursor or a long reaction time. The mesoporous silica microspheres prepared by using n-dodecylamine as a surfactant template in a recent report also show a heavily aggregated particles, and we have recently reported the stable mesoporous silica microspheres without any aggregation between particles successfully prepared by using n-dodecylamine as a surfactant template and bis(2-ethylhexyl)phosphate (HDEHP) as a cosurfactant. In this study, the structual properties and morphologies of nanostructured silica microspheres depending on the type of cosurfactant, the composition of the reactant solution, and other reaction conditions have been carefully investigated to elucidate the role of cosurfactants, including their potential applications in nuclear industries. Surface morphologies of the silica microspheres were significantly different depending on the type of phosphate surfactants. Phosphate surfactant with two alkyl chains rather than with three alkyl chains showed more stable pore structures as well as smoother and more stable surface morphologies regardless of the reaction conditions.

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Growth Control of t-Se Nanowires from a-Se Colloids and Array NWs in Polymer Thin Films

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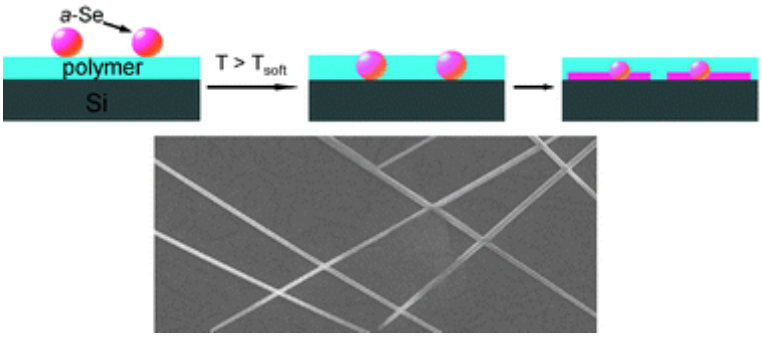
A one-dimensional nanostructure have been the subject of intensive researches, due to their potential uses as active components or interconnects in fabricating nanoscale electronic or electromechanical devices. In-situ parallel growth of NWs on the surface of solid substrates may be advantageous over handling the pre-made NWs due to its simpler process. This presentation suggests in-situ parallel growth control of NWs on the surface of solid substrates and a novel approach to fabricate arrayed NWs on the pretreated PDMS pattern in polymer thin film. The in-plane growth of the nanowires along the substrates made possible the creation of a chemically interconnected nanowire network. The t-Se nanowire can be further converted to a variety of other chalcogenide semiconductor nanowires with high carrier mobility. Since the process is solution-based and the production scale is readily enlarged, we expect the approach may find immediate industrial applications.



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Norepinephrine: Material-Independent, Multifunctional Surface Coating Reagent

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A facile approach for material-independent surface modification using norepinephrine, a small catecholamine molecule, was investigated. pH-induced oxidative polymerization of norepinephrine in alkaline aqueous media forms adherent films on virtually all material surfaces (noble metals, metal oxides, semiconductors, ceramics and synthetic polymers. Poly(norepinephrine) coatings can serve as a platform for protein bioconjugation as well as ring-opening polymerization of biodegradable polymers. Many types of materials can be modified by this surface modification strategy, which is accomplished under mild aqueous conditions via a dip-coating process.

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Template-free synthesis and characterization of hematite α-Fe2O3 nanostructures with tailored morphology

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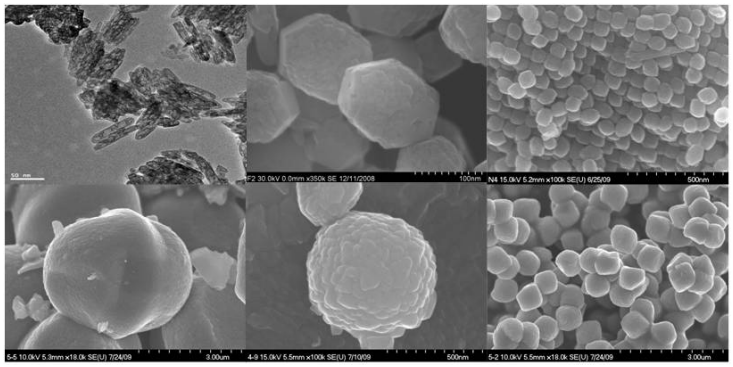
*고려대 소재화학과 *고려대 신소재화학과 **고려대 신소재 화학과*

The ability to control the structure of metal oxide materials on a nano and micrometer-length-scale and the unique properties of these materials may give rise to entirely new technologies. Assembly of one-dimensional nanostructures into two-dimensioanl (2D), and three-dimensional (3D) ordered superstructures are of great interest in the area of materials chemistry. Because different shapes and sizes are generally believed to be responsible for their widely varying properties and applications, fabrication of metal oxide architectures with controlled structures and morphologies is highly desirable. However, methods to manipulate such nanostructures often include the use of templates, which have to be removed after the reaction. Thus, to create spontaneous generation of novel patterns with tailored structures and shapes by a template-free and simple method remains a challenge. We have sucessfuly controlled the shape, size and morphology of hematite α-Fe2O3 without any template or surfactnt. Various sized rod, hexagonal-prisim, cube, hemisphere, shpere, bowl-like shape can be obtained by varying reaction parameters. We believe this synthesis method will give new insight to the development of magnetic nanostructures for the potential applications.



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Synthesis of Ultrathin MFI Zeolite with a Single-Unit-Cell Thickness

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KAIST 화학과

Zeolites are microporous crystalline aluminosilicates, which have been widely used as catalysts in petrochemistry and fine-chemical synthesis. Strong acid sites in the uniform micropores (diameter < 1 nm) enables size- and shape-selective catalyses. Despite the advantages, the sole presence of microporosity often imposes a diffusion limitation. Reactions involving larger molecules than micropores cannot be hosted by zeolites. In the diffusion-controlled regime, only the outer rim of zeolite crystals (typically synthesized in micrometer length scale) participates in catalytic reactions, leading to cokes formation and a loss of catalytic activity. Syntheses of zeolite nanocrystals, exfoliation of layered zeolites, and mesopore generation via templating strategies or demetallation processes were demonstrated as a means of reducing zeolite thickness and thereby achieving a minimal diffusion path length. In this presentation, we present a zeolite synthesis strategy using bifunctional surfactants that can direct structures in meso- and micro-length scales simultaneously. This led to direct crystallization of MFI zeolite nanosheets, in which the framework thickness corresponded to only a single unit cell dimension along b-axis (2.0 nm). Due to the large amount of acid sites on the external surface, the zeolites were highly active for catalytic conversion of large organic molecules. Furthermore, as compared with bulk zeolite crystals, the zeolite nanosheets exhibited a dramatic increase of catalyst lifetime in methanol-to-gasoline (MTG) conversion.

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화학 I 의 실험 수업에 대한 교사와 학생의 인식 조사 및 실태 분석

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*한국교원대 화학교육과 *서운고 과학실*

이 연구의 목적은 화학 I 의 실험 수업 실태를 분석하고 실험 수업에 대한 교사와 학생의 인식을 조사하는 것이었다. 이 연구를 위하여 화학 I 교수 경험이 있는 화학 교사 30 명과 인문계 고등학교 자연계열 2 학년 학생 120 명을 상대로 설문조사를 실시하였으며, 학생의 설문 결과는 학업성취 수준 및 성별에 따라 분석하였다. 연구결과, 화학 I 수업에서 실험 수업은 주로 개념 이해 및 형성을 목적으로 실시되고 있었으며, 이러한 실험 목적을 달성하기 위해 주로 결과가 잘 나타나서 학습의 이해도를 높일 수 있는 실험 주제 위주로 모둠별, 확인 실험의 형태로 실험 수업이 이루어졌다. 교사들은 학생들이 직접 실험하는 것을 통해 실험 원리나 결과에 대한 파지 효과가 보다 크게 나타날 것이라고 생각하고 있었고, 모둠별 실험을 통해 사고력 및 협동심이 향상될 것이라고 생각하고 있었다. 또한 원하는 지식을 빠른 시간 내에 더욱 쉽게 습득시키기 위하여 확인 실험을 선호하는 것으로 나타났다. 실험 수업을 통해 학습동기가 유발이 되고 화학에 대한 흥미를 가질 수 있으므로 화학 I 수업에서 실험 수업이 필요하다고 생각하는 교사의 수는 많았으나, 실제 수업에서는 입시 위주의 교육 현실, 가르쳐야 할 내용의 방대함 등을 이유로 개념 중심의 설명식 수업을 더 선호하는 것으로 나타났다. 화학 I 의 실험 수업에 대한 학생들의 인식에 있어서 성별에 따른 차이는 거의 없는 것으로 조사되었다. 학업성취 수준별로 분석한 결과, 성취 수준에 관계없이 실험을 통한 수업을 선호하는 경향이 높았으며, 상위 그룹에서 하위 그룹으로 갈수록 개념 중심의 설명식 수업을 선호하는 학생의 비율이 높게 나타났다. 상위 그룹과 남학생의 경우 탐구 실험의 형태를, 중·하위 그룹과 여학생의 경우 확인 실험의 형태를 더 선호하는 것으로 나타났다. 실험 수업의 유용성면에 있어서 교사와 학생 모두 실험 수업이 학습 동기 유발이나 기본 개념 이해에 매우 도움이 된다고 생각하나 실생활에 적용하는 능력이나 과학적인 문제해결력, STS 적인 사고를 신장하는데 있어서는 도움이

된다고 인식하는 경향이 매우 낮게 나타났다. 이러한 연구결과로 볼 때, 교사와 학생 모두 실험 수업의 필요성에 대해 깊이 인식하고 있으므로 실험 수업을 고려한 화학Ⅰ수업 시수의 조정 및 화학Ⅰ 내용의 적정화가 요구되며, 화학Ⅰ의 실험 수업에 대한 안전 교육 실시 및 실험실 현대화 등 실험 수업이 가능한 실험실 환경 여건이 마련되어야 할 것이다. 또한 학생들이 실험 수업의 목적의 다양성과 유용성에 대해 긍정적인 인식을 가질 수 있도록 다양한 목적과 형태를 갖춘 실험을 개발할 필요가 있다.

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고등학교 1학년 반응속도 학습에서 활성화에너지 도입이 학생들의 학업성취수준에 따라 개념형성과 학습만족도에 미치는 영향

최병순

한국교원대 화학교육과

6 차 교육과정에 따른 공통과학에서는 반응속도 학습에서 활성화 에너지를 다루고 있으나, 7 차 교육과정의 고등학교 1 학년 과학에서는 활성화 에너지를 다루지 않는다. 따라서 이 연구에서는 온도와 촉매 요인에 의한 반응속도변화를 설명할 때 활성화 에너지를 도입하지 않은 수업과 도입한 수업 후 학생들의 학업성취 수준별 개념 형성 정도와 학습만족도에는 어떠한 차이가 있는지 알아보았다. 연구 대상은 경기도 G 시에 소재한 인문계 B 고등학교 1 학년에 재학 중인 학생 120 명 이었다. 연구결과, 온도와 촉매에 따라 반응속도가 변화하는 이유에 대한 설명으로 활성화 에너지를 도입하지 않은 수업 후의 개념형성 정도에 대한 조사에서 학업성취 '상'수준의 학생들은 과학적 개념형성에 어려움이 없었고, '하'수준으로 내려갈수록 분자 개념에 대한 이해 부족으로 인하여 주관적인 생각에 의존하는 경향이 있는 것으로 나타났다. 또한 학업성취 '상'수준, '중'수준의 학생들은 온도에 의한 반응속도변화 이유로 주요 원인인 반응물의 에너지 변화에 의한 영향보다 충돌빈도수 변화에 의한 영향으로 생각하는 경향이 많았다. 활성화 에너지를 도입한 수업 후에는 학업성취 '상'수준과 '중'수준의 학생들에게서 온도에 의한 반응속도변화에 대한 이유로 충돌빈도수 변화에 의한 이유진술보다 활성화 에너지 이상의 에너지를 가진 분자 분율 변화로 진술하는 경우가 증가하였다. 온도에 따른 반응속도의 변화가 분자들의 충돌빈도수 변화에 의한 영향보다는 에너지 변화에 의한 영향이 훨씬 큰 것으로 볼 때, 활성화 에너지를 도입한 수업이 더 과학적인 개념형성에 도움을 주는 것으로 생각할 수 있다. 하지만 학업성취 '하'수준의 학생들은 활성화 에너지 개념을 거의 이해하지 못하고 있으며, 활성화 에너지 도입으로 인하여 오히려 개념형성에 혼란이 생기는 경우도 있었다. 활성화 에너지 개념을

도입한 수업에 대한 학습만족도 설문에서, 학업성취 '상'수준의 학생들은 과학적이고 체계적으로 이유를 진술할 수 있는 활성화 에너지를 도입한 수업에 만족도가 높았다. 반면에 학업성취 '중', '하'수준 학생들의 경우 활성화 에너지를 이해하는 데 어려움이 있는 경우가 많았으며, 이는 개념 이해의 어려움과 동시에 그래프를 이해하는 능력이 부족한 데서 오는 개념이해에 대한 자신감의 결여가 그 이유로 나타났다. 연구결과로부터 반응속도 단원에서는 7 차 교육과정에 따라 학생들의 탐구능력 향상에 목적을 두면서도 학업성취수준을 고려한 수준별 심화.보충 수업을 통하여 각 수준에서 학생들이 요구하는 수업으로 학생들의 학습만족도를 높이면 과학 수업에 대한 긍정적인 영향을 줄 수 있을 것으로 기대된다.

대 한 화 학 회
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멘토링을 통한 초임중등과학교사의 탐구지향적 교수실행 변화

고미례, 남정희, 김현옥

부산대

이 연구는 초임중등과학교사 3 명의 수업을 관찰하여 그 특징을 분석한 후 멘토링을 실시하고, 멘토링 과정에서 탐구지향적 교수실행이 어떻게 변화하는가를 보고자 하였다. 이를 위해 교직 경력 3 년 이하의 중학교 과학교사 3 명을 멘티교사로 선정하고, 멘토교사 3 명이 짝을 이루어 멘토링을 실시하였다. 멘티교사들은 각자의 학교상황과 학사일정에 따라 자유롭게 수업주제와 방법을 선택하여 총 5 차시의 수업을 녹화하였으며, 멘토교사는 멘티교사의 수업을 관찰한 후 멘토링을 통해 멘티교사들에게 지속적인 지원과 피드백을 제공하고 전문성 발달을 유도하였다. 초임 중등과학교사의 수업에서 탐구지향 수준을 알아보기 위해 ACEPT(The Arizona Collaborative for Excellence in the Preparation of Teachers)에 의해 개발된 RTOP(The Reformed Teaching Observation Protocol)을 수업분석도구로 활용하였다. 4 명의 수업분석자들이 3 명의 멘티 교사 수업들을 모두 관찰하여 교차 분석결과 상이한 부분은 여러 차례의 협의회를 통해 합의점에 도달한 후 교수관찰기록지(RTOP)를 최종 완성하였다. 멘토링 실시 전 초임중등과학교사의 수업에서 나타난 특징은 교사주도의 내용전달에 치중한 수업으로 학생들의 다양한 탐구활동이나 문제해결이 장려되지 못 하고, 학생들의 자유로운 의사소통도 부족한 것으로 분석되었다. 그러나 협력적 멘토링이 진행되는 동안 멘티교사들은 교사 위주의 설명식 수업 형태를 학생활동이 강화된 실험활동과 주제발표 및 토론 수업 등으로 다양하게 시도하는 변화를 보였다. 또한 멘토링 후반부로 갈수록 교사가 학생들의 다양한 표현을 격려하고 토론을 통해 자신의 생각과 의견을 제시해 볼 수 있는 기회를 제공하려고 노력하였다. 그러므로 교사와 학생이 함께 지식을 구성해 나가는 학습공동체 모습으로 발전하였다. 이렇나 변화의 원인은 멘토링 과정을 통해 초임과학교사들은 교과에 대한 다양한 레퍼토리를 축적해 나가는 기회를 제공 받았고, 수업내용의 단편적인 제시가 아닌 무엇을 어떻게 가르칠지에 대한 방안을

구체화시켜 나감으로써 자신감을 가지게 되었으며, 자신의 실제교수행위를 반성해 볼 수 있는 계기가 되었던 것으로 판단된다. 이러한 연구결과로 볼 때 교사양성과정에서의 과학교수학습에 관한 이론교육과 함께, 교직초기단계에서는 초임과학교사들을 교실상황 중심의 멘토링에 참여하게함으로써 교사 스스로 자신의 실제교수행위를 반성적으로 검토하게 하고, 이를 개선하고자 하는 의욕과 능력을 증진시킬 수 있는 기회를 제공해야한다. 이러한 멘토링 과정은 교사의 전문성을 향상시키는데 효과적이라고 할 수 있다.

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분자 확산에 대한 고찰과 탐구실험을 통한 예비교사의 개념변화

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이 연구에서는 확산에 대한 이해를 높이기 위해 확산을 이론적으로 정리하고, 예비교사의 개념을 바탕으로 확산을 이해하기 위한 탐구실험을 개발.적용하였다. 설문과 면담에 참여한 예비교사는 3 개 대학, 45 명이었다. 탐구실험은 이 중 한 대학에서 물리화학실험 수강생 24 명에게 수업의 일환으로 수행하였으며, 3 개 모둠에서 6 명의 실험과정을 녹음, 녹화하였다. 학생들은 실험과정에서 보고서를 작성하였으며, 이 후 관련내용이 기말고사문제로 출제되었다. 예비교사의 개념에 대한 이해를 돕기 위해 면담과 녹음자료의 전사본, 보고서와 설문지, 확산에 대한 시험 답안지를 분석하였으며, 공동연구자와 결과에 대해 논의하였다. 연구결과는 다음과 같다. 첫째, 기체의 이동과정은 다양한 방법이 존재하지만, 특히 분자의 자발적인 움직임에 의한 이동은 분출, 등압확산, 등흐름확산으로 나누어 이해할 수 있다. 둘째, 예비교사들은 분출과 확산 등을 그레이엄의 확산속도법칙에 의해 기계적으로 이해하고 있었으며 대부분의 학생들이 오인을 가지고 있는 것으로 조사되었다. 셋째, 탐구실험과정에서 예비교사들은 두 가지 확산과정에 대해 직접 관찰하였으나, 매우 빠른 평형이라는 새로운 대안개념을 제시함으로써 기존개념에 불만을 느끼지 못하고 개념변화에 실패하는 경우가 많았다. 탐구실험을 통하여 개념변화가 전부 또는 부분적으로 이루어진 예비교사는 약 40%였다. 이에 대한 교육적 시사점을 논의하였다.

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미래형 초중등 과학교과과정 모형 개발 현황

김희준

서울대 화학부

대한화학회는 한국과학창의재단이 발주한 미래형 초중등 과학교과과정 모형 개발을 주관하고 있다. 새로운 과학교육은 전 세계적인 요구이다. 뉴욕의 카네기재단과 프린스턴의 고등연구소가 중심이 되어 최근 발표한 보고서는 “너무 많은 내용을 깊이 없이” 가르치는 현 과학교육과정의 문제점을 지적하고, "우주에서 인간의 위치" 그리고 "우리는 어떻게 여기까지 왔는가?" 등의 주제를 중심으로 과학의 여러 분야를 통합적으로 교육하는 방향을 제시하고 있다. 공통과학 수준에서 거시세계와 미시세계를 통합적으로 바라보고 이해하는 관점으로 화학의 핵심 내용을 다루면 문과, 이과를 떠나 흥미를 가지고 중심 과학인 화학의 기초를 배울 수 있을 것이다. 심화 화학 과목에서는 화학의 원리들을 심도있게 다루어야 한다. 교과과정 모형 개발 중간 단계에서 현황을 보고하고 화학교육 전문가, 교사, 연구자들의 다양한 의견을 청취하여 최종 모형에 반영하고자 한다.

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국제 화학의 해와 화학 교육과 관련된 국제 학술 대회에 대한 소개

도춘호

순천대 나노신소재응용공학부

국제 화학의 해 (International Year of Chemistry (IYC)) 행사를 2011 년 전세계적으로 거행하기로 UN 과 IUPAC 에서 정하였다. 각국은 이것을 이미 준비를 시작하였다. 우리나라는 2006 년 화학의 해 행사를 치른 경험을 살려서 더욱 화학을 알리고 발전시킬수 있는 계기로 만들어야 할 것이다. IUPAC 의 화학교육위원회, 아시아화학 교육자 연맹 (Network of Inter-Asian Chemistry Educators (NICE)), 미국화학회의 연례학회중의 화학교육 심포지움, 미국화학회의 BCCE, 2010 년 Pacifichem 2010 중의 화학 교육 심포지움, 2011 년 IUPAC Congress 의 화학교육 심포지움 등 국제적 화학교육 활동을 알리고 우리나라 회원들의 참가 활동 등에 대해서 논의하고자 한다.

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화학 교육의 관심 분야

도춘호

순천대 나노신소재응용공학부

화학 교육은 매우 중요한 주제이고 다루는 범위도 매우 넓다. IUPAC, 미국화학회, NICE 심포지움 등에서 다른 심포지움 등의 제목과 발표 내용그리고 정책, 목표 등에서 우리나라 화학 교육에서 관심을 가져야 할 부분들을 살펴보고자 한다.

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중학교 과학교사들이 인식하는 탐구실험 활동을 저해하는 요인 분석

박현주

조선대 과학교육학부

The purpose of this study was to investigate middle science teachers' views on barriers in implementing inquiry-based instructions. For this, semi-structured in-depth interviews were performed with 58 middle science teachers who have served for more than five years. The data of teachers' views on barriers were categorized into external and internal factors of teachers. The study found that the external factors referred by teachers included the following: lab safety and unexpected accidents(38%), the shortage of a unit time(37%), lack of materials and equipments(25%), number of students in a class(22%), too much content to cover in a certain period for curriculum(22%), and difficulty in the assessment of students' inquiry activities(15%). Internal factors included the following: lack of self-confidence for student's learning through inquiry-based instructions, and lack of preparation for inquiry activities, lack of patience for students' activities and movements. The various barriers presented and their causes were analyzed in detail, and possible efforts in activating inquiry activities in middle science education were suggested.

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On the Formation Mechanism of Yellow Brown Color in Polystyrene Sulfonic Acid

이창훈, *고광환, 김준섭

*조선대 응용화학소재공학과 *조선대 첨단부품소재공학과*

Polystyrene sulfonic acid (PSSA) has long been known to be one of diverse precursor polymers for polystyrene-based ionomers. Our group has studied various physical properties of such ionomers including structural, mechanical signatures. Interestingly, in recent, we found the fact that the PSSA's color could be switched from white to yellow brown by temperatures used in the process of evaporating organic solvents remained. In room-temperature annealing it was white, but was changed to be yellow brown in 80 ^{O}C. In order to reproduce and identify such a phenomenon, we employed differential scanning calorimeter (DSC), thermogravimetric analysis (TGA), X-ray, UV-vis and infrared (IR) spectroscopy, electron magnetic resonance (EMR), ^{1}H nuclear magnetic resonance. In results, it can be verified as a result of a formation of SO_3^- radical in the PSSA. In connection with this, the low-field microwave absorption reported previously [1] is suggested to be originated from a possible coupling mechanism between the Zeeman magnetic energy and the rotational degrees of freedom of the SO_3^- radical in non-zero magnetic fields. [1] Chang Hoon Lee, Joon-Seop Kim, J. Appl. Polymer Sci. 11, 3355 (2008), "Apparent low-field microwave absorption properties of styrene-based copolymers containing acid groups"

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Observation of drying-induced cracks in thin film prepared from partially neutralized poly(styrene-*ran*-methacrylic acid) ionomers in DMF

고광환, *김준섭, **유정아

*조선대 첨단부품소재공학과 *조선대 응용화학소재공학과 **조선대 과학교육학부(화학)*

To understand the unexpected aggregation behaviors in poly(styrene-*ran*-methacrylic acid)[PSMAA] ionomers with very low ionic group content,[1-2] we studied partially neutralized poly(styrene-*ran*-methacrylic acid)[PSMA-Na] using a Scanning Electron Microscope(SEM). Neutralization degrees of methacrylic acid (MAA) units in PSMAA were 1%, 2% and 20%, and we kept ionomer concentration at $2x10^{-2}$ ~ $2x10^{-4}$ g/mL(CMC < 10^{-5} g/mL). For the SEM measurement, ionomer solutions were cast onto silicon wafers and dried under atmospheric conditions for 3days. Depending on drying conditions, concentration and ion content, cracks with few 10 nm-um thickness were observed. For the acid form of PSMAA and homo polystyrene, either no cracks or irregular patterns of cracks were formed. As the neutralization degree increases crack patterns became regular and the average thickness of cracks increased.[1] J.-A Yu, Y.-R. Park and J.-S. Kim, J. Nanosci. Nanotechnol. (in press).[2] J-A Yu, Kwang-Hwan Ko and Joon-Sup Kim, AsianalysisX book of abstracts, 150, 2009.

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Role of ionic groups on the aggregation behavior of partially neutralized poly(styrene-*ran*-methacrylic acid) ionomers

고광환, *김준섭, **유정아

*조선대 첨단부품소재공학과 *조선대 응용화학소재공학과 **조선대 과학교육학부(화학)*

In previous studies, we found that the content of ionic groups on the aggregation behavior of ionomers is significant even when the ionic units are less than 4 out of 10,000 repeating units(*ran*-methacrylic acid)[PSMAA][1-2]. To understand the effect of the ion content we varied neutralization levels of methacrylic acid(MAA) to 0, 1,2 and 20%. The content of acid groups was 3.6, 5.9 and 9.6 mol%, and morphological study was performed by using a Scanning Electron Microscope (SEM). Upon 1% neutralization, as previously reported result, the aggregation behavior of ionomers changed for all PSMAA samples used in this study; large spherical particles of the acid sample become contacted spheres covered with much smaller spheres (ca. 20 nm).[1] As neutralization level increases, the portion of the smaller spheres increases. In addition, when we compared particle size, 5.9 mol% behaves differently from 3.6 and 9.6 mol%. When the sample dried incompletely, smaller spheres were not shown instead large hemispheres separated by flat region. The result indicates that the ionic groups play an important role as the drying process proceeded . [1] J.-A Yu, Y.-R. Park and J.-S. Kim, J. Nanosci. Nanotechnol. (in press).[2] J-A Yu, Kwang-Hwan Ko and Joon-Sup Kim, AsianalysisX book of abstracts, 150, 2009.

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Mechanical properties of Poly(Styrene-co-3-Sulfopropyl Methacrylate) ionomer containing amphiphilic plasticizer

고광환, *김준섭

*조선대 첨단부품소재공학과 *조선대 응용화학소재공학과*

The mechanical properties of poly(styrene-co-3-sulfopropyl methacrylate) ionomers plasticized by sodium dodecylbenzene sulfonate (SDBS) were studied. It was found that the addition of SDBS decreased the ionic modulus of the ionomer. In addition, the matrix and cluster Tgs moved to lower temperatures slowly and significantly, respectively. This implied that the SDBS behaved like "cluster" plasticizer. These mechanical data were compared to the data obtained from SDBS-containing sulfonated polystyrene ionomers.

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광가교성 단량체를 이용한 새로운 전해질 고분자의 제조 및 특성 조사

김재욱, *박형석, 김종규, 공명선

*단국대 화학과 *단국대 나노바이오의과학과*

전기 전도성을 가지는 polyelectrolyte(전해질 고분자)는 센서, 연료전지 및 전색소자 등 정보화 첨단소재로서 여러 분야에 응용되고 있다. 감습막을 구성하는 전해질 고분자의 단량체 화학구조를 변화시킴으로서 흡습성이 우수하고 안정한 감습 재료가 개발되었으며 전극과의 접착성, 막의 유연성, 그리고 내수성들이 향상된 습도센서의 제조가 가능해졌다. 이러한 이온전도성 고분자는 4 차 암모늄염 형태의 친수성기를 가지고 있어 고습에서 해리되거나 급격한 swelling 현상으로 인한 성능 저하와 안정성이 저하되는 결과를 가져온다. 본 연구에서는 광가교성 단량체로는 4-benzoylphenyl acrylate 를 이용하고 감습성 단량체로는 N-[acryloyloxyethyl]-N,N-dimethylpropan-1-aminium bromide 를 이용하였다. 소수성 단량체로는 styrene 을 도입하였고, 감습막과 센서의 접착성 증진을 위하여 glycidoxy propyl trimethoxy silane 를 센서 표면과 가교결합을 하여 내수성 및 내구성이 좋은 습도센서를 제작하였다. 이러한 습도센서를 항온항습기와 impedance analyzer 를 이용하여 상대습도 대 임피던스값을 측정하여 감습특성을 조사하였다. 그 밖의 상대습도에 따른 여러 가지 습도센서로서의 특성을 조사하였다.

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New Cyclopentadithiophene-Based Copolymer Containing Electron Deficient Unit for Organic Photovoltaic Cell Applications

배영주, 김인태, 정주희

광운대 화학과

Thiophene based linear π-conjugated oligomers have their potential applications for active materials in organic electronic and photonic devices.Herein, We synthesized new conjugated copolymer containing coplanar cyclopentadithiophene units.The resulting copolymer was characterized by ^{1}H NMR, ^{13}C NMR, GPC and TGA.Electochemical and optical experiments of the resulting copolymer were observed by Uv-vis spectroscopy, PL spectroscopy and cyclovoltammetry.The resulting copolymer will be developed for the applications of polymer solar cells(PSCs).

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Preparation and Characterization of PEG Microcapsule for Sustained Drug Release Using Water-Insoluble Polymer

박정민, 박수진

인하대 화학과

In this work, alfuzosin•HCl was encapsulated using poly(ethylene glycol, PEG) mixed with Eudragit RS 100 (EuRS) as water-insoluble polymeric barrier, which was expected to be effective in preventing premature drug release. The microcapsules containing alfuzosin•HCl were prepared by oil-in-water (O/W) solvent evaporation method and confirmed by FT-IR and XRD. The morphology and particle size of the microcapsules were observed by SEM. Also, the drug release behaviors of the microcapsules with different contents of EuRS were determined by UV/Vis spectrophotometer. From the experimental we found that results, the microcapsules were successfully fabricated in all cases with 25-43 μm in size. And the drug release rate of the microcapsules was decreased with increasing the EuRS ratio, which was likely attributed to the increasing of the quaternary ammonium groups of EuRS.

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Effect of trimesic acid on thermogelling PEG-PA aqueous solutions

장지혜, 정병문

이화여대 화학나노과학과

Reverse thermogelling polymer aqueous solutions have been extensively studied during last decade. They undergo sol-to-gel transition as the temperature increases. Typically, they are aqueous solution at room temperature (20 ^{o}C) or lower, and form a semisolid gel at body temperature (37 ^{o}C) of a warm-blooded animal. In this research, we investigated that the sol-to-gel transition temperature could be controlled by adding trimesic acid by ionic complex formation.

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Enzymatically degradable polypeptide block copolymer aqueous solution

문효정, 정병문

이화여대 화학나노과학과

The aqueous solution of polypeptide in a concentration range of 3~10 wt% underwent sol-to-gel transition as the temperature increased from 10 to 50 ℃. The sol-to-gel transition temperature could be controlled by varying the molecular weight of each block, and composition. Measurement of dynamic light scattering, hydrophobic dye solubilization, and transmission electron microscope image suggest the formation of micelles in aqueous solution. The secondary structure of the polypeptides were investigated by circular dichroism and FT-IR spectroscopy. The polypeptide was degradable by elastase, chymotrypsin, cathepsinB, cathepsinC, and MMP-2 in vitro.

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Effect of Structure and Element of Novel Polyimides on LC Alignment Properties

이택준, 함석규, *권순기, 박삼대, 진상우, 김동민, 노예철, 김진철, 안병철, 권원상, 김경태, 김미희, 정정운, 고용기, 이문호

*포항공과대 화학과 *경상대 나노신소재공학부*

New organosoluble polyimides are synthesized (BBPD-ODA, BBPD-MDA, BBPD-FDA, BTPD-FDA, and BBBPAn-FDA) to study the anisotropic interactions between the oriented polymer chain segments and the LC molecules and to define the contribution of the chemical components of polymer segment to the film surface topography, the LC alignment, pretilt, and anchoring energy. We synthesized a series of new organosoluble polyimides: BBPD-ODA, BBPD-MDA, BBPD-FDA, BTPD-FDA, and BBBPAn-FDA to elucidate the anisotropic interactions between the oriented polymer chain segments and the LC molecules and to define the contribution of the chemical components of polymer segment to the film surface topography, the LC alignment, pretilt, and anchoring energy.the LC alignment, anchoring energy, surface morphology, and polymer segmental orientation results indicate that LC alignment on the surfaces of rubbed PI films is determined by the interplay between the directionally anisotropic interactions of the LC molecules with the oriented segments of the polymer main chains, and also the chemical component making up the segments of the polymer chain is significantly influencing the LC alignability of polymer chain.

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Excellent Biocompatible Brush Polymer with Phosphorylcholine Bristle Ends.

김미희, 김가희, 박삼대, 정정운, 김진철, 노예철, 안병철, 진상우, 이택준, 김동민, 권원상, 김경태, 고용기, 이문호

포항공과대 화학과

New brush polymers with various numbers of bristle ends incorporating phosphorylcholine (PC) moieties are synthesized. The polymers are thermally stable up to 175℃ and form good-quality films with conventional spin-, roll-, and dip-coating, and subsequent drying processes. These brush-polymer films exhibit excellent water wettability and water sorption whilst retaining the remarkable molecular multi-bilayer structure, and thus have hydrophilic surfaces. These novel multi-bilayer structured films repel fibrinogen molecules and platelets from their surfaces but also have bactericidal effects on bacteria. Moreover, the brush-polymer films are found to provide comfortable surface environments for the successful anchoring and growth of HEp-2 cells, and to exhibit excellent biocompatibility in mice. These newly developed brush polymers are suitable for use in biomedical applications including medical devices and biosensors that require biocompatibility and the reduced possibility of post-operative infection.

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Electrically programmable memory device with stable polyimide

권원상, 이택준, *Cha-Wen Chang, 함석규, 김경태, 박삼대, 김동민, 김진철, 진상우, 정정운, 노예철, 안병철, 김미희, 고용기, **Guey-Sheng Liou, 이문호

*포항공과대 화학과 *National Chi Nan University, Taiwan **National Taiwan University, Taiwan*

The electrically programmable memory devices based on nanoscale thin film of a thermally and dimensionally stable 6F-2TPA PI films were fabricated and investigated their switching characteristics and reliability. The 6F-2TPA PI films exhibit versatile memory characteristics that depend on the film thickness. All the PI films are initially present in the OFF state. The PI films with thicknesses in the range 34-74nm exhibit excellent WORM (i.e. fuse-type) memory characteristics with and without polarity depending on the thickness. The WORM memory devices are electrically stable, even in air ambient, for a very long time. The devices' ON/OFF current ratio is high, up to 10^{10}. Therefore, these WORM memory devices can provide an efficient, low-cost means of permanent data storage. On the other hand, the 100nm thick PI films exhibit excellent DRAM memory characteristics with polarity. The ON/OFF current ratio of the DRAM devices is as high as 10^{11}. These extreme thickness-dependent I –V results can be understood by considering the HOMO and LUMO levels and thicknesses of the 6F-2TPA PI film, the work functions of the top and bottom electrodes.These properties open up the possibility of the low-cost mass production of high density and very stable digital nonvolatile WORM and volatile DRAM memory devices.

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X-ray Scattering Studies on Molecular Structures of Star and Dendritic Polymers

진상우, *Tomoya Higashihara, *Takumi Watanabe, 이택준, 박삼대, 김동민, 김진철, 정정운, 노예철, 안병철, 권원상, 김경태, 김미희, 고용기, 이문호

*포항공과대 화학과 *Tokyo Institute of Technology*

We have studied the molecular shapes and structural characteristics of a 33-armed star polystyrene (PS-33A) and two 3rd-generation dendrimer-like star-branched poly(methyl methacrylate)s with different architectures (PMMA-G3a and PMMA-3Gb) and 32 end-branches under good solvent and theta solvent conditions by using synchrotron small angle X-ray scattering (SAXS). The SAXS analyses were used to determine the structural details of the star PS and dendrimer-like star-branched PMMA polymers. PS-33A has a fuzzy-spherical shape, whereas PMMA-G3a and PMMA-G3b have fuzzy-ellipsoidal shapes of similar size even though they have different chemical architectures. The star PS polymer's arms were found to be more extended than those of linear polystyrene. Furthermore, the branches of the dendrimer-like star-branched polymers are more extended than those of the star PS polymer, even though they have almost the same number of branches as PS-33A. The differences between the internal chain structures of these materials might be due to their different chemical architectures.

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Performance improvement of P3HT:PCBM solar cell by using water soluble conjugated polymer and nonconjugated polymer.

이준성, 박동규

경성대 화학과

A new type of P3HT:PCBM bulk heterojuncton solar cell was fabricated by using water soluble conjugated polymer (Poly(AHF-alt-PFN)) and water soluble nonconjugated polymer(PU). The device structure ITO/PEDOT:PSS/P3HT:PCBM/ Poly(AHF-alt-PFN)/ Al and ITO/PEDOT:PSS/P3HT:PCBM/PU/Al. The device has short circuit current density(Jsc) of 6.40mA/cm^2 and power conversion efficiency (η) of 1.006% without Poly(AHF-alt-PFN) layer. The device has short circuit current density(Jsc) of 8.01mA/cm^{2}and power conversion efficiency (η) of 1.943% within Poly(AHF-alt-PFN) layer. And the device has short circuit current density(Jsc) of 8.65mA/cm^2 and power conversion efficiency (η) of 2.058% within Poly(AHF-alt-PFN) layer. Also the device has short circuit current density(Jsc) of 8.5mA/cm^2 and power conversion efficiency (η) of 2.45% without PU layer. The device has short circuit current density(Jsc) of 8.09 mA/cm^2 and power conversion efficiency (η) of 2.39% within Poly(AHF-alt-PFN) layer.

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Photo- and Rubbing-Alignable Brush Polyimides Bearing Three Different Chromophores

고용기, 함석규, 이택준, 장태현, *정진철, 진상우, 박삼대, 김진철, 김동민, 정정운, 노예철, 안병철, 권원상, 김경태, 김미희, 이문호

*포항공과대 화학과 *포항공과대 재료공학과*

Three new photoreactive brush polyimides (PSPIs), each bearing a different type of chromophore (cinnamoyl (CA), 3-(2-furyl)acryloyl (FA), and methacryloyl (MA)) in their bristles, are successfully synthesized, and are found to produce good-quality films with smooth surfaces through conventional spin-casting and drying processes. These PSPI polymers are thermally stable up to 320 °C. This is the first quantitative investigation of the photoaligning and rubbing-aligning processabilities of PSPI polymer films, and of the abilities of the resultant films to control the orientation and anchoring of liquid-crystal molecules. The chromophores of both 6F-DAP-CA and 6F-DAP-FA PSPIs are found to undergo photodimerization in thin films and, to a lesser extent, photoisomerization, resulting in insoluble, crosslinked films. The MA chromophores of 6F-DAP-MA PSPI are found to undergo photopolymerization in thin films, which might include photodimerization to a lesser extent, resulting in insoluble, crosslinked films. Thin films of the PSPI polymer chains are found to have excellent unidirectional orientation ability as a result of either photoexposure with linearly polarized UV light or rubbing. Both the photoaligned and the rubbing-aligned polymer chains in the PSPI films are demonstrated to effectively induce the alignment of nematic LCs along their orientation directors by anisotropic interactions between the preferentially oriented polymer chain segments and the LCs. The contribution to LC alignment of the microgrooves developed in the rubbed films is found to be very low. The anchoring energies of the LCs on the photoaligned film surfaces are comparable to those on the rubbing-aligned film surfaces.

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발표종류: 포스터, 발표일시: 목 16:30~18:30

Crosslinkable Hole Transporting Materials for Solution Processed Polymer Light Emitting Diodes

한우택, 김인태, 이상우, 이지용

광운대 화학과

One of the most challenging tasks in fabricating multilayer Organic light-emitting diodes (OLEDs) by solution processes is to avoid the interfacial mixing between different layers because most of the commercially available emissive and charge-transporting materials are soluble in common organic solvents. To overcome this difficulty, extensive efforts have been invested in developing novel crosslinkable hole-transporting materials (HTMs). After thermo- or photo- crosslinking, all these crosslinked HTMs possess very good solvent resistance which greatly facilitates the subsequent processing of the emitting layer. As well as using the thermally cross-linked copolymer as a hole-transporting layer, solution processed multilayer light emitting diodes were prepared that exhibited performance with various optical properties. The new copolymer was characterized by ^{1}H-NMR, ^{13}C-NMR and FT-IR.

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Synthesis and Characterization of New Copolymers containing Electron-Transporting and Hole-Transporting Segments for Polymer Light-Emitting Diodes (PLEDs)

조청화

경상대 고분자공학과

Polymer light-emtting diodes (PLED) have been the subject of intense research interests due to their application in large-area flat panel displays. To achieve highly efficient PLED devices, charge (holes and electrons) injection and transport from both the anode and the cathode should be balanced at the junction of the emitting layer to yield the maximum exciton formation. So, it is important to achieve conjugated polymers which have both functions of hole/electron affinity in the single layer LEDs. In this communication, we synthesized a series of polymers with different ability and different ratios. Their photophysical and thermal properties would be investigated and further discussed.

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Biodegradable Poly(propylene carbonate) Prepared from Copolymerization of Carbon Dioxide with Propylene Oxide and its biological affinity.

정정운, 김가희, 박삼대, 진상우, 김진철, 김동민, 노예철, 안병철, 권원상, 김경태, 김미희, 고용기, 이문호

포항공과대 화학과

We synthesized poly(propylene carbonate) (PPC) films by copolymerization of carbon dioxide with propylene oxide. We investigated bacterial and cell adhesion to PPC in vitro, and biocompatibility and biodegradability in mice. Adhesion of human cells (cell line HEp-2) and five bacterial species [Staphylococcus epidermidis (S. epidermidis), Staphylococcus aureus (S. aureus), Enterococcus faecalis (E. faecalis), Pseudomonas aeruginosa (P. aeruginosa) and Escherichia coli (E. coli)] to PPC films was examined. PPC was also implanted subcutaneously in mice to assess biocompatibility by examining tissue reactions around implant sites and to assess biodegradation causing morphologic changes to the film surface. In addition, in vitro oxidative degradation tests were carried out to understand the mechanism of PPC biodegradation in mice

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Macromolecular and Supramolecular Complexation of the Anticancer Drug Paclitaxel and Cytotoxicity Study

이연주, 강희정, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*
의료시스템공학학제전공 Institute of Medical System Engineering (iMSE)

Among the anticancer drugs, paclitaxel is an important and effective representative, which is extracted from the bark of Taxus brevifolia. Although it has been shown to be highly effective for the treatment of various types of cancers, especially ovarian and breast cancer, it is very hydrophobic and, consequently, totally insoluble or only very slightly soluble in aqueous media. Thus, we applied the supramolecular concept to overcome the hydrophobicity and insolubility as well as to increase the anticancer effect by using a cyclodextrin polymer. In this study, the supramolecular polymer complexes were prepared by a solid-state reaction with the polymer and paclitaxel. The water-solubility of the resulting complexes were significantly increased and their properties were characterized by UV-vis, FT-IR, and NMR spectroscopy as well as by SEM. They were found to exhibit a pronounced anticancer effect on human breast cancer and human lung cancer cell lines in aqueous media.

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Broad absorption carbazole-based copolymers for bulk-heterojunction polymeric solar cells

정은재, *우한영

*부산대 나노융합기술학과 *부산대 나노기술대학 나노정보소재공학과*

Bulk heterojunction (BHJ) solar cells based on polymer semiconductors and fullerene derivatives give potential promise for the realization of a low-cost, easy-processable and renewable energy source. Particularly polycarbazole derivatives are attracting much attention as a photoactive structure. Leclerc and colleagues demonstrated a PCE value of 3.6% from a BHJ cell using a poly(2,7-carbazole) derivative, poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'- benzothiadiazole) (PCDTBT). PCDTBT presents two absorption peaks at 390 nm and 545 nm with an absorption valley around 450 nm. Wide-band absorption carbazole-based copolymers containing 2,1,3-benzothiadiazole (BT) and 4,7-bis(2-thienyl)-2,1,3-benzothiadiazole (DBT), were synthesized by Suzuki coupling with changing the feed ratio of DBT and BT (mol%:mol% = 50:50, 75:25 and 25:75) to fine-tune the resulting absorption and photovoltaic properties. Their optical, electrochemical, morphological and photovoltaic characteristics will be discussed.

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Synthesis and electroluminescent characteristics of carbazole and fluorene-based copolymers

남상훈, 정은재, *우한영

*부산대 나노융합기술학과 *부산대 나노기술대학 나노정보소재공학과*

Carbazole and fluorene-based copolymers were synthesized and their light-emitting characteristics were investigated. Their emission colors could be fine-tuned over the entire visible region by incorporating narrow bandgap comonomers such as 4,7-bis(2-thienyl)-2,1,3-benzothiadiazole (DBT), 2,1,3-benzothiadiazole (BT), 2,1,3-benzoselenadiazole (SeBT), 2,5-bis(4-hexyl-thiophen-2-yl)-thiazolo[5,4-d]thiazole (TZ) and 9,9-dioctyl-9H-fluorene (Fl). Synthetic approach involves the Suzuki copolymerization of alkylcarbazole diboronic ester (or dialkylfluorene diboronic ester) and the electron deficient units such DBT, BT, SeBT, TZ and Fl. The optical, photophysical, electronic properties and EL characteristics of the resulting copolymers will be discussed in detail.

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Isospecific Behavior of Lewis Base Functionalized Unbridged Metallocenes in Propylene Bulk Polymerization

윤승웅, *김화규, 도영규

*KAIST 화학과 *호남석유화학(주)*

Since the first disclosure of C2-symmetric metallocenes for isotactic polypropylene (iPP) by Ewen and Brintzinger, a huge number of metallocenes for propylene polymerization have been synthesized. Main focus of the synthesis has been centered on the increase of molecular weight and isotacticity of polypropylene by change of structure of the metallocenes. Although significantly high molecular weight and isotacticity have been attained until now, metallocenes which have complicated structures are needed for these properties. In this regard, our group recently disclosed new isospecific unbridged metallocenes which have much simpler structures than known C2-symmetric metallocenes for polypropylene. Activated by methylaluminoxane (MAO), the unbridged metallocenes showed isospecificity in propylene polymerization through the formation of in situ C2-symmetric-like cation anion pairing between Lewis basic functional groups in the metallocene and Lewis acidic sites in methylaluminoxane anion ([Me-MAO]-). As this property was investigated mainly at atmospheric pressure of propylene, in this study, brief details of polymerization behavior of these new isospecific unbriged metallocenes in bulk polymerization conditions and commercial significance of the results will be presented.

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Controlled Self-Assembly and Bio Appplication of Cyclic Peptide Building Block

정은경, *임용범

*연세대 화학과 *연세대 신소재공학과*

In aqueous solution, the spontaneous self-organization of the supramolecular building blocks is driven by noncovalent interactions including hydrophobic, electrostatic, $\pi-\pi$ stacking, and hydrogen bonding. Depending on the molecular structure of the building blocks, it has been possible to fabricate various supramolecular architectures, such as spherical micelles, vesicles, fibers, supramolecular helices, nanoribbons, and nanotubes. Especially nanostructures assembled from functional supramolecular building blocks where the bioactive function and the self-assembling segment are conjugated together are used for biotechnology like gene delivery, drug delivery, biomineralization and so on.We have designed amphiphilic molecule for self-assembly. We have used arginine peptide and fluorinated chain as for hydrophilic segment and hydrophobic segment. To conrol the nanostructure of building block, the molecule was cyclized that is expected to increase the surface area of hydrophobic part. The cyclic molecule is self assembled into vesicle structure. This vesicle structure is arginine coated. Positively charged arginine residues are cell penetrating. So the arginine coated nano capsule can be used for drug delivery system by loading the hydrophilic drug in the capsule. We have loaded calcein dye in the capsule and did intracellular delivery experiment. The calcein is efficiently delivered to the cell that is comformed by fluorescence microscopy.

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Hydrogen Bonding Mediated, Chain-Folded Lamellar Crystals of Multi-Block Polyureas Containing Oligoanilines

김택경, 박지웅

광주과학기술원 신소재공학과

Nanostructured materials with novel functional properties may be derived from conjugated oligoanilines utilizing their well-defined chain length, good solubility, controlled oxidation states, and structural design with various functional groups. In this study, the aniline heptamer diamine, whose secondary amine groups were protected with the tert-butoxycarbonyl (t-BOC) groups, was synthesized, and then polymerized with 1,12-diisocyanatododecane to produce a multi-block polymer with urea moieties. The resultant polymer exhibited good solubility in common solvents such as chloroform and dichloromethane in the presence of 20 % (v/v) of methanol. The t-BOC groups were removed by refluxing in NMP solution in the presence of a small amount of oxygen to yield emeraldine base (EB) form of the polymer. As the polymers were dried on silicon substrates from dilute solutions in the EB state, chain-folded lamellar crystals formed via folding of the chain in the alkane segments which were most likely to be driven by intra-molecular hydrogen-bonding of urea moieties. Detailed structural characterization of the polymer was carried out using atomic force microscopy (AFM), transmission electron microscopy (TEM), and small/wide angle X-ray scattering (SAXS/WAXS).

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Synthesis and Characterization of Fluorescent Magneto Polymeric Nanoparticles (FMPNs) for Bimodal Imaging Probes

박요셉

연세대 화공생명공학과

Magnetic nanocrystals (MNCs) have recently demonstrated excellent magnetic properties and low toxicity that can be applied to magnetic resonance imaging systems. [1] Also fluorescent-dye conjugated nanoparticles are representative examples of optical nanoprobe systems. [2] In a concept to develop a new type of nanoprobes which can amplify each of advantageous components, novel fluorescent magnetic poly methyl methacrylate (PMMA) nanoparticles (FMPNs) were synthesized for the application of highly efficient bimodal imaging probes; magnetic resonance (MR) and optical imaging. Nanocomposites, composed of hydrophobic lauric acid-coated 10nm MNCs embedded in fluorescent (rhodamine B) labeled PMMA nanoparticles, were fabricated in a simple way by nano-emulsion method. The obtained nanocomposites have a homogeneous size of 80 nm. In the spin-spin relaxation time (T2) weighted MR images, FMPNs solution presented high relaxivity coefficient (720.62 mM-1sec-1) because of large amounts of fabricated magnetic components on PMMA. The potential of FMPNs as optical imaging probes estimated in the microtube before and after the application of permanent magnet. Then their corresponding optical images clearly demonstrated that FMPNs produced excellent fluorescent intensities ensuring successful application as effective optical imaging agents. Conclusively, FMPNs, as bimodal imaging probes, not only demonstrated excellent sensitivity as MR probes but also produced clear fluorescent intensity as optical imaging agents.

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Preparation of graphene dispersion by exfoliation of graphite in surfactant/water medium

김진화, 오응주

명지대 화학과

In this study, water dispersions of hydrophobic graphene were prepared using various surfactants. The formation of graphene and its structure was confirmed by XRD, IR spectra, SEM and TEM images. Stability of the dispersion was confirmed by zeta potential measurement. The effect of surfactants on the properties and the stability of dispersion will be discussed.

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Synthesis of poly(3,4-ethylenedioxythiophene) using graphite oxide as a dopant and its properties

김방한, 오응주

명지대 화학과

In this study, aqueous dispersion of PEDOT [poly(3,4-ethylenedioxytiohphene)] was synthesized. In the synthesis, APS (Ammonium persulfate) were used as anoxidants and graphite oxide were used as a dopant. Transmittance and absorbance were measured by UV-Vis./NIR spectrometer and surface resistance were measured. Surface resistance measured was 10^6Ω/□ and transmittance at 550 nm appeared to be 27%. Effect of dopant on the properties of PEDOT will be discussed.

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Polypyrrole as counter electrode in dye sensitized solar cell

김기연, 오응주

명지대 화학과

In this study, polypyrrole (Ppy) was synthesized by oxidative polymerization using NSA [2-naphthalenesulfonic acid] as a dopant. To check the possibility of polypyrrole for application to DSSC as a counter electrode, electrical conductivity was measured using 4-probe method and porosity was measured by SEM. Current density of the I_3^- / I^- redox reaction peak for the Ppy electrode was measured using cyclic voltametry. DSSC with the structure of FTO / TiO_2 / electrolyte / Ppy / FTO was fabricated and its efficiency was obtained from I-V curves. From the results, the performance of Ppy as a counter electrode in DSSC will be discussed.

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Preparation of polymeric counter electrode in dye sensitized solar cell and its properties.

이상범, *오응주

*명지대 전도성 고분자 연구실 *명지대 화학과*

In this study, polyaniline (PANI) was coated on FTO by spray coating. To check the performance of PANI as a counter electrode in DSSC, electrical conductivity was measured using 4-probe method and current density of the I3- / I- redox reaction peak for the PANI electrode was measured using cyclic voltametry. In addition to, morphology of the counter electrode and adhesion between PANI and FTO were measured by SEM. From the results, potential application of polyaniline to counter electrode in DSSC will be discussed.

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Self-labeled magneto nanoprobes using tri-aminated polysorbate 80 fordetection of human mesenchymal stem cells

임은경

연세대 화공생명공학과

Self-labeled magneto nanoprobes (SLMNs) were synthesized for one-step labeling of humanmesenchymal stem cells (hMSCs) via non-invasive magnetic resonance (MR) image tracking. Thesurface of superparamagentic nanocrystals (SMNCs) were enveloped by tri-aminated polysorbate 80 (TP80) not only for enhancement of the affinity for hMSCs, but also to achieve increasedcolloidal stability in aqueous phase by the nanoemulsion method. The synthesized SLMNsexhibited excellent labeling efficiency of hMSCs and produced highly sensitive MR signals as wellas safe cell cytotoxicity.

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Anti-EGFR antibody conjugated gold nanorods for targeted imaging and photothermal therapy of epithelial cancer

최지혜

연세대 화공생명공학과

We studied a new class of targeted photothermal agents employing the PEGylated gold nanorods conjugated with Cetuximab for epidermal growth factor receptor (EGFR) specific tumor-cell targeting. The gold nanorods having an optical resonance peak in the NIR region were synthesized by the seed-mediated growth method. Then CTAB bilayer was replaced with heterobifunctional polyethyleneglycol (COOH-PEG-SH) as a biocompatible stabilizer on gold nanorods. Further, the carboxylated gold nanorods can be easily functionalized with Cetuximab to produce Cetuximab conjugated gold nanorods by using EDC-NHS chemistry. In order to assess the potential of the CET-PGNRs to serve as targeted photothermal agents, we investigated their optical properties, biocompatibility, colloidal stability and affinity for tumor cells as well as in vitro/vivo therapeutic efficacy.

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Nanoscale Thin Films of a Fully Conjugated Polymer with Memory Characteristics.

박삼대, 이택준, 진상우, 김진철, 김동민, 정정운, 노예철, 안병철, 권원상, 김경태, 김미희, 고용기, 이문호

포항공과대 화학과

This paper reports for the first time the programmable digital memory characteristics of the nanoscale thin films of a fully conjugated polymer, poly(diethyl dipropargylmalonate) (pDEDPM) in the absence of doping. This conjugated polymer was found to exhibit good solubility in organic solvents and to be easily processed to form nanoscale thin films through the use of conventional solution spin-, roll-, or dip-coating and subsequent drying. Films of the p-conjugated polymer with top and bottom metal electrodes exhibit excellent dynamic random access memory (DRAM) characteristics or write-once-read-many-times (WORM) memory behavior without polarity, depending on the film thickness. All the PI films are initially present in the OFF-state. Films with a thickness of 30 nm were found to exhibit very stable WORM memory characteristics without polarity and an ON/OFF current ratio of 10^6, whereas films with a thickness of 62-120 nm were found to exhibit excellent DRAM characteristics without polarity and an ON/OFF current ratio as high as 10^8. These memory characteristics are governed by trap-limited space-charge limited conduction and heterogeneously local filament formation. In these polymer films, both the ester units and the conjugated double bonds of the polymer backbone can act as charge trapping sites. The excellent bistable switching properties and processibility of this conjugated polymer mean that it is a promising material for the low-cost mass production of high density and very stable digital nonvolatile WORM memory and volatile DRAM devices.

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Electrochemically Active Vesicles, Reversible Redox Control

김훈, 박지웅

광주과학기술원 신소재공학과

We report the formation of electrochemically active vesicles by the rod-coil polymer consisting of a tetraaniline (TANI) block and a polyethylene glycol (PEG) block. TANI-b-PEG550 was synthesized by coupling of TANI and polyethylene glycol monocarboxylic acid. Transmission electron microscopy (TEM) indicates that the rod-coil form the vesicular aggregate in aqueous solution. The aggregation size in the LEB state is bigger than those in the EB state with tens of nanometers, which were confirmed by dynamic light scattering (DLS). The redox states of vesicles as well their corresponding size were reversibly controlled by external potential at -0.2V and 0.6V, respectively. The redox cycles were also confirmed by UV/Vis absorption spectra. Detailed characterization of the vesicles will be presented. This work was supported by the Program for Integrated Molecular Systems (PIMS) at Gwangju Institute of Science and Technology and the Korea Science and Engineering Foundation (KOSEF) grant (R01-2008-000-12246-0) funded by the Korean Government (MEST).

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Preparation of calcium alginate from sodium alginate in presence or absence of additive & their characterization

윤정호, Tara Sankar Pathak, *백대진, 팽기정

*연세대 화학과 *한서대 화학과*

Alginates are linear unbranched biopolymers containing β-(1→4)-linked D-mannuronic acid (M) and α-(1→4)-linked L-guluronic acid (G) residues. Naturally occurring biopolymers like alginate have been known to exhibit excellent adsorption ability for metal ions. Alginic acid converted into the metal alginate is confirmed using FTIR spectroscopy. In presence of additive (PVA & PVP mixture), total intrusion volume of calcium alginate (0.0077 mL/g) is lower compared to blank calcium alginate (0.0097 mL/g) i.e prepared without additive. The presence of additive also affects the porosity % and pore size distribution of calcium alginates. Thermal degradation of calcium alginates prepared in presence or absence of additive showed a stepwise weight loss during thermal sweep, indicating different types of reactions during degradation.

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Facile and Versatile Method for Heparin Coating Inspired by Mussel

유인성, *강성민, 이해신

*KAIST 화학과 *KAIST 화학과*

Heparin immobilization on the surfaces has gained a great deal of attention in the development of biomedical devices such as catheters, grafts, implants and stents for enhancement of blood compatibility. However, existing methods for heparin immobilization have some limitations in practical use; complexity of surface modification and lack of versatility for heparin coating due to chemical specificity of interfacial modifiers with heparin and surfaces. In this work, we conjugated dopamine to heparin in order to develop a facile and versatile method for heparin coating. Dopamine was conjugated to heparin after activation of carboxylic groups of heparin, and the reaction was confirmed by UV-Vis spectroscopy and FT-IR spectroscopy. For investigating the effect of the dopamine-conjugated heparin, it was coated on metal and polymeric surfaces, and bioactivity of the surface was evaluated by protein adsorption and cell adhesion test.

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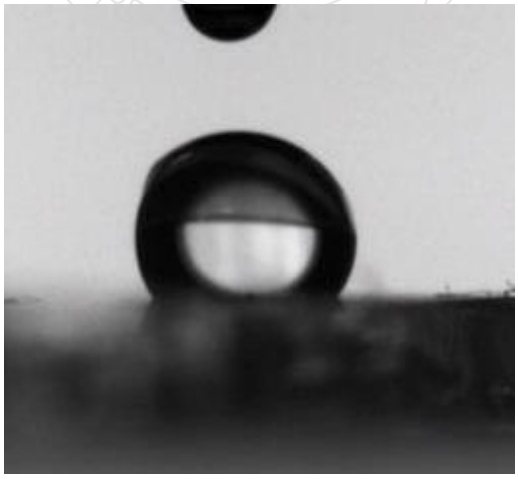
Hybrid organic-inorganic coatings with phosphonate functionalities on glass

박연화, 안용현

단국대 화학과

Superhydrophobic surface have been focused for self-cleaning properties. Water drop onsuperhydrophobic surface remains spherical and roll off easily. In order to obtain superhydrophobic surface on solid substrates, we synthesized diphosphate alkane and prepared the hybrid organic-inorganic sol-gel. We are investigating wet chemical method such as dip coating and obtained surface with a water contact angle of 150°.In this poster, we will present the synthesis of substrate, preperation of sol-gel and analysis of modified surface with SEM, NMR.



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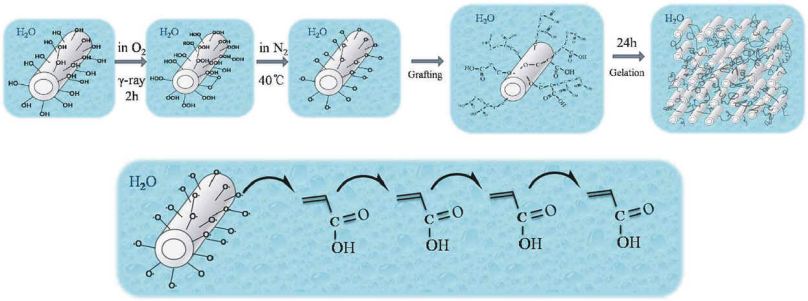
Synthesis and Characterization of Rod/Polymer Hybridgel

이호익, 구준모, 손대원

한양대 화학과

Imogolite has new attention as a new nano-scale material because of its unique nano-scale tubular structure similar to that of a single-walled carbon nanotube. Imogolite is a hollow nanotube which has hydrous aluminosilicate with a chemical formula of $(HO)_3Al_2O_3SiOH$. We reported easy way of synthesizing hydrogel by ramma-ray. The hydrogel was directly prepared by polymerization on hydroxide surface of imogolite. When particles are irradiated with ^{60}Co gamma-ray at ambient condition, the surface is changed to peroxide acting as both an initiator and a cross-linker. The hydrogel was made from a mixture of peroxideized imogolite and acrylic acid.We have researched for increasing specific surface area and the property of gas storage ability. We measured specific surface area by BET method, and confirmed the property of gas storage ability by BELSORP-HP.



Scheme 1. Formation mechanism of the Imogolite-hydrogel.

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Synthesis and Characterization of New Selenophene Based Polymers for Organic Thin-Film Transistors

이우형, *공호열, *심홍구, 강인남

*가톨릭대 화학과 *KAIST 화학과*

In the presentation, we report the syntheses and electrical properties of the selenophene based polymers. These polymers, poly(3,3-alkylterselenophene) (P1), poly(3,3-alkylquaterselenophene) (P2) and poly(3,3-alkylquaterselenophene-co-biselenophene) (P3), were synthesized via Yamamoto and Stille coupling reaction. The synthesized polymers were well dissolved in common organic solvents, such as chloroform, THF and chlorobenzene due to the incorporation of the long alkyl side chains in the polymer backbones. Thin solid films of P1, P2, and P3 exhibited the UV-visble absorption maxima at 566, 584 and 532 nm, respectively. And the optical band gap (eV) of the P1, P2 and P3 showed 1.73, 1.74 and 1.75 eV, respectively. The field-effect transistors using the polymers as a channel layer were characterized.

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Synthesis and Properties of Photocurable Biphenyl Modified Aromatic Acrylates

김백선, *김동국, 고윤석, **김지은

*한양대 응용화학과 *한양대 화학과 **한양대 응용화학*

최근 디스플레이 제품은 LCD, LED 등 점점 얇고 가볍게 변모되고 있으며 거기에 장착되는 BLU(Back Light Unit)도 얇고 가벼운 Light 방식으로 발전하고 있다. 이에 따라 BLU 에 고휘도 필름이 요구 되어지면서 고굴절 원료에 대한 관심이 상당이 집중되고 있다. 이중 고굴절 원료인 바이페닐계의 아크릴레이트가 각광받고 있으며 이에 대한 이용도가 증가될 것으로 보고 있다. 본 연구에서는 이러한 바이페닐계의 아크릴레이트인 하이드록시 페닐페놀 아크릴레이트에 이소시아네트를 도입하여 광경화형 바이페닐 아크릴레이트를 합성하였다. 이소시아네이트별로 합성된 바이페닐 아크릴레이트의 각각의 굴절률과 점도 변화를 조사하였다. 또한 합성된 바이페닐 아크릴레이트에 페녹시아크릴레이트를 희석하여 광개시제인 2-hydroxy-2-methyl-1-phenyl-1 propanone 을 혼합, 자외선을 이용하여 광경화 특성을 조사하기 위해 경화된 필름을 제조하였다. 경화된 필름은 바이페닐 아크릴레이트의 구조에 따라 나타나는 경도, 내마모성, 인장강도, 신장율 등의 물성을 조사하였다.

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Synthesis and investigation of [1,3]oxazine based pH switching ionic valve

PK JOUSHEED, 홍종달

인천대 화학과

Polyelectrolyte multilayer (PEM) films layer-by-layer deposited on porous supports have been potentially investigated as membrane skins for selective ion separation applications. The PEM films are known to possess high selectivity of ions due to Donnan-exclusion effect in comparison with conventional polymer membrane. The development of stimuli-responsive or switchable membrane is important for technical applications such as filtration system, membrane-based separations, and sensors. In this study, a PEM membrane was functionalized with [1,3]oxazine derivative that can act as a valve for ion permeation. [1,3]oxazine derivatives are known to have pH and photoresponsive properties by UV-Vis irradiation and pH change. Here we demonstrate a pH switch for controlling ion permeation with the PEM films, which was dip coated on porous alumina support. At different pH condition, the PEM membrane functionalized with [1,3]oxazine show different permeation rates. Surprisingly we found that the charge of ions has dominate effect on the mass transport in acidic condition (at pH 2.50) over the ionic size.

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The variation of specific surface area of Imogolite dependent on carbon/carbon + silicon ratio

정재우, 양정윤, 손대원

한양대 화학과

Aluminosilicate nanotubes as Imogolites were synthesized in Lab. In previous our work, we measured a variation of specific surface area of pure-Imogolite and outer surface modified-Imogolite. So, we also measured different sample like inner elements substituted Imogolite for confirmation of porous property.We synthesized inner elements substituted Imogolite by different carbon ratio instead of silicon. And carbon substituted Imogolites were confirmed by powder X-ray diffraction (powder XRD), and Fourier transform infrared (FT-IR) spectroscopy. Their morphology variations were also investigated by transmission electron microscopy (TEM) and images analysis. At last, we determined porous properties of carbon substituted Imogolites (different ratio) using BET methods with N_2/77K adsorption isotherms. The specific surface area of the carbon-imogolites (C/C+Si=0.5) was 282.71 (m^2/g) and carbon-imogolites (C/C+Si=1) was 207.77 (m^2/g).

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Biodegradable, injectable, *in-situ* polymerizable polymer networks based on PCL and amino acid

김수연, 정일두

부산대 고분자공학과

Degradable synthetic polymers have found diverse applications in medicine ranging from resorbable vascular grafts to tissue-engineering scaffolds. However, these polymers have limited applications in such areas as *in situ* orthopedic bone filling and fixation or soft-tissue repairs. To be used in orthopedic applications, it should have the properties that possess a liquid- or putty-like consistency that can be easily polymerized and molded to any shape under physiological conditions. In this work, novel biodegradable, injectable and *in situ* crosslinkable polymer networks based on hydroxyl polycaprolactone acrylate and acryloyl glutamic acid were synthesized and characterized. The polymer networks and their composites with β-tricalcium phosphate(β-TCP) were prepared by photo- and redox polymerization, respectively. The composites with different formulations were prepared and their properties were investigated.

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Effects of dendrimer as adsorbent on dye-sensitized solar cells

신봉하, 원종옥

세종대 화학과

One main reason for the low performance of dye-sensitized solar cells (DSSCs) is a recombination at the surface of TiO_2. Since recombination can be reduced by blocking the bare TiO_2 surfaces with adsorbent, we studied the effect of adsorbent on DSSC using different generation of dendrimers. DSSCs were prepared with 13nm sized TiO_2 nanocrystalline, $RuL_2(NCS)_2$:2TBA (L = 2,2'-bipyridyl-4,4'-decarboxylic acid, TBA = tetrabutylammonium) (N719) as a dye, and 1-methyl-3-propyl imidazolium/I_2/acetonitrile as a liquid electrolyte. The size effect of the dendrimer was investigated by the DSSCs performance.

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POSS® 첨가에 따른 epoxy 접착제의 기계적, 물리적 특성 연구

이영선, 민정식, 원종옥

세종대 화학과

Polyhedral oligomeric silsesquioxane (POSS®) 는 $(RSiO1.5)_n$ (n=8, 10, 12) 의 실리콘과 산소를 기반으로 이루어진 무기계열 입방면체로 내부가 core 형태이고, 외부엔 유기 계열의 작용기들로 둘러쌓인 구조를 가진 유기-무기 혼성화합물이다. epoxy 기를 갖고 있는 POSS®는 외부에 유기 계열의 작용기를 도입함으로써 유기 물질과의 친화력을 증가 시켜 다양한 유기 계열의 고분자들과도 분산이 잘 되는 장점이 있다. 이러한 장점을 가진 POSS®를 다른 epoxy 수지와 혼합하여 사용함으로써 기존의 epoxy 수지가 가진 문제점을 보완하는 연구를 진행하였다. HBA 는 Bisphenol-A 계열의 epoxy 인데 벤젠 고리에 있는 이중 결합을 완전히 수소화시킴으로써 기존의 Bisphenol-A 형 epoxy 수지의 단점인 자외선을 받으면 색이 변하는 황변 현상이 일어나지 않기 때문에 epoxy 수지로 선정했다. 사용한 POSS®들로는 Cyclohexyl epoxy 기를 가진 EP0408 과 한 개의 Cyclohexyl epoxy 기와 나머지는 I-butyl 기로 치환된 EP0402, Glycidyl 기를 가진 EP0409, 한 개의 Glycidyl 기와 나머지는 I-butyl 기로 치환된 EP0418 를 사용하여 0~30wt.%의 POSS® 의 첨가량을 다르게 하고, HBA 와 POSS®를 혼합하여 사용, 접착제의 성능을 측정하였다. 경화제로는 무색 투명하여 접착부분의 색상을 파괴 하지 않는 poly(propylene glycol) bis(2-aminopropyl ether) 을 사용하였다. FT-IR 을 사용하여 평균 경화시간이 72 시간이라는 것을 확인하였고, 색 투명도, 인장강도, 압축강도, 굴곡강도, 압축전단 접착강도를 측정하여 POSS®의 첨가량과 비율에 따른 기계적 성질을 분석 하였다.

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기능성 POSS®를 이용한 에폭시 수지 접착제의 개발 및 특성 연구

윤일녕, 강덕기, *김정진, 원종옥

*세종대 화학과 *안동대 지구환경과학과*

에폭시 접착제의 기계적 강도를 증가시키기 위해 에폭시 기능기를 갖고 있는 Polyhedral Oligomeric Silsesquioxane (POSS®)를 이용하여 새로운 에폭시계 접착제를 개발하였다. 투명성 및 시간에 따른 색 안정성을 위해 에폭시의 주제는 bisphenol-A 를 수소화시켜 이중 결합을 제거한 형태인 hydrogenated-bisphenol-A(HBA)를 선정하였고, amine 계열의 투명한 경화제인 Isophorone-diamine (IPDA)를 사용하여 경화시켰다. Epoxy 작용기를 가진 POSS® 중에 epoxycyclohexyl 기를 가지고 있는 POSS® EP0408 과 glycidyl 기를 가지고 있는 액상 형태의 POSS® EP0409 를 다양한 조성으로 연구하였으며, epoxycyclohexyl 기와 glycidyl 기를 각각 가지고 있는 분말 형태의 POSS® EP0402 와 EP0418 를 혼합하여 총 4 종류의 POSS®를 이용하여 연구하였다. FT-IR spectrum 을 이용하여 경화 시간을 확인하였으며, 각각의 기계적 특성을 파악하기 위해 인장강도, 압축강도, 굽힘강도, 압축전단강도를 측정하여 성능을 비교하였고, 이를 화강암에 사용하여 접착강도와의 관계를 확인하였다.

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Solution-processable acene derivatives for organic field-effect transistors

권제호, *박성연, 김태동, *이광섭

*한남대 신소재공학 *한남대 신소재공학과*

Much progress on organic field-effect transistors (OFETs) has been made in various organic-based electronic circuits, such as displays, sensors, inverters, and logic elements. Currently, the best values of the field-effect mobility ( ) of OTFT devices based on vacuum-deposited polycrystalline small molecules are in the range of a few cm2V-1s-1. Acene-type molecules consisting of a fully extended π conjugation system have shown excellent OTFT performances but have been still necessary to pursue suitable molecular engineering for solution processability and good film forming properties in OFET applications. In the presented work we have designed and synthesized a series of new acene derivatives and characterized their OTFT properties in various conditions.

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Pseudo gel 전해질을 이용한 DSSC 성능 연구

강덕기, 유순동, 원종옥

세종대 화학과

Dye-sensitized solar cell (DSSC) 에 사용되는 액체 전해질의 주요 단점인 누액현상을 막고 long term stability 를 향상시키기 위해 공중합체 물질인 triblock copolymer 를 ionic liquid (IL) 와 iodine 으로 이루어진 액체 전해질에 첨가하여 pseudo-solid 형태의 ionic gel 전해질을 제작하였다. Triblock copolymer 는 5wt%의 시료만으로도 solvent 와 함께 mixing 으로 간단한 solution 을 형성하고, 70℃ 의 vacuum oven 에서 solvent 를 증발시켜 ionic gel 을 형성하는 등 사용되는 시료의 양이 적고 제작과정이 단순하다는 장점이 있다. 또한, copolymer 를 구성하고 있는 poly(ethylene oxide) 의 조성비에 따라 종류가 다른 두가지의 triblock copolymer 는 각기 free standing 형태와 film 형태의 ionic gel 을 형성하기 때문에 각각의 특성을 살려 DSSC 에 도입한다면 pseudo solid 전해질로써의 충분한 가능성을 기대할 수 있다. 1-methyl-3-propylimidazolium (PMII) 과 Iodine 의 몰비율이 12:0.5 로 구성된 전해질에 5wt%의 triblock copolymer 를 첨가하여 이를 Ruthenium 535-bis TBA (N719) 과 13nm sized TiO_2 DSSC 에 도입하고 J-V curve 을 측정하여 액체 전해질과 pseudo-solid 전해질의 성능을 비교하였다.

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Supported ionic gel membranes for CO_2 separation

유순동, 원종옥

세종대 화학과

Supported ionic liquid membrane (SILM) for CO_2 separation has long term stability over conventional supported liquid membranes due to the negligible vapor pressure of ionic liquids. However SILM has a problem in practical application due to the formation of defects at relatively high operation pressure. In order to improve the long term stability as well as the mechanical strength of the selective ionic liquid layer, we prepared supported ionic gel membrane by the formation of ionic gel on the surface of Nylon support (Magna Nylon membrane filter by Osmonics). The ionic gel was prepared by the addition of poly(styrene-block-ethyleneoxide-block-styrene) triblock copolymer in 1-hexyl-3-methylimidazolium hexafluorophosphate ([hmim][PF_6]) using methylenechloride as a solvent. Four different gases (CO_2, N_2, O_2 and CH_4) permeance were measured at room temperature and the membrane morphology was investigated. The ideal selectivity of CO_2/CH_4 was 11.8 for supported ([hmim][PF_6] gel membrane, which is lower than that of SILM.

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Anthracene-type fluorescent crack sensors in polymeric materials

조성열, *김중곤, 정찬문

*연세대 화학과 *한화석유화학(주) 바이오연구센터*

Anthracene and its derivatives have been studied extensively in the fields of photochemistry. Photodimerization of anthracene is one of the oldest known photochemical reactions and a classical example of photocycloaddition. Since the fluorescence properties of an anthracene-type monomer and its dimer are different from each other, if the dimer returns to its monomer by mechanical cleavage upon cracking, the dimer structure is applicable as a crack sensor. A novel anthracene-type monomer, AHME, was synthesized and polymerized. The photocrosslinking of polyAHME was investigated by UV-*vis* spectroscopy, photoluminescence spectroscopy and ^{1}H NMR. The crosslinking of polyAHME were confirmed by ^{1}H NMR. Fluorescence microscopic images of microcracks in the polymeric material were obtained. In this work it was demonstrated that an anthracene based polymer could be used as a crack sensor.

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Photochromic- and thermochromic properties of PDA-based liposomes

최혜, 안난영, 심영정, 최준식

충남대 생화학과

Polydiacetylene(PDA) shows unique color transition by various stimuli such as heat, pH, and solvent. After the color of PDA liposome was switched from blue to red, we also measured the fluorometric properties. Polyethylene glycol(PEG) is a polymer which is commonly used for various applications due to high water solubility, biocompatibility, and low immunogenicity. In this report, we prepared various concentrations of PEG-PDA based liposome and induced the color transition properties by applying some external stresses, such as polycationic polymer, α-cyclodextrin, and heat. The photochromic properties were measured by UV/vis spectrophotometer and the fluorescence was measured by spectrofluorometer.

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Fabrication of printable single crystal micro/nano silicon structures for flexible electronic devices

양유미, 고홍조

광주과학기술원 신소재공학과

Printing technology using organic/inorganic electronic elements onto a plastic or a rubbery substrate is one of the key processes to realize flexible electronic devices. Among them, dry-transfer-printing method via a slightly sticky platelet such as polydimethylsiloxane (PDMS) enables the transfer of key elements from a wafer to a plastic substrate. The important step in the method should be 'how we can make easily transferable elements of a donor substrate?'. The common process is to use the structure of electronic elements on the sacrificial layer which provide easy detachment of the elements after etching. In this study we propose a simple and powerful method to fabricate printable element structure with high transfer efficiency using post in the edge of the elements. The posts prevent not only misalignment of elements but also total sagging down of Si isolation which causes poor transfer yield. This method provides high transfer yield (> ~99%) with no dependence on thickness of the top silicon. We believe this strategy will give a powerful processing aspect in the flexible electronics based on Si wafer and others.

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Synthesis and Characterization of Polyethylenimine-grafted Polydiacetylene Liposome

심영정, 이혜원, 최혜, 최준식

충남대 생화학과

Polyethylenimine(PEI) is one of the most widely studied as a non-viral gene carrier. In this report, polycationic PEI was grafted onto the surface of PDA liposome which can be used as a liposomal vector for gene delivery. Polydiacetylene(PDA) liposome system has been widely studied for biosensor applications using the colorimetric or fluorescent transition properties of PDA under various conditions. When the specific wavelength of UV was irradiated, the PDA monomers were polymerized and the blue color has appeared as the polymerized backbone is constructed. The construction of PEI-grafted PDA liposome and formation of complexes with plasmid DNA was characterized by 1H-NMR, dynamic light scattering, and zeta-potential measurement. The PEI-grafted PDA liposome system is expected to be an efficient gene carrier system with low cytotoxicity.

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Photoconversion of *o*-hydroxycinnamates to coumarins and its application to fluorescence imaging

송영규, 조성열, *김중곤, 정찬문

*연세대 화학과 *한화석유화학(주) 바이오연구센터*

(E)-o-Hydroxycinnamates were synthesized and their photochemical behavior was investigated in liquid and solid states. It was confirmed by ^{1}H NMR spectroscopy that the *(E)-o*-hydroxycinnamates converted into the corresponding coumarins via *(Z)-o*-hydroxycinnamate intermediates. The photoconversion was greatly accelerated in the presence of *p*-toluenesulfonic acid. The optical properties of the cinnamates were compared with those of the corresponding coumarins. Fluorescence imaging was successfully accomplished by photoirradiation of PMMA films containing the cinnamates.

KOREAN CHEMICAL SOCIETY

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Preparation and Characterization of Nanoporous Thin Films of Alicyclic Polyimides

유환철, VIJAY S. WADI, 조성열, *김중곤, **Kazuaki Kudo, 정찬문

*연세대 화학과 *한화석유화학(주) 바이오연구센터*
***Institute of Industrial Science, The University of Tokyo*

It is required to develop insulating materials with low dielectric constants for achievement of high integration and speed in semiconductor.1 In this work ABA-type triblock copolymers consisting of an aliphatic polyimide block and a thermally labile polymer block have been prepared from an alicyclic dianhydride, four alicyclic diamines, and an amine-terminated poly(propylene glycol) (PPG).2 Rel-[1S,5R,6R]-3-oxabicyclo[3,2,1]octane-2,4-dione-6-spiro-3'-(tetrahydrofuran-2',5'-dione) (DAn) was used as the alicyclic dianhydride.3 The thermal properties of the copolymers were investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Thermal decomposition of the labile block in the copolymers was carried out to obtain porous polyimide films, which were characterized with a scanning electron microscope(SEM).

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Study of diffusion in PLA polymer by DOSY NMR

임성철, 정민환, 조혜성

LG화학기술연구원 CRD연구소

Pulsed field gradient spin echo NMR is generally the method of choice for diffusion measurements on liquid samples. An attractive technique is to characterize mixtures without first having to separate the components. DOSY(Diffusion Ordered Spectroscopy NMR can yield quite useful analytical information. A careful choice of DOSY NMR experiment and its processing strategy is required to obtain optimum results. In this study, PLA polymer is prepared to investigate the spectrums obtained from PLA polymer and its lactide monomer. Through the study we can confirm the seperation of lactide monomer and PLA polymer spectrum peaks.

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Hydrophobic modification of poly(amidoamine) dendrimer and its application to gene delivery carrier in vitro

유광식, 유하나, 최윤희, 최준식

충남대 생화학과

In this study, we prepared poly(amidoamine) dendrimer derivatives conjugated with 6-aminohexanoic acid and amino acids. The 4th generation of poly(amidoamine) dendrimer was used because it displays relatively good transfection efficiency and low cytotoxicity than other generations. 6-aminohexanoic acid was selected as a spacer molecule to enhance the hydrophobicity. Because they have six carbon chain in their structure, it is expected that conjugation of 6-aminohexanoic acid into poly(amidoamine) dendrimers could enhance their hydrophobicity. Also, further modification of the poly(amidoamine) dendrimer derivative with amino acids. The transfection efficiency of the derivatives was evaluated by luciferase assay and the cytotoxicity was assessed by EZ-Cytox reagent based on WST-1 method.

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Preparation of Pore Size Controllable Macroporous Poly(methacrylic acid-co-methyl methacrylate) (PMAA-co-PMMA) Bead

박주영, 전봉현, *강호만, 이윤식

*서울대 화학생물공학부 *서울대 협동과정 나노과학기술전공*

Macroporous polymer beads have been used in various fields as solid supports in solid-phase organic synthesis and combinatorial chemistry, adsorbents in column chromatography, and etc. Such broad applications have stimulated many researchers to develop macroporous polymer bead. However, despite of a lot of efforts, it is still hard to control the porosity and the pore size distributions within the polymer beads by previously reported methods.In this study, we prepared silica nanoparticles (NPs) embedded poly(methyl methacrylate) (PMMA) beads by polymerization of methyl methacrylate monomer with mono dispersed silica NPs. Then, the silica NPs embedded PMMA beads were hydrolyzed with sodium hydroxide for obtaining macroporous structure by removing the embedded silica NPs. At the same time, part of methyl methacrylate turned to methacrylic acid, which led PMMA beads to macroporous poly(methacrylic acid-co-methyl methacrylate) (PMAA-co-PMMA) beads. By this method several beads that have different pore size were prepared. The pore size of the beads could be easily controlled by controlling silica NP's size.

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Delivery of siRNA using cell penetrating peptide modified silica particles

김희석, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

One of the fundamental issues for gene therapy in gene delivery system is how to deliver siRNA, which inhibits the adverse gene expression, into normal cells. We synthesized FITC incorporated silica nanoparticles having various sizes (from ~200 nm to ~800 nm) and modified their surfaces with HIV-1 trans-activator factor (TAT) peptides, which are known as very efficient cell penetrating agents. Previously, We found that most of the nanoparticles could penetrate into the cytoplasm of the cells, regardless of their sizes. In this presentation, we prepared the silica nanoparticles attached with Alex305 labelled siRNA together with TAT peptides and observed the particles are internalized into the mammalian cells. Finally, we will discuss the effectiveness of siRNA-mediated gene silencing effects using TAT-modified particles.

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Synthesis and Characterization of a novel p-type polymer based on Thiophene for organic thin film transistor(OTFTs)

KANG PENGTAO

경상대 고분자공학과

A new p-type polymer was synthesized by the Suzuki coupling reaction. The monomers were prepared with highly overall yields and the obtained polymer is confirmed by elemental analysis, 1H NMR, 13C NMR, FT-IR, UV absorption, photoluminescence (PL), and cyclic voltammetry (CV). The polymer contains alkyl-substituted thiophene and we are expected to have a high solubility by introducing the alkyl-chain. Furthermore, the introduction of the alkyl chain can increase the degree of orderness by self-assembly. The thermal property of polymer was confirmed by using the thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The polymer was showed 5% weight losing temperature at 401.89 oC. The number-, weight-average molecular weight of the polymers were 9814 and 18817, determined by gel permeation chromatography (GPC) using polystyrene standards for calibration in the eluent THF. The band-gap of polymer is 2.01 eV and the HOMO is 5.37 eV.

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A Study on the Synthesis and Properties of Novel Silicon Containing Polybenzimidazoles

이석영, 윤국로, 이수민

한남대 화학과

Polybenzimidazole (PBI) was widely used in astronauts space suits, firefighters protective clothing and electrically conductive materials.1 The silicon containing monomers that the acid dichlorides bis(4-chlorocarbonylphenyl)diphenylsilane (DCPS) and bis(4-chlorocarbonylphenyl)di-methylsilane (DCMS) were synthesized by a previous report.4 Novel PBIs containing DCPS/ DCMS were synthesized by polycondensation with suitable aromatic tetraamines at temperatures around 250℃. We attempted synthesis of stable polymers possessing Si atom in the main chain expected higher values of thermal and mechanical parameters due to the higher ionic character of the C-Si bond compared with the C-C bond, and due to the lower size of the Si atom that presents lower rotational barriers.2,3 The resulting polymer was characterized by infrared spectroscopy, 1H NMR spectroscopy and GPC. The glass transition temperatures and the thermal stability were determined by TGA and DSC.

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High-Performance n-Type Organic Thin-Film Transistors Using Solution-Processable C60 Derivatives

남선영, *김신태, *이성형, 김태동, *이광섭

*한남대 신소재공학 *한남대 신소재공학과*

Organic thin-film transistors (OTFTs) have shown great potential in various electronic applications, such as low-cost, light-weight, large-area, and flexible panels/circuits. Much of the work carried out on p-type OTFTs has focused on designing new organic molecules suitable for solution processing, that is, stable under ambient conditions with a high charge mobility. Despite significant progress in p-type OTFTs, only a few n-type semiconductors have been reported so far due to their poor OTFT performance. Here we report new C60 derivatives, which contain an alkylated thiophene unit, for solution-processable n-type OTFTs. More importantly, we have fabricated high-performance n-type OTFT devices by means of the ink-jet-printing method. The fabrication process was carefully optimized in order to achieve a uniform morphology and the desired molecular orientation.

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Crosslinkable Polymers containing Sulfonated Poly(ether sulfone) and Poly(phenylene phthalamide) segments for the Preparation of PEMFC Membrane

정현진, 김정민, *조창기

*한양대 섬유고분자공학과 *한양대 응용화공생명공학부*

Nafion membrane is presently the major membrane used in polymer electrolyte membrane(PEM) fuel cells. However, application of Nafion membrane is limited by relatively high methanol permeability, high cost, and loss of membrane performance at elevated temperatures. So it is very necessary to find out novel proton conductive membranes with low cost and low methanol permeability. Recently, crosslinked polymer membranes have been studied extensively for low methanol permeability, water uptake, and swelling ratio. Aromatic polyamides such as poly(p-phenylene terephthalamide) (Kevlar), poly(m-phenylene isophthalamide) (Nomex) show high temperature stability and strength, so they are attractive in many applications. In this study, sulfonated poly(phenylene ether sulfone) and m-phenylene isophthalamide or p-derivatives were copolymerized in the presence of end capping agents to prepare crosslinkable prepolymer and to check the possibility as membrane materials for fuel cell application. The prepared proton exchange membranes were characterized. Detailed results will be presented.

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Encapsulation of phase change material using miniemulsion polymerization

강길준, *김성훈, **조창기

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

Microencapsules are fine particles whose size ranges from 50nm to 2,000um, composed of an excipient polymeric shell and incipient active core component. Microencapsulation of phase-change materials (PCM) has been studied in thermal energy storage area. Microcapsule containing PCM has application to heating, air conditioning of buildings, thermal adaptable fibers, etc. Size of microcapsule using miniemulsion can be smaller than 1um. Miniemulsion is generally consist of oil, water, surfactant, and cosurfactant that is very in-soluble in the water. In the miniemulsion, oil droplets are stable even though the size is smaller than 1um due to the cosurfactant. In this work, poly (methyl methacrylate) or polystyrene was used for the encapsulation of octadecane. The size of the obtained nanoparticles was measured by dynamic light scattering.

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Colloidization of chitosan nanopowders prepared from a top-down method in water by self-assembly

은채정, 서영수

세종대 나노공학과

Chitosan, a deacetylated derivative of chitin, is a biodegradable cationic polymer, which has been known as a potential biomaterial for a food ingredient, artificial skin, and drug delivery system. As food and cosmetics ingredients, applications of chitosan are currently restricted because it is insoluble in water. Here we present how nanosized chitosan powder can be dispersed in water by surface modification, where chitosan nanopowder was prepared from a top-down method. Chitosan nanopowder can be treated with small amount of acid in water, from which it renders hydrophilic to be dispersed in water. Successively surfactants added are self-assembled onto it so as to be well-dispersed colloidal solution. The colloidal solution is stable even after the solution is neutralized. Colloidization and self-assembly process are monitored using dynamic light scattrering (DLS) and colloidal interactions using static light scattering (SLS). And also it will be presented that colloidal chitosan nanpowders in water are viewed using Cryo-EM.

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Preparation of Ionic Liquid Resin and Its Application on Peptide Synthesis

조홍준, *정성원, 이윤식

*서울대 화학생물공학부 *서울대 나노융합*

Ionic liquids (ILs) have been used as metal ligand, lewis acid catalyst, electrolyte, soluble support and environmentally benign reaction media because of their versatile properties, which can be easily controlled by exchanging counter anion. ILs as reaction media and catalytic support were used in various chemical reaction such as enzymatic reactions, Diels–Alder reactions, hydrogenation reactions and peptide coupling reaction. To apply ILs as a support for Solid-Phase Peptide Synthesis (SPPS), we designed several ionic liquid linkers. Various ionic liquid resins were prepared by treating chloromethyl polystyrene (CMPS) resin with ionic liquid linkers. We measured the swelling property and coupling kinetics of amino acids on ionic liquid resins which contained different counter anions (Cl-, BF4-, OTf-, PF6-, TFSI-). To evaluate the properties of ionic liquid resins as a polymer support for SPPS, several peptides were synthesized and the results were compared with other resins.

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Diffusion Dynamics of Flame Retardants in Polymeric Matrices Studied by DSIMS and TOFSIMS

윤여은, 윤동환, 권계민, 정현태, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

One of major disadvantages for polymeric products, which often have a significant chance of being exposed to an ignition source, is their high flammability upon heat. Therefore, incorporation of flame retardants becomes a very important process for the most of housing electronic products. Although there have been many scientific approaches to reduce the flammability of polymeric materials, particularly, phosphorus-containing flame retardants are important issue corresponding to environmental concern. When fires start with an ignition event, where heat comes into contact with fragmented polymers generated by the heating of the polymer products, polymer fire starts. Therefore, one of well known flame-retardant strategies is to effectively scavenge free radicals and to form the char layer upon the surface of product produced by polymeric materials in high temperature, by the formulation of flame retardants. In order to design more efficient flame retardants, although polymer combustion test might provide the efficiency of the target flame retardants directly, one has to understand why and how a specific flame retardants acts in a polymer matrix in high temperature. In this regard, it is clear that the flame retardant mobility in a polymer matrix is a particularly important, because the mobility is closely related to the fundamental properties, such as the interaction between the polymer and the flame retardants, which is important to develop novel flame retardants having different molecular structures specifically tailored for applications. Increased viscosity can also occur when attractive interactions exist which can pin the flame retardant molecules to the polymer matrix. In this experiment with BDP which is a kind of flame retardant, we can show the diffusion as annealing time. Hence we chose to directly measure the depth profiles, providing effect of diffusion properties for various flame retardants, using dynamic secondary ion mass spectrometer. In near future, we are further planning to use the neutron

reflectometry to obtain several critical issues, which only can be answered with the depth profiles with a subnanometer scale.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Aggregation induced holographic patterning on photopolymers containing bipyridazine derivatives

서석재, 도재권, 김은경

연세대 화학공학과

Aggregation induced emission enhancement (AIEE) properties of bipyridazine derivatives were investigated in solid mixture as well as in solution. The materials having AIEE property show strong fluorescent in aggregation state or solid phase but they show weak emission when they are dissolved in solution. AIEE property of bipyridazine derivatives was confirmed by comparison with analogue compounds which have biphenyl as core instead of bipyridazine. Through the holographic recording, the concentration of fluorophores became significantly localized to unrecorded area. Since the concentration of the localized fluorophores were enough to show AIEE property, aggregation induced pattering was possible on the photopolymer film.

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Ethene-Norbornene Copolymer with High Norbornene Content Produced by (Cyclopentadienyl)(aryloxy)titanium(IV) Complex: Synthesis, Characterization, and Catalytic Activities of Cp'TiCl2(O-2-R-Ph)

김범준

고려대 소재화학과

Ethene-borbornene copolymerizations were carried out by Cp'TiCl2(O-2-R-Ph) [Cp' = C5H5 (1), C5Me5 (2); R = Me (a), i-Pr (b), t-Bu (c), Ph (d)] activated with Ph3CB(C6F5)4/m-MAO at room temperature. Effect of Cp fragment in copolymerization of ethylene with norbornene by Cp'TiCl2(O-2-R-Ph) has been explored and (t-BuNSiMe2Flu)TiCl2 (3) was chosen as the reference. The 1 showed higher activity than others at NBE 1M concentration. The activities of 1 and 2 increased with increasing the NBE concentration. In the same NBE 5M concentration, It was revealed that 2 was the highest NBE incorporation with (N = 32.12 mol%).. Effect of both cyclopentadienyl and aryloxy groups plays an essential key role in the copolymerization not only to exhibit high catalytic activity but also to afford relatively high molecular weight copolymer with narrow polydispersity. It also turned out that norbornene incorporation into the copolymer is highly affected by the substituents on the cyclopentadienyl group. The copolymer was analyzed by GPC, DSC, and 13C NMR spectroscopic investigations.

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Synthesis and Characterization of New Copolymers containing Electron-Transporting Groups for Polymer Light-Emitting Diodes (PLEDs)

yuanwei, *조청화, **권순기, ***김윤희

*경상대 고분다 *경상대 고분자공학과 **경상대 나노신소재공학부 ***경상대 화학과*

Polymer light-emtting diodes (PLED) have been the subject of intense research interests due to their application in large-area flat panel displays. To achieve highly efficient PLED devices, charge (holes and electrons) injection and transport from both the anode and the cathode should be balanced at the junction of the emitting layer to yield the maximum exciton formation. So, it is important to achieve conjugated polymers which have both functions of hole/electron affinity in the single layer LEDs. In this communication, we synthesized a series of copolymers with electron-transporting and hole-transporting segments. Their photophysical and thermal properties would be investigated and further discussed.

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The Blister Defect Study of Organic Insulator Photoresist

조문철, *이영범

*삼성전자(주)/삼성전자공과대 LCD총괄 공정개발그룹/Display *삼성전자(주) DS총괄 LCD사업부*

우리는 포토레지스트의 공정진행시, 발생될 수 있는 블리스터 결함 (blister defect)에 대하여 아크릴계 수지가 주성분인 유기절연막 포토레지스트를 이용하여 초기 세정 조건, PR 도포전 베이크 조건, 전면노광 공정 조건을 통해 그 원인, 평가 및 개선을 위한 연구 결과를 보고한다. 본 연구에 사용된 유기절연막 포토레지스트는 박막 액정 소자, 능동형 유기발광소자나 플랙서블 디스플레이소자를 구성하는 보호박막(passivation thin film)의 하나로 활용될 수 있다. 본 연구 결과는 기존에 보고된 블리스터의 발생원인이 유기절연막과 하부기판인 SiNx 의 접착력에 영향을 주는 공정변수인 초기세정 및 베이크 조건에 기인하기보다 현상 후, 후속공정인 전면노광 공정에서 발생하는 것을 확인하였다. 이 결과를 토대로 원인된 전면노광 공정의 노광파장 및 에너지를 조절하여 노광기인성 블리스터 결함의 근원적인 제거가 가능하였다.

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Preparation and Characteristic of Poly-ɣ-Glutamic Acid Hydrogel

박효진, *변지영, *최재철, **곽미선, **성문희

*국민대 생명나노화학과 *(주)바이오리더스 **국민대*

We prepared several types of hydrogel using poly-ɣ-glutamic acid (ɣ-PGA). ɣ-PGA is naturally synthesized by *Bacillus subtilis* (chungkookjang), and it is biodegradable. Naturally occurring polymers have attracted considerable interest among polymer scientists in recent years. ɣ-PGA hydrogel could be used as compatible biomaterials for many applications. ɣ-PGA hydrogel by ɣ-irradiation showed individual specific water content and fast swelling property. They have cross-linked networks and pore structures of various sizes. It is able to regulate physical property of hydrogel by degree of ɣ-irradiation and molecular weight of ɣ-PGA. Also, we prepared chemical cross-linked gel and physical gel using by ɣ-PGA. These each have different physical characteristics. ɣ-PGA hydrogel may be used as functional cosmetics material, biomedical material, and so on. This indicates that ɣ-PGA hydrogel could be used in the various fields of industrial application. [This work was supported by the 'Seoul R&BD Program (10580)']

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Fabrication of ɣ-PGA-Levan Nanofiber using electrospinning method

최두열, *최동환, **박청, ***Hiroshi Uyama, *성문희

*국민대 생명나노화학과 *국민대 **(주)바이오리더스 ***Graduate School of Engineering, Osaka University, Suita, Japan*

Poly-gamma glutmamic acid (ɣ-PGA) is naturally synthesized by *Bacillus subtilis* with glutamic acid. ɣ-PGA was spun to form a fiber using general electrospinning method. But ɣ-PGA fiber was a microsized fiber and quickly soluble in humid condition. We carried a out experiment for ɣ-PGA and levan mixtures spinning method, and successfully fabricated. The average ɣ-PGA-Levan fiber diameter was in the range between 200 nm and 500 nm. These results will be shown and discussed its applications. [This work was supported by the 'Seoul R&BD Program (10580)']

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Characteristics of Ultra High Molecular Weight Poly-γ-Glutamic Acid and its Applications

박청, *김철중, *임용택, **성문희

*(주)바이오리더스 *충남대 **국민대*

Poly-γ-glutamic acid (γ-PGA) is an anionic, water-soluble, safe biomaterial that is naturally synthesized by *Bacillus subtilis*, and the α-amino and γ-carboxy groups of D- and/or L-glutamic acid are polymerized via γ-amide linkages. Its multifunctionality, biodegradability, nontoxicity, compatability and edibility have made it a promising biopolymer in the various industrial fields. Since the discovery of *Bacillus subtilis* (chungkookjang) that produces high molecular weight γ-PGA, specific applications have continued to be developed. Recently, we have found that ultra high molecular weight of γ-PGA produced from *Bacillus subtilis* (chungkookjang) shows a unique characteristics and increases density, Ca-solubility, immune stimulating ability. Interestingly our results suggest that higher molecular weight g γ-PGA induced more innate immune responses in macrophages and dendritic cells (DCs) than lower molecular weight γ-PGA. The highlights of these studies will be shown and discussed. [This work was supported by the 'Seoul R&BD Program (10580)']

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Comparison of Poly-γ-glutamic acid Production between *Bacillus megaterium* and *Bacillus subtilis*

박성빈, 최인복, *곽미선, *성문희

*국민대 생명나노화학과 *국민대*

Poly-γ-glutamic acid (γ-PGA) is edible and biodegradable polymer with repeated-chain structure of glutamic acid. γ-PGA has different characteristics and properties depending on molecular weight and D/L-glutamic acid ratio. To obtain microorganisms, that can produce the γ-PGA of different molecular weight and D/L-glutamic acid ratio, we screened of γ-PGA producer from Toha-jeot (salt-fermente Toha shrimp). We isolated four strains that could grow and form a highly mucous colony on the medium containing 5% NaCl. Finally we selected one strain as new sources of produce the γ-PGA of different D/L-glutamic acid ratio. The 16s ribosomal RNA sequence of isolated strain revealed the highest homology score with *Bacillus megaterium*. We compared different characteristics of produced γ-PGAs from *Bacillus megaterium* and *Bacillus subtilis*. [This work was supported by 'Seoul R&BD Program (10580)]

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Mono-, bis-, tris-2-phenylphenoxy 리간드가 치환된 Cp*Ti(2-R-PhO)nCl3-n의 폴리올레핀 중합 활성과 메커니즘

김태진, 김범준, 고재중, 강상욱

고려대 소재화학과

R 치환체에 methyl, iso-propyl, tert-butyl, and phenyl 이 치환된 Cp*Ti(2-R-PhO)nCl3-n 형태의 폴리올레핀 중합용 타이타늄 촉매를 합성하였다. 페녹시 리간드의 2 번 위치에 치환기가 치환되었기 때문에 리간드의 구조적 크기가 작아서 mono-, bis-, tris-페녹시 리간드를 가진 촉매를 합성할 수 있었다. Cp*Ti(2-Ph-PhO)Cl2 (1PhCl2), Cp*Ti(2-Ph-PhO)2Cl (2PhCl), Cp*Ti(2-Ph-PhO)3 (3Ph)를 X-ray 분석을 통해서 구조를 확인해보았을 때 모든 화합물의 구조는 중심 금속에 배위된 Cp*와 페녹시 리간드, 그리고 클로린 치환기가 pseudo-tetrahedral 형태를 취하고, Ti-O 거리는 리간드의 수가 증가함에 따라서 1.784(3), 1.798(5), and 1.81(1) Å 로 커지는 것을 확인하였다. 페녹시 리간드의 수가 증가함에 따라서 UV-visible 스펙트럼은 단파장 이동을 하고, cyclic voltammogram 은 환원 포텐셜이 큰 값을 가지는 것을 확인하였다. R 치환체에 methyl, iso-propyl, tert-butyl, and phenyl 이 치환된 Cp*Ti(2-R-PhO)nCl3-n 형태의 폴리올레핀 중합용 타이타늄 촉매를 Ph3CB(C6F5)4 and mMAO-7 로 활성화 시켜 고온 에틸렌 중합에 적용을 하면 alkyl 기가 치환된 화합물에 비해 phenyl 이 치환된 화합물이 높은 활성을 보였고, 이 때 페녹시 리간드가 2 개 치환된 화합물 2PhCl 이 가장 높은 활성을 보였다 [65.4 Kg/(mmol of Ti•h)]. 이러한 활성의 원인을 밝히기 위해 1Ph2Cl, 2PhCl, 3Ph 와 각각 aluminum scavenger [trimethylaluminum (TMA), triisobutylaluminum (TIBA), methylalumoxane (MAO)]와의 반응을 진행해 본 결과 활성을 나타내는 Cp*Ti(OPh)MeCl 이 2PhCl 의 경우에 가장 높은 수율로 합성되는 것을 확인하였다.

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Synthesis of 3,5-diaminofluorobenzene from TNT

조훈, 김석찬

국민대 화학과

폐탄약에서 얻은 TNT 를 사용하여 내마모성을 향상시킬 수 있는 fluorine 과 polymer 의 가지연장제로 사용할 수 있도록 dual function 을 갖는 3,5-diaminofluorobenzene 을 합성함으로써 고부가가치를 창출하고자 한다

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

정스런, *허은수, 정민석, 김훈식

*경희대 화학과 *경희대 이학부 화학과*

Composite membranes based on room temperature ionic liquids (RTILs) bearing a basic anion were highly effective for the selective separation of acetylene in ethylene. The high affinity of the RTILs to acetylene was supported by the comparison of solubility data measured at 313.15 K and at atmospheric pressure. For instance, the solubility of acetylene in 1,3-dimethylpyrrolidinium methylphosphite ([DMPyrr][MeHPO3]) is about xx times higher than that of ethylene. Computational and 1H NMR results with [DMPyrr][MeHPO3] clearly demonstrate that there are substantial interactions between the acidic hydrogen atoms of acetylene and the phosphite anion.

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fluorine계 난연성 세정제의 합성 연구

김재현, 송혜선, *김석찬

*국민대 생명나노화학과 *국민대 화학과*

유기 용제를 사용한 세정법은 인체와 환경에 치명적인 해를 끼친다.그리고 VOC 방출에 있어서 법적으로도 제재를 받고 있다. 이에 대해 휘발성 용제로 알려진 톨루엔 이나 아세톤이 새로운 환경 친화적 용제로 인체에 보다 적은 유해를 끼치는 물질로 시장에 등장하고 있다. 하지만 톨루엔이나 아세톤은 낮은 인화점으로 인하여 세정시 여러가지 문제점을 가지고 있다. 그래서 fluorine 을 도입한 화합물을 합성하여 세정력도 높이면서 난연성을 도입할 수 있는 세정제 합성을 연구한다.

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발표종류: 포스터, 발표일시: 목 16:30~18:30

Characterization of Disk type Mesoporous Carbon Nitride using SBA-15 Material

민병훈, 정승민, 정은영, 박상언

인하대 화학과

Carbon nitride (CN) is a well-known and fascinating material that has attracted worldwide attention because of the incorporation of nitrogen atoms in the carbon nanostructure. Recently, Vinu et al. successfully reported the preparation of mesoporous carbon nitride with a uniform pore-size distribution (MCN-1) using SBA-15 as a template.[12]Recently, our group was successful synthesized of disk type esoporous silica. Because of the short channels of disk type materials, it was observed the serious diffusion or mass transfer limits in Knoevenagel condensation of benzaldehyde with ethyl cyanoacetate.[3] So, disk type mesoporous carbon nitride material also has several advantages, including disk type SBA-15 material. The characterization of disk type MCN material was shown by small angle XRD powder patterns, scanning/transmission electron microscopy and nitrogen sorption analysis.

1. A. Vinu, K. Ariga, T. Mori, T. Nakanishi, S. Hishita, D. Golberg, Y. Bando, Adv. Mater. 2005, 17, 1648.
2. A. Vinu, Adv. Funct. Mater. 2008, 18, 816–827
3. Sujandi, Sang-Eon Park,* Dae-Soo Han, Sang-Cheol Han, Myung-Jong Jin and Tet su Ohsuna, Chem. Commun., 2006, 4131–4133

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장소: 대전컨벤션센터
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Catalytic oxidation of cycloolefins over microwave synthesized Ti containing mesoporous TUD-1 material

정승민, Jiang Nanzhe, 정은영, 민병훈, 박상언

인하대 화학과

Ti-incorporated mesoporous silica has been used as an excellent catalyst for various industrial fundamental applications such as epoxidation reaction. The 3-dimensional Ti- mesoporous TUD-1 was prepared by one pot surfactant free method using TEA (Triethanolamine) instead of surfactant via microwave. The TEA assisted well homogeneously dispersion of metal complex onto mesoporous surface. In addition, microwave synthesis could accelerate the preparation even under large quantity of water due to its characteristic of selective heating and enhance hydrophobicity onto surface.In our research, we tested epoxidation reaction using high contents of titanium containing 3-D Ti-TUD-1 via microwave synthesis as catalytic precursor. The epoxidation of cyclooctene under Ti-TUD-1, even high titanium content of the TUD-1 at Si/Ti=10 ,exhibited the highest catalytic activity and selectivity especially compared with other catalysts due to well dispersion of metal and metal oxide onto mesoporous surface, and its more hydrophobiciy onto surface.

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One-Pot Synthesis of tetrakis(4-carboxyphenyl)porphyrin Compounds Prepared by Microwave

정은영, Eko Adi Prasetyanto, 정승민, 민병훈, 박상언

인하대 화학과

Porphyrins as macrocyclic compounds are nowadays revoking great interests due to easy synthesis and various application such as nonlinear optical materials, photodynamic therapy, solar energy. we now report the preparation and some properties of 5,10,15,20-tetrakis(4-carboxyphenyl)-porphyrin. Microwave synthesis without solvent was adopted as an one-pot synthesis of tetrakis(4-carboxyphenyl) porphyrins from pyrrole and 4-carboxybenzaldehyde by using propionic acid. And one-pot synthesized M-TCPP having Zn, Cu and Fe by microwave were characterized by UV-Vis spectroscopy and raman spectroscopy and CV analyzer and so on. Catalytic activities in the hydrogen transfer reaction of a variety of ketones by a typical liquid phase and microwave-induced reactions were investigated over TCPP and M-TCPP (M=Zn, Cu and Fe) catalysts

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Melamine tri-silsesquioxane bridged periodic mesoporous organosilica as an organocatalyst for CO_2 utilization

Eko Adi Prasetyanto, 박상언

인하대 화학과

Periodic mesoporous organosilica is a special type of ordered mesoporous silica, in which organic moieties are integrated into the silica framework to form hybrid organic-inorganic material. In this work, we successfully incorporate T-type large sized melamine based tri organosilsesquixane as organic linker in the periodic mesoporous organosilica. Melamine-bridged PMOs were prepared with highly reproducibility by co-condensation using N2,N4,N6-tris(3-(triethoxysilyl) propyl)-1,3,5-triazine-2,4,6-triamine (TBTS) and sodium metasilicate in the presence of poly(ethylene oxide)-poly-(propylene oxide)-poly(ethylene oxide) triblock copolymer (Pluronic P123, $EO_{20}PO_{70}EO_{20}$,Aldrich) at highly acidic concentration. The resulted melamine PMO had high orderness mesostructure in p6mm form and its organocatalytic behaviour in hydrogen transfer reaction was investigated. Catalysis via organo functional groups has been interested as green method to produce high valued fine chemicals without metallic contaminants

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Synthesis and Photovoltaic properties of efficient organic dyes containing the unsymmetrical quinacridone moiety for DSSCs

사공천, 김재필

서울대 재료공학부

New organic dyes composed of the unsymmetrical quinacridone donor, thiophene or benzene-conjugated bridge and cyano acrylic acid acceptor were designed and synthesized for dye-sensitized solar cells (DSSCs). Nanocrystalline TiO2 dye-sensitized solar cells were fabricated using these dyes and their photovoltaic properties were measured.

THE KOREAN CHEMICAL SOCIETY

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Synthesis and photovoltaic properties of phenothiazine-based novel organic dyes containing additional donor for dye-sensitized solar cells

김세훈, *김현우, *김재필

*서울대 공과대 재료공학부 *서울대 재료공학부*

We designed and synthesized phenothiazine-based novel organic dyes containing additional donor for dye-sensitized solar cells (DSSCs). New organic sensitizers are composed of phenothiazine(PTZ) moiety as an electron donor, ethylthiol as an additional donor, and cyanoacrylic acid group as an electron acceptor. In addition, N-butyl, N-methoxyphenyl and N-butoxyphenyl units were introduced for increasing a solubility and a donating power. Photovoltaic cells were prepared with the synthesized organic dye-sensitizers. The influences of N-substituents and ethylthiol both on their solubility and photovoltaic properties were studied.

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Surface treatment of TiO_2 films for dye-sensitized solar cells usingby atmospheric pressure plasma treatment of TiO_2 films

노진희, *황철균, **조성우, ***김민지, ****한주탁, *오지훈

*경북대 나노과학기술학과 *나노부품실용화센터 나노소재개발팀 **나노부품실용화센터 나노융합개발팀 ***영남대 디스플레이 화학공학부 ****나노부품실용화센터 경영기획실*

In this paper, we report that atmospheric-pressure plasma treatment as means for the preparation of TiO_2 films of fluorine dope tin oxide (FTO) coated glass substrates used for dye-sensitized solar cells (DSSCs). The effect of atmospheric-pressure plasma treatment on the cell performance describe as shown by the SEM, AFM, the I-V characteristics, etc. Considering the effect on plasma treatment, we believe that the specific surface area and photocurrent density of TiO_2 film was influenced by the plasma surface treatment which contributed to influence significantly on the energy conversion efficiency of DSSCs.

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Effect of ester functionalized zwitterionic imidazolium compounds as membrane materials for separation of olefin/paraffin mixtures

김대원, 정스런, **Nguyen Dinh Quan**, 정민석, 김훈식

경희대 화학과

Zwitterionic imidazolium compounds containing an ester group at 1- or 2-position and a propylsulfonate group at 3-position were prepared and used as the membrane materials for separating ethlyene/ethane and propylene/propane mixtures. The location of the ester group on the imidazolium ring significantly affected the performance of the membranes consisting of a silver salt and a zwitterionic imidazolium compound bearing an ester group. The interaction between a zwitterionic imidazolium compound and silver nitrate was investigated by using density functional theory method and FT-IR study. The results indicated that the silver ion bonded to the propylsulfonate group interacts intra-molecularly with the ester group only when both ester and propylsulfonate groups are located on the same side of the imidazolium ring.

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Nonimidazolium Ionic liquid-based extractants for the removal of alkynes from isoprene

김진형, 정민석, *안병성, 김훈식

*경희대 화학과 *KIST 청정에너지연구센터*

Various nonimidazolium ionic liquids were tested as extractants for the removal of alkynes from isoprene. The removal of acetylenic hydrocarbons in olefins is very important. Because terminal alkynes often serve as catalyst poisons in the process of producing polyolefins and also lower the product quality of polyolefins. When the feed containing 1% of isopropenyl acetylene (IPA) in isoprene was contacted with nonimidazolium ionic liquids, about 50~70% of IPA was extracted from isoprene to the ionic liquid layer. Further more we used metal containing nonimidazolium ionic liquids. The extraction ability of the ionic liquids was greatly enhanced, resulting in the removal of 80~90% IPA in the feed.

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Effect of ether group on the electrochemical stability of zwitterionic imidazolium compounds

김희환, 강제은, 김대원, 정민석, 김훈식

경희대 화학과

The cathodic stability of the zwitterionic imidazolium compounds was significantly enhanced by the introduction of an ether group at 1 or 2-position on the imidazolium ring. The cycle performance tests showed that the initial cell capacity was maintained almost unchanged up to 100 cycles at 0.5 and 1 C when 2.5 wt.% of 2-butoxymethyl-1-methylimidazolium-3-propylsulfonate or 2-butoxymethyl-1-butylimidazolium-3-propylsulfonate was added to the model electrolyte (1 M LiPF6 in ethylene carbonate, dimethyl carbonate and ethylmethyl carbonate (1/1/1 v/v/v)).

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Carboxylation of amines employing ionic liquids as effective catalysts

Nguyen Dinh Quan, *허은수, 김대원, 정민석, 김훈식

*경희대 화학과 *경희대 이학부 화학과*

The synthesis of 1,3-disubstituted ureas from the carboxylation of amines by CO2 was investigated in the presence of conventional ionic liquids. Four series of dialkylimidazolium ionic liquids were employed for the experiments, including dialkylphosphate, alkylphosphite, dialkylsulphate, and halide. The results showed that the anion played a very important role in the catalytic properties of the ionic liquids. The optimal temperature was found to be 170oC in the pressure of CO2 (700-900 psi) to obtained ureas with good yields (61-93 %). In contrast with a previous study [1] the addition of solvents and co-catalyst, such as K2CO3, K3PO4, CsOH, ZnCl2, ZnBr2, Cs2CO3, CuCl, etc., did not improve significantly the reaction. Moreover, the use of one-pot-synthesized ionic liquids suggests a much more convenient procedure than that of using hydroxyl-based ionic liquid [2].1. F. Shi, Y. Deng, T. Sima, J. Peng, Y. Gu, and B. Qiao, Angew. Chem. Int. Ed., 2003, 42, 3257-3260.2. T. Jiang, X. Ma, Y. Zhou, S. Liang, J. Zhang and B. Han, Green Chem., 2008, 10, 465-469.

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장소: 대전컨벤션센터
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Ru-catalyzed hydrogenation of aromatic diamines: The effect of alkali metal salts

권오준, *이방숙, 김훈식, *이현주

*경희대 화학과 *KIST 청정에너지연구센터*

The influences of added alkali metal nitrates and nitrites on the performances of ruthenium catalysts in the liquid phase ring hydrogenation of 4,4'-methylenedianiline (MDA) and 1,4-phenylenediamine (PDA) have been examined. Sodium nitrate and sodium nitrite were shown to be the most effective promoters in enhancing the catalytic activity and in suppressing the formation of by-products. The effects of various solvents and the added water on the hydrogenation activity have also been investigated. The promoting effects of sodium nitrate and sodium nitrite were considerably enhanced in the presence of small amounts of water. XRD patterns of the Ru/Al_2O_3 catalyst sample obtained from the reaction performed in the presence of $NaNO_3$ or $NaNO_2$ revealed that the sodium aluminate ($NaAlO_2$) phase appears indicating that the cations of metal salts are interacting with the supporting material. An active species, $NaOCH(CH_3)_2$ was isolated and identified by spectroscopic and elemental analyses.

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ABS복합재료의 제조 및 특성 분석

조형준, *임정섭, **정동운

*원광대 생명나노화학부 *원광대 생명나노화학과 **원광대 화학과*

기존의 고분자플라스틱 재질은 표면이 수분을 배척하는 소수성이며 또한 통기성이 좋지 못하다. 이러한 물성을 개질하기 위하여 고분자플라스틱에 기능성충전제로 친수성인 점토 등의 무기물을 블렌드하여 친수성 및 통기성이 향상된 복합재료를 제조하였으며 공기투과율, 접촉각 측정을 통해 물성을 확인하였다.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Seed-Directed Formation of Micro-sized Hexapod Coordination Polymers

박성진, 조원, 오문현

연세대 화학과

Micro- and nanoparticles made from atomic or molecular building blocks have received great attention due to their utilizations in various applications in which their properties depend not only on their sizes and morphologies but also on their compositions. In this objective, controlling the sizes and morphologies of particles and introducing the new components within particles have been considered to be quite important. Here we present the formation of multicomponent fluorescent hexapod coordination polymer particles from a blend of fluorescent building blocks and transition metal ions.

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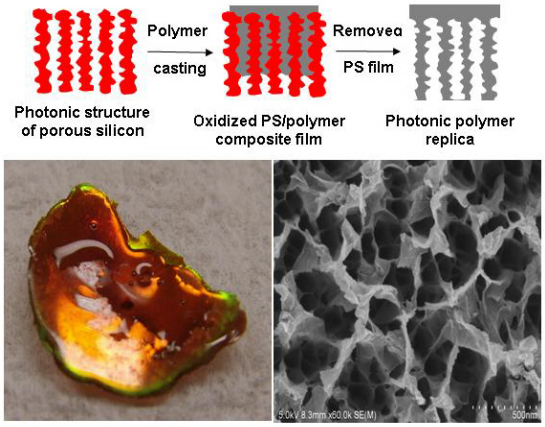
Novel Photoanode Structure of Polymer Replicas Templated from a Tunable Nanostructure of Oxidized Porous Silicon and Its Application for biosensor

김지훈, 조성동, 손홍래

조선대 화학과

Novel photoanode structures of polystyrene thin films containing many independent codes were fabricated by replicating the photonic features and the nanostructure of a multi-encoded rugate porous silicon master. A photograph and FE-SEM image of a rugate-structured polymer replica illustrate that its color results from the reflection of the polymer replica and that the morphology of the polymer film has a photoanode structure of multi-encoded rugate porous silicon. In a basic demonstration for biosensor application using polymer replica, the biotin-incorporated polymer replica using biocompatible polymer are used to detect of avidin. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.



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Rugate-Structured Porous Silicon for Application of Full Color Stop Band

손홍래, 김지훈, 조성동

조선대 화학과

Fabrication and optical characterization of rugate porous silicon (PS) were investigated by an electrochemical etching of silicon wafer in aqueous ethanolic HF solution. Rugate PS prepared by applying a computer-generated pseudo-sinusoidal current waveform displayed high reflectivity in a specific narrow spectral region and display a very sharp line in the optical reflectivity spectrum. Structures of periodic PS multilayer, which was formed by the current density modulation method, were investigated by cross-sectional scanning electron microscopy (SEM) observation. The reflection wavelength of ruagte PS was controllable by changing of sinusoidal current waveform in hertz (Hz). This line can appear anywhere in the visible range depending on the sine waveform of each Hz value. These spectral features can be much narrower than the fluorescence spectrum obtained from a molecule or core-shell quantum dot. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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Detcteton of Biomolecules Based on Biotinlyted Silole and Aggregation-induced emission (AIE)

고영대, 조성동, 손홍래

조선대 화학과

The aggregation of highly emissive organics and polymers into a solid state causes an emission-quenching effect, since the aggregation of molecules forms less emissive species such as excimers. In contrast, few results on aggregation-induced emission (AIE) properties have been recently reported. Recently, we reported an aggregation-induced emission enhancement of biotinlyted-silole. Here, we report the synthesis of the highly fluorescent siloles derivatized with biotin for searching a possible application as biosensor. Biotin-derivatized silole molecule was obtained from the reaction biotin tetrafluorophenyl ester. Optical properties and aggregation behavior will be discussed. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Application of Chemosensor based on Polysilole Nnanoaggregate and Polysilole/SiO2

손홍래, 고영대, 조성동

조선대 화학과

Polymetalloles such as siloles and germoles containing silicon and germanium have continuously received much attention because of their unusual electronic properties.1-3 Polytetraphenylsilole(PTPS)/porous silica nanoparticulates have been synthesized from the reaction of PTPS with tetramethoxyorthosilicate(TMOS) and used to detected explosives such as TNT, PA, DNT, and NB. Size of PTPS/porous silica nanoparticulates is about 300–400 nm measured by field emission scanning electron Mmicroscope(FE-SEM). Detection has been achieved through the measurement of quenching photoluminescence of PTPS/porous silica nanoparticulates by adding analytes. A linear Stern-Volmer relationship is obtained for each analyte. The quenching efficiency of PTPS/porous silica nanoparticulates for nitroaromatic compounds is greater than that of PTPS nanoparticulates. The possible reason and mechanism will be discussed-This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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발표분야: 무기화학
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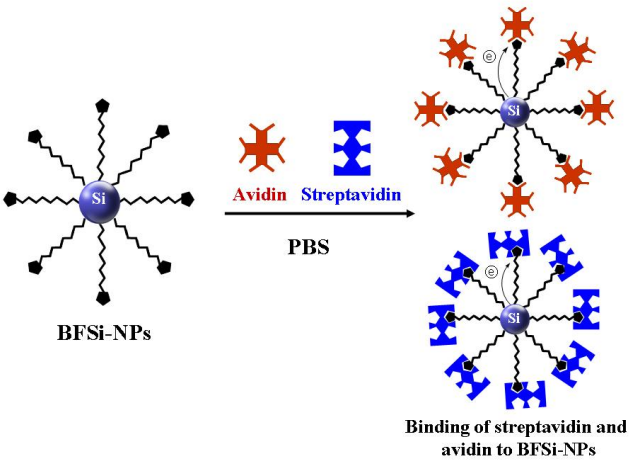
Synthesis and Characterization of Biotin-functionalized Silicon Nanoparticles and Their Application as a Biosensor

장승현, 최태은, 조보민, 손홍래

조선대 화학과

A new convenient and easy method for a simple room temperature synthesis of Biotin-functionalized Silicon Nanoparticles (BFSi-NPs) with strong blue photoluminescence (PL) for the detection of avidin and streptavidin has been developed. Hydrogen-terminated Si-NPs were synthesized from the reaction of Zintl salt (Mg_2Si) with ammonium chloride (NH_4Cl).Hydride-covered Si-NPs can be functionalized further by hydrosilylation process with allylamine to terminate amine groups for reaction to biotin group. Prepared BFSi-NPs were characterized by TEM, FT-IR, UV-vis absorption and PL spectrum. The sizes of BFSi-NPs ranged from 4 to 6 nm in diameter.The maximum intensity of emission spectrum was centered at 445 nm with an exitation of 360 nm. Further details will be presented. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation(KOTEF) through the Human Resource Training Project for Regional Innovation-



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장소: 대전컨벤션센터
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Synthesis and Characterization of Amin-substituted Silole Derivatives for sensing Inorganic Acids

장승현, 조성동, 손홍래

조선대 화학과

Chemical sensors, which are new approaches to the rapid detection of ultra-trace analytes from inorganic acids. Functionalized siloles have been a topic of interest because of their unique optical and electroluminescent properties. A new chemosensors for the detection of inorganic acids based on photoluminescent 1-amino-1-methyl-2,3,4,5-tetraphenylsilole and 1-methyl-1-(3-amino)propyl-2,3,4,5-tetraphenylsilole have been developed. The detection of inorganic acids is achieved from the measuring of quenching and enhancing photoluminescence of aminosiloles by adding the analytes. The aminosiloles are highly sensitive and selective to detect the inorganic acids without any other interference. TLC-based detection method with aminosilole is also developed. Our dectection limit for sensing inorganic acid was obtained using TLC-based technique. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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Synthesis, structure and physical properties of metal complexes (M = Fe, Co, Mn) containing *N,N*-bis(2-pyridylmethyl)-2-aminoethanol

신종원, *송전익, **김상우, **김태훈, **한성수, **이기석, ***민길식

*경북대 화학과 *울산과학고 - **울산과학고 ***경북대 사범대학 화학교육과*

We have synthesized and characterized several metal complexes having *N,N* –bis(2-pyridylmethyl)-2-aminoethanol (bpaeOH), i.e. $[Fe_4(bpaeO)_2(CH_3O)_2(N_3)_8]$ (1), $[Co_3(bpaeO)_2(N_3)_4(NO_3)_2]$ (2), $[Fe(bpaeOH)(NCS)_2]$ (3), $[Co(bpaeOH)(NCS)_2]$ (4), $[Mn(bpaeOH)(NCS)_2]$ (5), $[Mn(bpaeO)(N_3)_2]$ (6). Compound 1 is a linear tetranuclear iron(III) complex, while 2 is a mixed-valence trinuclear cobalt(II,III) complex. Unexpectedly, as using thiocyanate ions instead of azide ions, monomeric Iron(II) and cobalt(II) complexes are obtained like 3 and 4, respectively. In case of manganese compounds, manganese(II) complex (5) bonded with one bpaeOH and two thiocynate ions and manganese(III) complex (6) coordinated with a deprotonated bpaeO and two azaide ions are formed. That is, the Mn ions have different oxidation states depending on binding anions. In this poster, we will explain the detailed preparation, crystal structure, magnetic properties as well as interesting coordination chemistry.

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Synthesis, structure, and magnetic properties of methoxy-bridged dinuclear iron(III) complexes

신종원, *김승휘, 이유경, 로투산카라라오, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

The reaction of stoichiometric amount of iron(III) nitrate nonahydrate, (2-pyridylmethyl)(3-pyridylmethyl)amine (2,3-pyma) and sodium azide/sodium thiocyanate in methanol under aerobic conditions affords the dinuclear complexes, [(2,3-pyma)$(N_3)_2$Fe$(OMe)_2$Fe$(N_3)_2$(2,3-pyma)] (1) and [(2,3-pyma)$(NCS)_2$Fe$(OMe)_2$Fe$(NCS)_2$(2,3-pyma)] (2) in good yield. The coordination geometry around iron(III) ions in both compounds is a tetragonally distorted octahedron. The iron(III) ions are coordinated by two nitrogens of a 2,3-pyma, two nitrogens of two azide/thiocyanate ions, and two oxygens of two methoxy groups. Thus, both compounds are isomorphous. Additionally, both compounds display the C-H••• and - stacking interactions, respectively. Interestingly, the compounds show strong antiferromagnetic couplings between the iron(III) ions in the temperature range from 2 to 300 K. In this poster, we will explain the detailed preparation, crystal structure, and magnetic properties.

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Synthesis, Structure, Catecholase Activity, and Azide Binding of A Series of Phenyl-Based Cu(II) Complexes

shuranjan sarkar, 이홍인, *홍창섭, *윤정희

*경북대 화학과 *고려대 화학과*

Some active catalytic enzymes take a benefit of the combined action of nearby metal ions within their active site, specifically for electron redox transformations such as the activation of O_2. These ordinary systems represent a guiding line for the improvement of novel bioinorganic catalysts. Owing to this interest, we have prepared a series of highly preorganized copper complexes based on compartmental phenolate ligands, in which molecular parameters such as the number of metal can be tuned by proper modifications of the ligand gallows. The entire synthesized complexes were characterized by a combination of elemental analysis, FAB-MS, IR, EPR and UV-vis spectroscopy. Those complexes were structurally characterized and showed one or more open coordination sites which were established by the titration of azide anion into solutions of the complexes in methanol resulted in the appearance of a new band between 340–500 nm. In this poster, we have shown the catalytic action of those complexes by using the oxidizing agent 3,5-di-tert-butylcatechol.

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Synthesis, Characterization, Crystal Structures, and Spectroscopic Properties of Some Transition Metal Complexes Containing Novel Schiff-Base Ligands

shuranjan sarkar, 이홍인, *홍창섭, *윤정희, **나명수

*경북대 화학과 *고려대 화학과 **한양대 응용화학과*

Several Schiff-base complexes of transition metal have been widely working in the improvement of catalysis, photochemistry, medicine, gas sorption, molecular electronics and single molecule-based magnetism. Their magnetic, electronic, optical and physical, properties have been explored in different coordination atmosphere with organic chelators, blockers, and appropriate bridging units. These complexes are also relevant as models for the active sites of enzymes. Much effort has been spent on the synthesis of mono-, bi-, and multi-nuclear metal complexes as functional and structural models of multimetal enzymes. In this poster, we have explored some Schiff base transition metal complexes those were successfully synthesized and characterized by a combination of elemental analysis, UV-vis spectroscopy, IR, EPR and x-ray crystallography.

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Hydrogen Adsorption Behaviors of Nickel-dispersed MCM-48

이슬이, 박수진

인하대 화학과

In this work, the hydrogen adsorption behaviors of MCM-48 (Ni/MCM-48) were studied in the presence of nickel nano-particles. The Ni/MCM-48 was prepared using a hydrothermal process as a function of Ni content (0, 2, 5, and 10 wt.% in the pure silica MCM-48). The structure and morphology of the Ni/MCM-48 were characterized by X-ray diffraction (XRD) and field emission transmission electron microscopy (FE-TEM). Ni/MCM-48 showed the well-ordered cubic structure. The textural properties of the Ni/MCM-48 were evaluated using N_2/77 K adsorption isotherms. Specific surface areas and mesopore volume of the samples were determined from the BET equation and BJH method, respectively. The hydrogen adsorption capacities of the Ni/MCM-48 were investigated at 298 K/10 MPa. As a result, the hydrogen adsorption capacities of the Ni/MCM-48 were increased with Ni content. Consequently, it was found that the presence of Ni on mesoporous MCM-48 created hydrogen-favorable sites, resulting in enhancing the hydrogen adsorption capacity.

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Effect of Mixed Acid Ratio on Hydrogen Adsorption Behaviors of Multi-walled Carbon Nanotubes

이슬이, 박수진

인하대 화학과

In this work, we investigated the effect of mixed acid ratio on hydrogen adsorption behaviors of multi-walled carbon nanotubes (MWNTs). The surface functional groups and specific elements of the MWNTs were characterized with X-ray photoelectron spectroscopy (XPS) and atomic absorption spectroscopy (AAS), respectively. Also, the changes in the surface functional groups of the MWNTs were quantitatively detected by Boehm's titration method. N_2/77 K adsorption isotherms were analyzed by BET and D-R plot methods to characterize specific surface area, pore volume, and pore size distribution of the samples. From the experimental results, we found that the mixed acid ratio could largely influence on the hydrogen adsorption behaviors of the MWNTs, resulting from introducing the oxygen-functional groups on the MWNT surfaces.

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A Study on Hydrogen Storage of Ni-loaded Multi-walled Carbon Nanotubes/Metal-organic Framework-5

이슬이, 박수진

인하대 화학과

In this work, we prepared nickel (Ni)-loaded multi-walled carbon nanotubes (Ni-MWNTs)/metal-organic frameworks-5 (MOF-5) hybrid composites (Ni-MWNTs/MOF-5) in order to investigate the hydrogen storage behaviors at room temperature. The Ni-MWNTs/MOF-5 was obtained using a hydrothermal process with Zn (II) ion as a metal centre and telephthalic acid as organic ligands. The Ni-MWNTs/MOF-5 formed crystalline structures, measured by X-ray diffraction (XRD). Morphological characteristics and average size of the Ni-MWNTs/MOF-5 were also obtained using a SEM. The pore structure and specific surface area of the Ni-MWNTs/MOF-5 were analyzed by N_2/77 K adsorption isotherms. From the experimental results, we concluded that the Ni-MWNTs/MOF-5 would be potentially supporting materials for hydrogen adsorption and storage applications at room temperature.

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Synthesis of Various Macrocyclic Copper(II) Complexes Bearing Two Different Functional Pendant Arms

강신걸, 김현자, *이욱

*대구대 화학과 *부경대 화학과*

Various 14-membered tetraaza macrocyclic copper(II) complexes bearing two different functional pendant arms, such as $[CuL^2]^{2+}$ bearing one *N*-CH_2CONH_2 and one *N*-CH_2CN groups, $[CuL^3]^{2+}$ bearing one *N*-$CH_2C(=NH)NH(CH_2)_2CH_3$ and one N-CH_2CN groups, and $[CuL^4]^{2+}$ bearing one *N*-CH_2CONH_2 and one *N*-$CH_2C(=NH)NH(CH_2)_2CH_3$ groups, have been prepared by the reaction of $[CuL^1]^{2+}$ (L^1 = 2,13-bis(cyanomethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) with appropriate reagents. The reactivity of *N*-CH_2CN group in $[CuL^1]^{2+}$ is quite different from that in $[CuL^3]^{2+}$. The coordination behavior of the *N*-$CH_2C(=NH)NH(CH_2)_2CH_3$ group in $[CuL^4]^{2+}$ is also different from that in $[CuL^3]^{2+}$. Synthesis, characterization, and chemical properties of the copper(II) complexes are presented.

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Synthesis and Properties of a Macrocycle Bearing Two or Four *N*-methoxyethyl Pendant Arms and Their Complexes

강신걸, 김현자, *정수경, **곽지훈

*대구대 화학과 *김포대학 호텔조리학과 **순천대 화학과*

The *N*-methoxyethylated macrocycles 2,13-bis(2-methoxyethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (L^2) and 2,6,13,17-tetrakis(2-methoxyethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (L^3) have been prepared by the reaction of 3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (L^1) with 1-bromo-2-methoxyethane. The copper(II) complexes $[CuL^2]^{2+}$ and $[CuL^3]^{2+}$ as well as $[NiL^2]^{2+}$ have been prepared and characterized. The oxygen atoms of the methoxyethyl groups in the copper(II) complexes are coordinated to the metal ion in the solid state and in various solvents, whereas those in the nickel(II) complex are not involved in coordination. Synthesis, characterization, and chemical properties of the functionalized macrocyclic compounds are presented.

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Luminescent Polyethylenes with Side-Chain Triarylboranes: Synthesis and Fluoride Ion Binding Properties

박명환, 도영규, *이민형

*KAIST 화학과 *울산대 화학과*

The copolymerizations of ethylene with ω-triarylboryl-α-olefin monomer, 1-dimesitylboryl-4-(oct-7-en-1-yl)benzene (1) using a $[Me_2Si(\eta^5\text{-}C_5Me_4)(\eta^1\text{-}N\text{-}^tBu)TiCl_2]$ (CGC)/MAO catalytic system were investigated to prepare polyethylenes with pendent triarylborane groups. Despite the presence of sterically hindered triarylborane side groups, the catalytic system efficiently produces high-molecular-weight copolymers with a well-defined polymer structure. The copolymers exhibit borane-based fluorescence and particularly show high fluoride ion affinity. The details of synthesis, characterization, and fluoride ion binding properties of the copolymers will be discussed.

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Synthesis and X-ray structural characterization of novel tetrazol–thiolato Pd(II) and Pt(II) complexes

김용주, 이정현, 강지현, 이소명, *이경은, *이순원

*강릉대 화학과 *성균관대 화학과*

Pd(II)– and Pt(II)–azido complexes, [M(N3)(PMe3)2(C-L)] {LH = 2-(2')-thienyl pyridine; M = Pd (1), Pt(2)}, which contain σ-bonded heterocycles (L), were treated with aryl isothiocyanate (Me2C6H3–NCS) to afford the corresponding Pd(II) and Pt(II) tetrazol–thiolato complexes, trans-{M[SCN4(2,6-Me2C6H3)](PMe3)2(C-L)} {M = Pd (3), Pt (4)}. X-ray structural analyses of complexes 3 and 4 show a 1-D helical network formed by the intermolecular M•••S van der Waals contacts.

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Vinyl-Type Polynorbornenes with Triarylamine Side Groups: A New Class of Soluble Hole-Transporting Materials for OLEDs

박준하, 박명환, 도영규, *이민형

*KAIST 화학과 *울산대 화학과*

The soluble polynorbornenes bearing pendant triarylamine side groups were prepared by the vinyl addition polymerization of norbornene monomers with Pd(II) catalyst in combination with chain transfer agent (CTA). The polynorbornenes exhibit very high glass transition temperature (T_g > 268 °C) and good film forming ability. When being incorporated into the hole-transporting layer of tris(8-hydroxyquinolinolato)aluminum (Alq_3) based-electroluminescent devices through solution process, the polymers display excellent hole-transporting/injecting ability for the stable green emission of Alq_3. Details of synthesis, characterization, and hole-transporting properties of polymers will be discussed.

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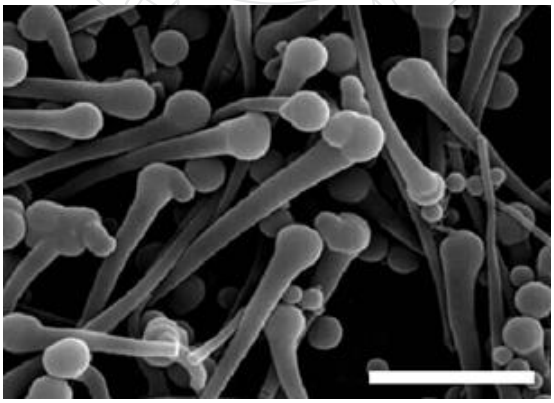
Keen Competition between Electrostatic and Argentophilic Interactions in the Formation and Behavior of Molecular Circles

노태환, 김치원, 김초롱, 정옥상, 안정민, 정옥상

부산대 화학과

The reaction of AgX (X^- = NO_3^- and $CF_3SO_3^-$) with bis(nicotinoyl)-4,4'-(9-fluorenylidene)diphenolate (L) as a hemicircle tecton has been studied. Discrete oblong circles and linked circles were constructed via the competition between the intercircular argentophilic interaction and the electrostatic interaction between Ag(I) and its anion, and the interconversion of the two species was attempted by means of anion. The delicate difference between both structures in solid state can be explained by the coordinating ability of anions.



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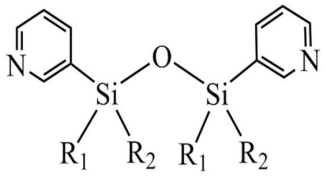
Anion Effects on Solution-behavior of Cyclodimeric Pd(II) Complexes

류윤경, 정옥상

부산대 화학과

The reaction of (dppp)Pd(OTf)$_2$ (dppp = 1,3-bis(diphenylphosphino)propane; OTf = trifluoromethanesulfonate) with L (L1 = 1,3-bis(pyridine-3-yl)tetramethyldisiloxane; L2 = 1,3-bis(pyridine-3-yl)dimethydiphenyldisiloxane; L3 = 1,3-bis(pyridine-3-yl)tetraphenyldisiloxane) in acetone affords single crystals consisting of cyclodimers, [Pd(dppp)(L)]$_2$(OTf)$_4$. Anion effects on the solution-behavior of each complex based on the ^{1}H NMR chemical shifts and conductivities, were carried out. The fluxionality of the cyclodimeric skeleton was found to be sensitive to the Hoffmeister series of anions.

L :



L1 : R_1 = methyl, R_2 = methyl
L2 : R_1 = methyl, R_2 = phenyl
L3 : R_1 = phenyl, R_2 = phenyl

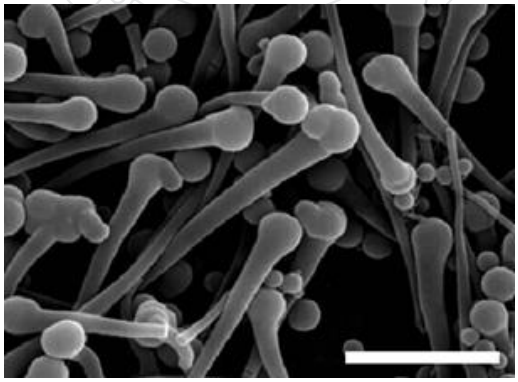
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P22포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Concentration Effects on the Formation of Morphology. Micro-sprout of Ionic Palladium(II) Complex

김초롱, 정옥상

부산대 화학과

The micro-sprout morphology is facilely formed by the reaction of *cis*-protected palladium(II) species in water with new pyridyl ligand in acetone in very dilute concentration, and followed by evaporation of acetone. The metallacyclodimer of ionic palladium(II) complex allows to form a micro-sprout morphology without any template or additive. However, the reaction produces the formation of microsphere in high concentration or fast evaporation of acetone. Furthermore, subtle surface modifications of the micro-sprout via typical anion exchange or sonication have been studied.



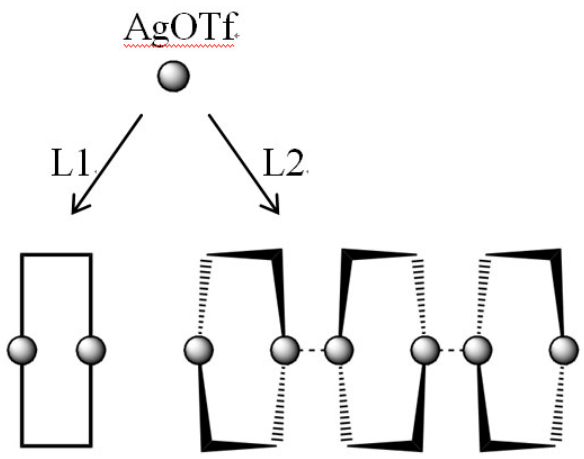
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P23포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Ring-Conformations via the Competition of Electrostatic Interaction and Argentophilic Interaction. Cyclodimeric Structures of Silver Trifluoromethanesulfonate Containing Isonicotinate Ester Ligands

김치원, 안정민, 정옥상

부산대 화학과

Metallacyclodimers, $[Ag(OTf)(L1)]_2$ and $[Ag(L2)]_2(OTf)_2$ (L1 = 1,3-dibromo-2,2-bis[(isonicotinoyloxy)methyl]propane; L2 = 2,5-dimethyl-2,5-bis(isonicotinoyloxy)hexane) were constructed and characterized. The crystal structure of $[Ag(OTf)(L1)]_2$ reveals a 32-membered cyclodimer, whereas that of $[Ag(L2)]_2(OTf)_2$ shows a linked 34-membered cyclodimer chain via intercyclic argentophilic (Ag…Ag) interactions. $[Ag(OTf)(L1)]_2$ affords racemic "twisted cyclodimer" whereas $[Ag(L2)]_2(OTf)_2$ produces "π-π interaction cyclodimer". Ring-conformation of the cyclodimers was affected via the competition of electrostatic interaction and argentophilic interaction.



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장소: 대전컨벤션센터
발표코드: **Ⅰ33P24포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Highly Efficient Aqueous Sensing of Cation and Anion by Fluorescent Dinuclear Zinc(II) Schiff Base Complexes

Snehadri Khatua, 김기봉, **D.G.Churchill**

KAIST 화학과

Design and synthesis of cation and anion-selective sensor has received considerable attention now a days. The development of selective receptors for phosphate anions and derivatives, such as HPO_4^{2-}, pyrophosphate (PPi), adenosine triphosphate (ATP), adenosine diphosphate (ADP) and phosphoproteins has been of particular interest because of the vital roles these chemical species play in a range of life processes. Cu^{2+} is an essential d-block metal ion in human health, but is also harmful to biological systems in excessive amounts. Accordingly, the development of Cu^{2+}-specific molecular probes have been of considerable interest in the biological and analytical sciences. Herein, we report the easy "one pot" synthesis of fluorescent dinuclear chiral zinc complexes $[Zn_2(slys)_2Cl_2]\bullet(CH_3OH)_2\bullet(H_2O)_3$ (1) and $[Zn_2(slys)_2(NO_3)_2]\bullet(H_2O)_2$ (2) in which the L-lysine based Schiff base ligand is generated in situ. Under neutral aqueous conditions (0.01 M HEPES buffer, pH 7.4), 1 and 2 exhibit intense blue fluorescence. The complex 1 is tested with several inorganic and biologically relevant anions in water at physiological pH. The dizinc species are found to act as a highly selective sensor for PPi in particular by fluorescence ON-OFF signaling. Both the fluorometric and colorimetric titration results suggest that compounds 1 is a highly selective sensor for PPi. Heavy metal ions such as Hg^{2+}, Pb^{2+}, Cd^{2+} and d-block metals such as Cu^{2+} are known generally to act as quenchers. As compounds 1 and 2 are highly fluorescent, significant quenching effect is expected from the aforementioned metal ions via direct displacement. The sensing behaviour of compounds 1 and 2 in presence of various metal cations has been investigated by various spectroscopic methods in water. The results confirm that 1 and 2 are highly sensitive and selective fluorescent ON-OFF probes for Cu^{2+} via direct displacement.

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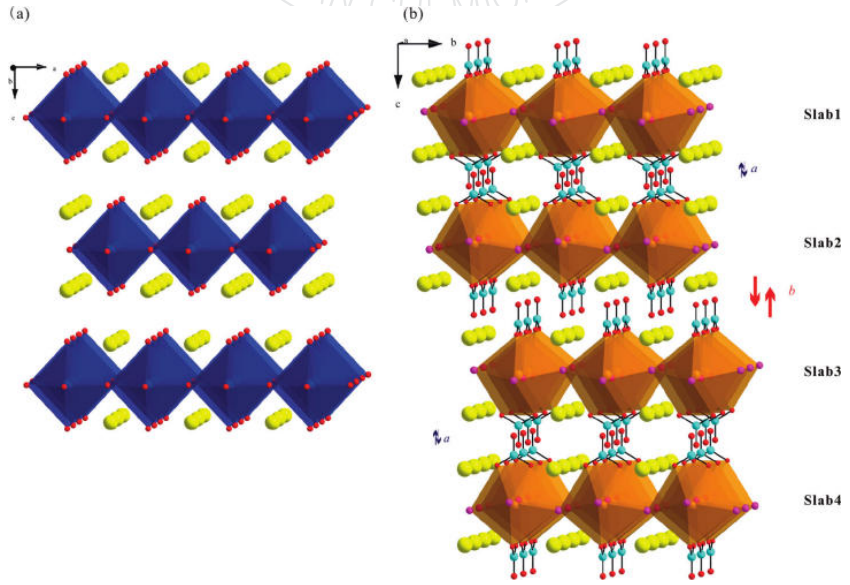
장소: 대전컨벤션센터
발표코드: **Ⅰ33P25포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

$Cs_2PbCl_2(NO_3)_2$: A new variant of layeredperovskite. Synthesis, charaterization, and Ion-exchange reaction to $CsPb_2Cl_5$.

김민경, 조빛나, 이동우, 옥강민

중앙대 화학과

A new variant of highly symmetric layered perovskite material with a NO_3^- ligand, $Cs_2PbCl_2(NO_3)_2$ has been synthesized by a hydrothermal reaction method using $Pb(NO_3)_2$, CsCl, and water at 240 °C. The structure has been determined by single-crystal X-ray diffraction. $Cs_2PbCl_2(NO_3)_2$ has a novel two-dimensional layered structure containing PbO_4Cl_4 polyhedra and NO_3 trigonal planes. $Cs_2PbCl_2(NO_3)_2$ is closely related to the n = 1 layered perovskite families. Detailed structural analysis, Infrared and UV−vis diffuse reflectance spectra, thermogravimetric analysis, and ion-exchange reactions of $Cs_2PbCl_2(NO_3)_2$ are reported.



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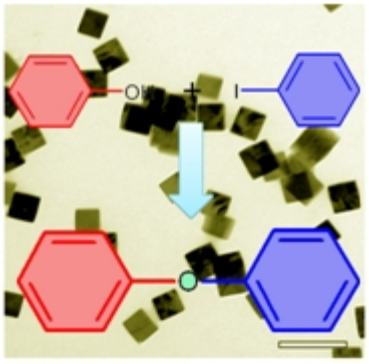
장소: 대전컨벤션센터
발표코드: **Ⅰ33P26포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Cu_2O Nanocubes-Catalyzed Cross-Couplings of Aryl halides with phenols via Ullmann coupling

김아영, 김지영, *박지찬, *송현준, 박강현

*부산대 화학과 *KAIST 화학과*

Thermal and air-stable uniform Cu_2O nanocubes developed an approach for gram-scale synthesis of by a one-pot polyol process. An efficient cross-coupling reaction of aryl halides and phenol using a catalytic amount (0.1 mol%) of Cu_2O nanocubes as recyclable catalyst with Cs_2CO_3 as the base in THF at 150 oC is reported. The process is simple and allows the formation of a diverse range of diaryl ethers in excellent yields.



일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P27포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Properties of Non-Framework Coordination Polymers Based on Metal-Organic Polyhedral Cages and Simple Diamine Linkers

정희진, 전형필

한양대 응용화학과

비선형 다이카르복실 리간드에 의해 이핵 외륜 (Paddlewheel) 단위가 꼭지점으로 연결된 다면체 형태의 금속-유기 거대 분자를 합성하였다. 이 거대 분자는 기체가 흡착할 수 있는 구 형태의 빈 공간 (d = 18 Å) 이 있으며, 각 외륜 마다 치환 가능한 용매 자리가 존재한다. 이 용매 자리에 간단한 다이아민 리간드를 연결하여 불규칙하게 확장된 비정질의 배위고분자를 얻었다. 이 배위 고분자는 거대 분자의 미세기공을 가질 뿐 아니라, 연결 리간드로 인해 메소기공이 추가로 생성된 것을 기체 흡착 실험으로 확인하였다. 이 다공성 배위 고분자에는 기능성 리간드를 연결할 수 있는 여분의 배위 자리가 존재한다.

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발표코드: **Ⅰ33P28포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Guest- and Temperature-Dependent Gate Opening in Gas Sorption Behavior of Flexible Metal-Organic Framework

서진우, 전형필

한양대 응용화학과

Zn(II)와 3,5-pyridinedicarboxylate (pydc)의 용매열 반응을 통하여 (10,3)-*a* 위상을 갖는 3 차원 골격구조를 합성하였다. Zn(II)와 pydc 리간드 모두 세 방향의 연결마디로 작용하여 골격의 상호침투가 없는 srs ($SrSi_2$) 구조를 이루고, 전체 확장구조는 지그재그 모양의 일차원 기공을 형성한다. 질소, 수소, 알곤 및 메탄 기체의 흡착실험 결과 이 MOF 는 비 다공성 물질의 거동을 보이지만 특정 압력범위에서 흡착량이 급격히 증가한다. 이러한 흡착거동은 기체의 종류와 온도에 따라 다르게 나타난다.

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발표코드: **Ⅰ33P29포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Topologies and Gas Sorption Properties of Metal-Organic Frameworks with 5-Pyrimidinecarboxylate

진나래, 서진우, 전형필

한양대 응용화학과

Co(II), Cd(II), Cu(II)와 5-pyrimidinecarboxylate (pmc) 리간드의 용매열 반응을 통해 세 가지 새로운 골격구조를 합성하였다. 이 MOF 들은 각각 bcu, rtl (rutile), nbo 의 구조를 가지며, 이는 위상기하학적 관점에서 중요하다. 특히 nbo 구조를 갖는 $[Cu(pmc)_2]$는 골격의 상호침투로 인해 선형 일차원 기공구조를 이루며, 손님분자가 접근 가능한 자유 부피는 전체 결정의 약 29%이다. 이산화탄소와 질소, 수소, 알곤, 산소, 메탄을 대상으로 한 기체흡착 실험 결과 $[Cu(pmc)_2]$는 이산화탄소만을 선택적으로 흡착하는 성질을 가지고 있다.

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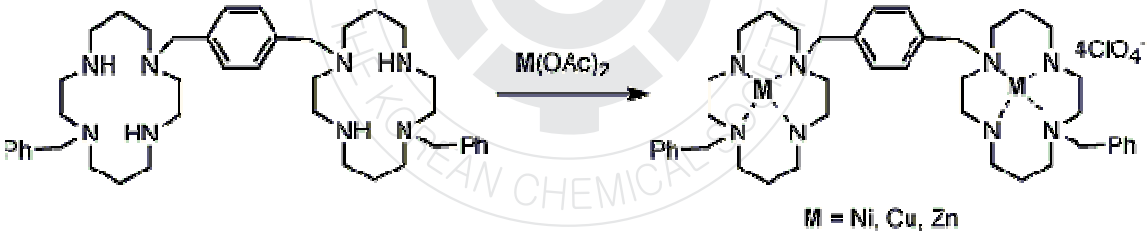
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis of Bicyclam Ligands and their Metal Complexes

오선화, 정미향, 김주창

부경대 화학과

Cyclams are of interest in the fields as diverse as catalysis, selective metal recovery and recycling sensors, therapy and diagnosis. The bicyclam containing two monobenzyl-cyclam units connected by a p-phenylenebis(methylene) linker. The oligomers were characterized by NMR, FT-IR and Elemental analysis. The syntheses and properties of Ni(II), Cu(II), Zn(II) complexes were investigated



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장소: 대전컨벤션센터
발표코드: **Ⅰ33P31포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Tetrameric Cu_4I_4 Coordination Polymers of 1,4-bis(2-(methylthio)ethoxy)benzene: Crystal Transformation and γ-CuI Nanocrystal Preparation

양호진

경상대 화학과

2D copper(I) coordination polymers $[Cu_4I_4L(CH_3CN)_2]_n$ (1) and $[Cu_8I_8L_3(CH_3CN)_2]_n$ (2) have been synthesized by the reaction of stoichiometric amounts of CuI and 1,4-bis(2-(methylthio)ethoxy)benzene (L). Heating both 1 and 2 near 105 ^oC has resulted in a new luminescent coordination polymer, $[Cu_4I_4L_2]_n$, 3 . Crystal structure of 3 by single crystal X-ray diffraction data analysis shows a 1D loop chain coordination polymer with inner metallomacrocycles based on cubane Cu_4I_4 clusters, which is topologically same as tubular 1D coordination polymers. Photoluminescence of 3 is a characteristic phenomenon of the cubane Cu_4I_4 cluster. Heating both 1 and 2 near 170 ^oC has yielded γ-CuI Nanocrystals.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Cu(I) Coordination polymer of N,N'-bis((methylthio)propyl) pyromellitic diimide : Vapochromism

박가람

경상대 화학과

Depending on the solvents used for crystallization, copper iodide and the flexible dithioether-type ligand incorporating pyromellitic diimide, N,N'-bis((methylthio)propyl) pyromellitic diimide (L) readily formed three distinct types of 1D (1) and 2D (2, 3) coordination polymers, which were previously reported. A new 2D network coordination polymer $\{[Cu_2I_2L_2]\bullet 2CH_2Cl_2\}_n$ (4) is prepared from the reaction of an equivalent amount of CuI and L in acetonitrile and dichloromethane. In this poster, single crystal X-ray structure, photophysical, and thermal studies of the coordination polymer 4 in solid state will be reported.

일시: 2009년 10월 28~30일(수~금) 3일간
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Mixed Valence Cu(I, II) Coordination Polymer from an NS Hetero-Donor Ligand

김태호, 양호진, 박가람, 김진은

경상대 화학과

An NS hetero-donor ligand with 4-pyridinylthiomorpholinomethanone (L) was prepared. Reaction of L with Cu(I) and Cu(II) salts afforded 3D network coordination polymers 1. We determined crystal structures by single crystal X-ray diffractometer. Structural, photophysical, and thermal studies of coordination polymers in solid state are reported.

일시: 2009년 10월 28~30일(수~금) 3일간
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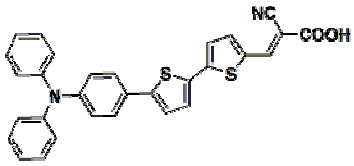
발표코드: **Ⅰ33P34포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Fastened effect of Triarylamine System for Organic Sensitizers

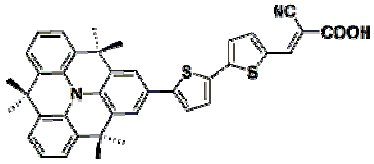
김덕현, 도광석, 김철우, 소슬기, 최혜주, 백상현, 강상욱, 고재중

고려대 소재화학과

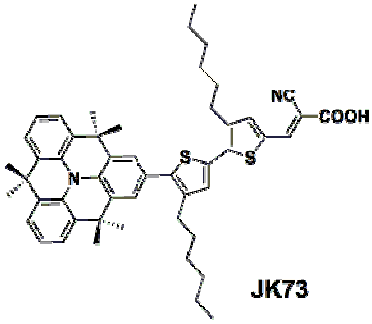
Four organic dyes, JK-72, JK-73, JK-74, and JK-75 containing dimethylmethylene bridged triphenylamine are designed and synthesized. Nanocrystalline TiO2 dye-sensitized solar cells were fabricated using these dyes. Under standard global AM 1.5 solar condition, the JK-72 sensitized solar cell gave a short circuit photocurrent density of 15.37 mA cm-2, open circuit voltage of 0.715 V, and a fill factor of 0.73, corresponding to an overall conversion efficiency η of 8.04 %. We found that the dimethylmethylene bridged triphenylamine is more efficient electron donor group than the no bridged triphenylamine due to the planar stable triphenylamine radical cation. And, the attachment of long alkyl chain causes the increase of open circuit voltage. The improved Voc value is attributed to the suppression of dark current owing to the blocking effect of a long alkyl chain.



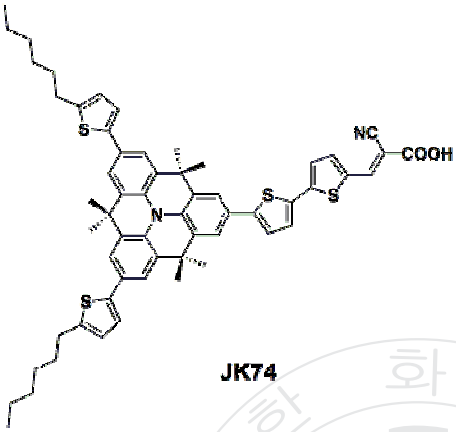
Reference(TNTT)



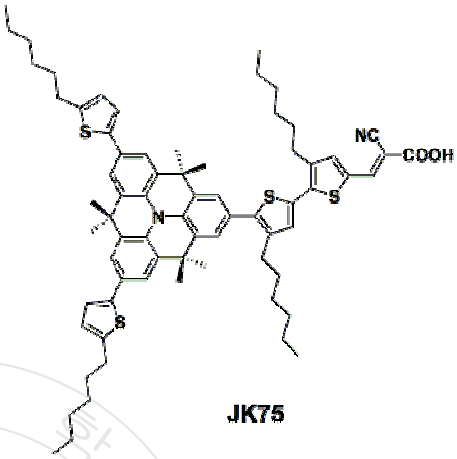
JK72



JK73



JK74



JK75

대한화학회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 목 12:30~14:30

New Spacer Group of Organic Sensitizer for DSSCs

백상현, 최혜주, 정반석, 김경준, 강상욱, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) have received attention due to their high performances and low cost. We designed organic sensitizer containing 3,4-Ethylenedioxy thoiphene (EDOT) moiety because of their planarity and rigidity. For increase π-conjugation, we introduced thieno[3,2-b]thiophene group to organic sensitizer. We made these two compounds as spacer group. We found difference between presence and absence of hexyl group. Consequently, we obtained new organic sensitizer having good power conversion efficiency.

일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P36포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

New Organic Sensitizer Containing Broaden Wavelength for DSSCs

최혜주, 백상현, 최홍식, 소슬기, 강상욱, 고재중

고려대 소재화학과

Dye sensitized solar cells(DSSCs) are currently attracting wide-spread interest as low-cost alternatives to conventional solid-state photovoltaic devices. Controlling the light harvesting in DSSCs is very important due to the scientific and industrial interest to enhance the photoenergy conversion efficiency. We introduce 3,4-ethylenedioxy thoiphene(EDOT) as spacer group, we expect to increase π-conjugation and electron donor ability. Since S-O intramolecular interations between the two central EDOT groups resilt in a planatizrion and rigidification of the conjugated system, and hence in an enhanced π-electron delocalization. So we made new organic compounds containing EDOT moiety. As a result, Absorption maxima(λmax) is red shifted. We expect to get high power conversion efficiency.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Electron-Donating Ability of 2,2':6',2"-Dithiatriphenylamine Sensitizers

김철우, 최현봉, 김점종, 강상욱, 고재중

고려대 소재화학과

Some p-substituted triphenylamine radical cations are stable species in a propeller-like structure in solid state. However, the unsubsitituted triphenylamine shows an irreversible oxidation peak in its cyclic voltammogram, indicating that the radical cation has much poorer stability. In order to obtain insight into their electron-donating ability and stability, we have investigated the lesser bridged triphenyl amines, 2,2':6',2"-dithiatriphenylamine. We were to get the JK-126, JK-150 contained 2,2':6',2"-dithiatriphenylamine.

일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
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발표종류: 포스터, 발표일시: 목 12:30~14:30

Molecular Engineering of Organic Sensitizers containing Fused-amine as Electron Donor Group for Dye-Sensitized Solar Cells

도광석, 김덕현, 정반석, 강상욱, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) are currently attracting considerable academic and industrial interest as low-cost, high-efficiency alternatives to the conventional silicon p-n junction photovoltaic devices. It have been used not only transition metal complex but also organic dye as photosensitizers for dye-sensitized solar cells. A planar stable triphenylamine radical cation is fascinating π-electron system that is potentially applicable to electronic and magnetic materials. The triphenylamine framework of fused-amine•+ is most likely planar. The dimethylmethylene bridges prevent to its π-π stacking. So JK-110 and JK-117 containing fused-amine for donor group are designed and synthesized. Under standard global AM 1.5 solar condition, We found that the η of JK-117 was higher than η of JK-110 due to the higher Voc. The improved Voc value is attributed to the suppression of dark current owing to the blocking effect of a long alkyl chain.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

An Efficient Dye-Sensitized Solar Cell with an Organic Sensitizer Encapsulated in a Cyclodextrin Cavity

최현봉, 조나라, 소슬기, 강상욱, 고재중

고려대 소재화학과

We encapsulated the JK-2 dye inside the cavity of CDs in order to retard the charge recombination and to prevent the aggregation of dyes. The β-CD/JK-2 device using a polymer gel electrolyte gave an overall conversion efficiency of 7.40%. The efficiency is the highest one reported for DSSCs based on the organic sensitizers. Moreover, the β-CD/JK-2 device showed an excellent stability under light soaking at 60 °C for 1000 h. The high efficiency and excellent stability may be attributed to the encapsulation of JK-2 inside the cavity of CD. We believe that the development of highly efficient DSSCs device with excellent stability is possible through various interfacial modifications and work on these is now in progress.

일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P40포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

The Introduction of EDOT-Vinyl Moiety into the Bridge Part of Dye for DSSCs

조나라, 김경준, 소슬기, 강상욱, 고재중

고려대 소재화학과

In these Dye Sensitized Solar Cells(DSSCs), sensitizing dye molecules have to be chemically adsorbed on the meso-porous nanocrystalline TiO_2 surfaces, and harvest solar light ranging from the UV to visible and near-IR regions just like photovoltaic semiconductor diode interfaces. As the introduction of 3,4-ethylenedioxy thiophene(EDOT)-Vinyl moiety into the bridging part, we expect to increase π-conjugation and electron donor ability. Hence, we also expect that these cells get high power conversion efficiency.

일시: 2009년 10월 28~30일(수~금) 3일간
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Neopentyloxybenzene-Functionalized Triphenylamine Dyes for Efficient Molecular Photovoltaics

임기민, 최현봉, 최홍식, 강상욱, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) are currently attracting considerable academic and industrial interest as low-cost, high-efficiency alternatives to the conventional silicon p-n junction photovoltaic devices. We designed and synthesized new organic dyes, which have a triphenylamine derivative as donating group and cyanoacrylic acid as withdrawing group and hexyl-substituted thienothiophene as bridging group. We expected that alkyl chain prevented the recombination, whereas adsorptions were decrease. Consequently we could find roles of alkyl chain, which were advantageous and disadvantageous, through this experiment.

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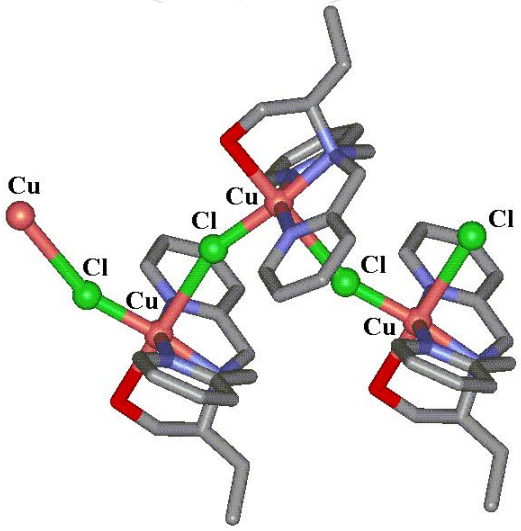
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Optically Active 1-D Coordination Polymer, (R)-2-(Bis(pyridin-2-ylmethyl)amino)butan-1-ol Copper(II) perchlorate

김미현, *신디, *데위, **민길식, 조정환, *김양, ***최지영, ****변종철

*고신대 화학신소재학과 *고신대 화학 신소재학과 **경북대 사범대학 화학교육과*
****제주대 화학과 ****제주대 자연과학대학 화학과*

A novel optically active ligand, (R)-2-(bis(pyridin-2-ylmethyl)amino)butan-1-ol (L), and its copper(II) complex as 1-D coordination polymer was prepared and characterized by crystallography, circular dichroism spectrum, and magnetic susceptibility. The X-ray structure of [CuLCl]ClO4 showed that the copper is bound to all four donor atoms of L, with N1, N2, N3 and a Cl1 ligand occupying equatorial positions while the alcohol oxygen (O1) of the 2-aminobutane-1-ol substituent is bound in an axial position of what approximates a distorted square pyramidal coordination geometry.



일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Investigation of Monolayer LB Film Properties of Silsesquioxane

신대식

동아대 화학과

In this study use silsesquioxane hybrid between dendrimer and polymer. We expect that dendritic branches have networking structure which is difficult to make uniformly monolayered film. We obtain easily uniform monolayer because molecule combination with interaction on water-air interface. Moreover, this networking structure would have regularly uniformed hole. The fabricated Langmuir-Blodgett (LB) films of carbosiloxane dendrimer was obtained as a thin film. We investigated the monolayer behavior by π-A isotherm at the air-water interface. The π-A curves indicated surface pressure of this LB film from liquid to solid state between 5 and 8 mN/m. The monolayer was deposited onto highly oriented pyrolytic graphite (HOPG) substrates by Y-type deposition at surface pressure 5.5 mN/m. We also observed the morphological of the silsesquioxane hybrid LB films using SPM and determined the electrical property of LB films using STM.

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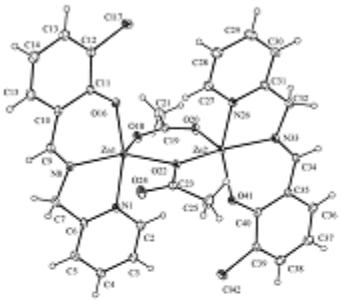
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

The Luminescent Zinc Complexes with 2-Substituted-6-((pyridin-2-ylmethylimino)methyl)phenol

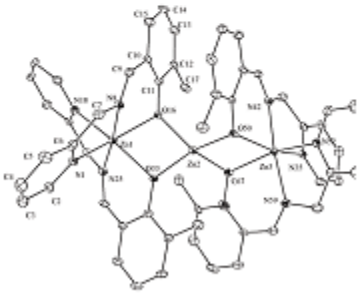
이진영, *서회주, **김지훈, ***강성권, 김영인

*부산대 화학교육과 *부산대 화학과 **부산대 첨단정보및디스플레이소재협동과정*
****충남대 화학과*

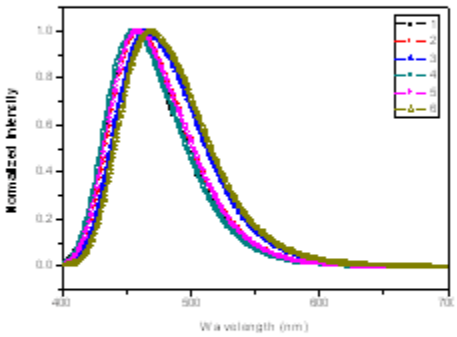
Dinuclear and trinuclear zinc complexes, $[Zn(PP)(OAc)_2Zn(PP)]$(1), $[Zn(ClPP)(OAc)_2Zn(ClPP)]\bullet CHCl_3$ (2), $[Zn(CH_3PP)(OAc)_2Zn(CH_3PP)]$(3), $[Zn(PP)ZnZn(PP)]\bullet(PF_6)_2$(4), $[Zn(ClPP)ZnZn(ClPP)]\bullet(PF_6)_2$(5) and $[Zn(CH_3PP)ZnZn(CH_3PP)]\bullet(PF_6)_2$(6) were obtained using N,N,O- tridentate Schiff base which was prepared from 3-substituted-2-hydroxybenzaldehyde (x=H, Cl, CH_3) and 2-picolylamine. The prepared complexes were characterized by optical, photoluminescence (PL) and cyclic voltammetry (CV) method. The complexes showed emission peaks in blue region (455~470nm) resulting from intraligand ($^1\pi$-π^*) fluorescences.The CV showed the oxidation potentials in the range of 1.03V~1.40V. The structure of complex 2, 6 were determined using X-ray crystallography.



complex 2 .



complex 6 .



대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

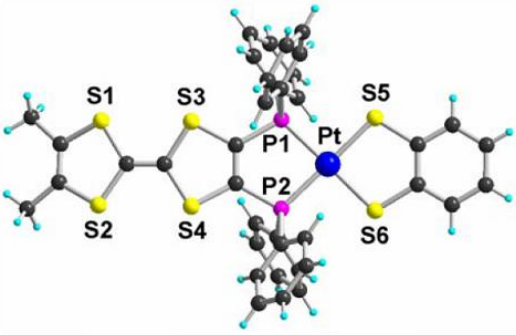
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P45포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Redox Multifunctionality in (P2)Pt(II)(dithiolene) Complexes

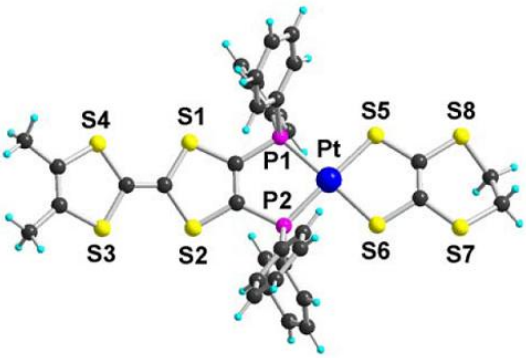
이수경, *Marc Fourmigué, 노동윤

*서울여대 화학과 *Université de Rennes 1*

[(P2)Pt(dithiolene)] complexes where P2 is 3,4-dimethyl-3',4'-bis(diphenylphosphino) tetrathiafulvalene and dithiolene is benzene-1,2-dithioltate (bdt), 1,3-dithiole-2-thione-4,5-dithiolate (dmit) or 5,6-dihydro-1,4-dithiin-2,3-dithiolate (dddt), were synthesized using (P2)$PtCl_2$ and the 1,2-dithiolate precursors. The molecular structures of complexes were determined from single crystal X-ray diffraction, together with a model compound [(dppe)Pt(dddt)] (dppe: bis(diphenylphosphino)ethane). Electrochemical studies using cyclic voltammetry (CV) show that at least three reversible oxidation waves are observed in the bdt and dmit complexes, but four sequential reversible redox processes are exhibited in the case of [(P2)Pt(dddt)]. The successive oxidations of the two covalently linked but electronically uncoupled Pt(dddt) and P2 electrophores, are supported by electrochemistry of the model compound [(dppe)Pt(dddt)] containing only Pt(dddt) electrophore and DFT calculations of HOMO of the neutral [(P2)Pt(dddt)] and SOMOs of the $[(P2)Pt(dddt)]^{1+/2+/3+}$ cation.



[(P2)Pt(bdt)]



[(P2)Pt(dddt)]

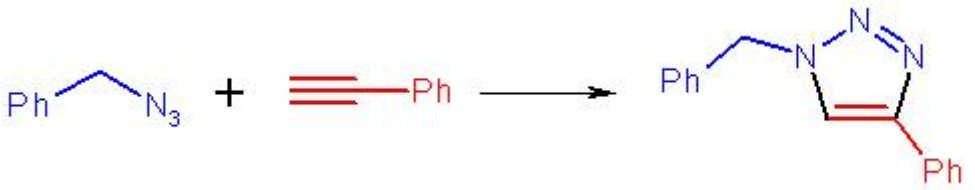
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ33P46포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

CuO Hollow Nanostructures Catalyzed Alkyne-Azide Cycloadditions

강현태, 김지영, *박지찬, *송현준, 박강현

*부산대 화학과 *KAIST 화학과*

The reaction forming a triazole-containing carbon-heteroatome bond through Huisen [3+2] cycloadditions is a representative example of click reactions. (Eq1) This reaction makes triazoles from azide and terminal alkynes. We show here that CuO nanoparticles have been used for the catalytic [3+2] Cycloaddition of Azides with Terminal Alkynes to provide the products in good yields with high regioselectivity. Reaction conditions are amazingly improved in comparison with previous catalytic systems and commercial available micro size CuO(II).



Eq 1.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Metallasupramolecular Frameworks Constructed by Self-assembly of Calix[4]arene spacer and Lanthanide-Transition-Metal ions

강은주, 김진은, 이심성, 박기민

경상대 화학과

Of a variety of macrocyclic molecules, the calixarene has been spotlighted as one of the most attractive macrocycles in supramolecular chemistry because of not only well-defined their molecular structures but also the ease of modification from simple calixarenes to functionalized calixarene derivatives. Although syntheses and applications of many calixarene derivatives have already been investigated and reported, a lot of effort has been only devoted to develop of sensory materials against cations or anions. In order to utilize not only as a strong multi-nucleating ligand but also as a spacer with cavity, we have designed and synthesized the potassium salt of calix[4]arene tetracarboxylate ($CTCK_4$, $\{[K_2(K_2@CTC)]\bullet G\}_n$, G = solvent molecules) with 1,3-alternative conformation and four carboxyl groups. Self-assembly of the lanthanide-transitio-metal ions (Er, Eu,and Sm) and $CTCK_4$ leads to the formation of 3D metallasupramolecular frameworks. We present here the crystal structures of 3D supramolecular frameworks consisting of the lanthanide-transition-metal ions and calix[4]arene spacer ligand.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

NBO-Functionalized Magnetic Silica Nanoparticles as a Selective Fluorogenic Chemosensor for Cu^{2+} Ion

박민성, 정종화

경상대 화학과

The nitrobenzoxadiazolyl (NBO)-based receptor was synthesized of the nitrobenzoxadiazolyl, aminodiethyl alcohol and triethoxysilane in dried THF. The fluorogenic NBO-based receptor was immobilized by grafting reaction in toluene under reflux condition. 1 was characterized by transmission microscope (TEM), scanning microscope, TGA, and FT-IR. The NBO-based receptor was attached onto the surface of magnetic silica nanoparticles with 40 nm of diameter by covalent-bonds. Then, we carried out fluorogenic changes of 1 upon the addition of metal ions such as Na^+, K^+, Ca^{2+}, Ba^{2+}, Ag^+, Cd^{2+}, Mn^{2+}, Hg^{2+}, Co^{2+}, Fe^{2+}, and Cu^{2+} ions in aqueous solution. In the fluorescence spectrum, free 1 exhibited an emission maximum at 536 nm. Very interestingly, the fluorescence intensity of 1 dramatically decreased upon addition of Cu^{2+} ion. On the other hands, no significant changes were observed for other metal ions. These results indicate that 1 selectively recognize only Cu^{2+} ion. Upon addition of increasing Cu^{2+} ion concentrations, the λem gradually quenched at until mole ratio 1:1, whereas the fluorescence intensity of 1 did not change at above mole ratio 1:1. The results support the view that NBO moiety attached onto 1 forms 1:1 complex with Cu^{2+} ion. Therefore, 1 is useful as solid chemosensor and adsorbent for Cu2+ ion.

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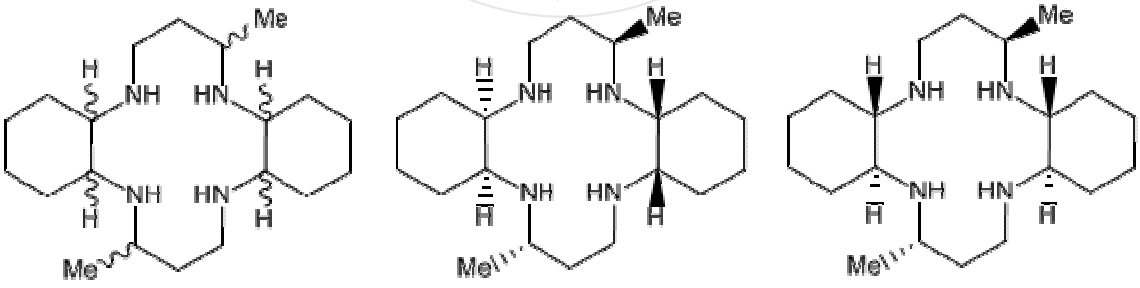
Different Cp (Cp = cyclopentadienyl) conformations induced by zinc(II) macrocycles

곽진숙, 김주창

부경대 화학과

Two new zinc(II) coordination polymers $\{[Zn(L1)(Fe(\eta^5\text{-}C_5H_4COO)_2)]\cdot 3H_2O\}_n$ (1) and $\{[Zn(L2)(Fe(\eta^5\text{-}C_5H_4COO)_2)]\cdot 2H_2O\}_n$ (2) (L = 3,14-dimethyl-2,6,13,17-tetraazatricyclo[14.4.0^{1,18}.0^{7,12}]docosane) have been prepared and structurally characterized. Although complexes 1 and 2 showed similar 1D coordination polymers, their ferrocenyl conformations were totally different, where the ferrocenyl groups of fdc (fdc = 1,1´-ferrocenedicarboxylate) ligands were staggered (in 1) and eclipsed (in 2). It is believed that the introduction of diastereomerically related macrocycles L1 and L2 cause different ferrocenyl conformations in complexes 1 and 2.



L **L1** **L2**

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Optical Characterization of ZnS:Mn/ZnS core-shell quantum dot

이재욱, *황청수

*단국대 무기화학실험실 *단국대 화학과*

The preparation of semiconductor nanocrystal ZnS:Mn/ZnS core-shell quantum dot is described. This compound was synthesized by a thermal decomposition reaction of diethylzinc, bis(acetylacetonato)manganese(II), and Hexamethyldisilthiane at various temperature (50℃, 100℃, 135℃, 150℃, 175℃, and 200℃) in a hydrophobic media (n-trioctylphosphine). This nanocrystal was optically characterized by UV-Vis and Photoluminescence spectroscopies. The particle sizes were measured via HR-TEM images and atomic ratio was measured EDXS.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Surface Analysis of Histidine and Cysteine Capped Water ispersible ZnS Nanocrystals

김송이, *황청수

*단국대 무기화학실험실 *단국대 화학과*

The surface of histidine and cysteine capped water dispersible ZnS nanocrystals was analyzed Raman spectroscopy. In this work, water dispersible ZnS nanocrystals were synthesized by using various amino-acids as polar surface capping agents in aqueous solvent. These compounds were characterized by FT-IR, Photoluminescence(PL) spectroscopy and Raman spectroscopy. The particle sizes were measured via HR-TEM images and atomic ratio was measured by EDXS.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Surface analysis by Raman spetroscopy for L-valine capped ZnS nanoparticles.

이상민, *황청수

*단국대 *단국대 화학과*

In this work, water dispersible ZnS nanocrystals were synthesized by using L-valine as polar surface capping agent in aqueous solvent.Surface characterization was performed by FT-IR and Raman spectroscopies. The specific coordination mode of the valine molecules on the nanocrystal surface was determined by comparing the obtained peaks of certain vibratinal modes, such as stretching peaks of NH and C=O groups, to that for a precursor complex, [Zn(val)2(H2O)], and free valine.The particle sizes were measured via HR-TEM images and atomic ratio was measured EDXS.

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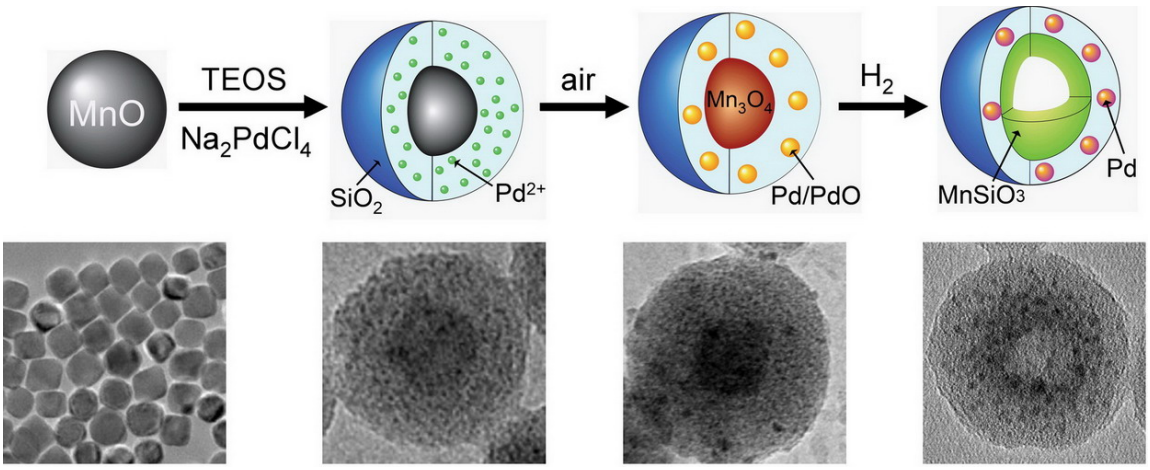
Generation of Hollow Nanostructure of $MnSiO_3$ through the Solid-state Reaction of Mn_3O_4 and Pd/PdO Nanocrystals Dimensionally Confined within Nanosized Silica Sphere

신종민, 이인수

경희대 응용화학과

An important research direction in nanoscience is to synthesize and fabricate hollow nanoparticles having attractive potentials in diverse field including catalysis, energy storage, drug delivery, and medical imaging. This poster presentation will report the generation of a hollow nanostructure through a novel solid-state approach using nanoparticles co-encapsulated within a silica nanosphere. In the course of annealing the silica nanosphere incorporating Mn_3O_4 and Pd/PdO nanocrystals, it was found that the Mn_3O_4 nanocrystals were reduced and transformed into a hollow $MnSiO_3$ nanostructure. It was also revealed that the formation process of hollow nanostructure was facilitated by the co-encapsulated Pd nanocrystals. Such a solid-state conversion of nanoparticles into a hollow structure is very unique and can be achieved only by a reaction dimensionally confined within nano-sized matrix.



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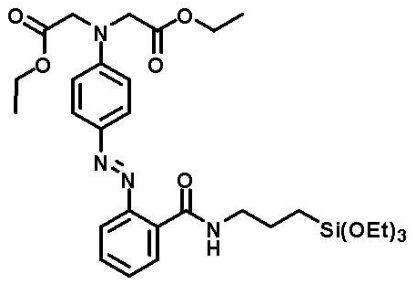
Introducing Distinctly Different Chemical Functionalities onto the Interanl and External Surfaces of Silica Nanotubes

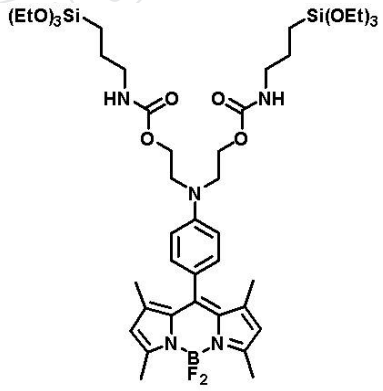
김은정, 서성민, 이혜영, 배두리, 정종화

경상대 화학과

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



Ligand 1



Ligand 2

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Surface Modification of Exfoliated Layered Gadolinium Hydroxide for Development of Multimodal Contrast Agent for MRI and Fluorescence Imaging

윤영수, 이경식, 변송호, 이인수

경희대 응용화학과

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

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Synthesis of $CuIn(S_{1-x}Se_x)_2$ nanoparticles through a simple sonochemical method

황차환, 박재영, 박종필, 옥강민, 심일운

중앙대 화학과

Synthesis of $CuIn(S_{1-x}Se_x)_2$ nanoparticles through a simple sonochemical method were tried in various solvents under the multibubble sonoluminescence (MBSL) conditions. For the synthesis, we used copper nanoparicles, $InCl_3 \cdot 4H_2O$, thioacetamide, and selenium powder. Methanol was used as solvent with ethylenediamine. The prepared $CuIn(S_{1-x}Se_x)_2$ nanoparticles are examined by XRD, ICP, UV-vis spectrophotometer, and HR-TEM.

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Bandgap Engineered ImP/CdSe and CdSe/InP Core/Shell Quantum Dots

박재현

아주대 분자과학기술학과

Various nanostructures have attracted considerable attention on account of their novel properties and potential applications. One of the most interesting fields of these nanostructures is the heterojuction formed between semiconductor materials with different band offsets, particularly a core-shell structure in colloidal nanocrystals. These structures exhibit good electronic properties, such as high emission quantum yield (QY) and enhanced photo-stability, which are difficult to be achieved with a single component. Therefore, many studies have examined core/shell materials with a heterojunction in the interface, which are called type-I, type-II and reverse type-I band offsets. Among them, the recently developed type-II structures, which were triggered by the creative works of Bawendi's group, have attracted considerable attention because the staggered band offsets between the core and shell may allow tuning of the emission wavelength and photo-stability. We report the synthesis of InP/CdSe and CdSe/InP core/shell nanocrystals with a heterojuction of both the II-VI and III-V family. The optical properties of the core-shell nanocrystals are affected by the energetic offsets between the valence and conduction band edges of the two constituents.Both showed a red-shift in absorption and emission, which was expected from the modeled wave function and probability density. The staggered band alignment separates the wave functions of the electron and hole, which results in many novel properties including a red-shift in emission and a long decay life time because the emission originates from the radiative recombination of an electron-hole pair across the core/shell interface.

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Fabrication of Mn-Ferrite Nanoparticles from MnO Colloids and Their Toxicity Studies

한안나

아주대 분자과학기술학과

Colloidal magnetic nanocrystals have been studied extensively on account of their peculiar magnetic properties resulting from their nanosized domains. They are core materials in many applications related to data storage, magnetic separation, drug delivery and magnetic resonance image(MRI) contrast enhancement. Magnetic ferrites, which are expressed by MFe_2O_4 (M: Fe, Co, Mn, Ni, Cu, Zn), have attracted considerable attention and been well studied because of their easy magnetic property engineering by adjusting the M^{2+} ion. Various methods have been used to synthesize ferrite nanocrystals, including reverse micelle and nonhydrolytic methods.we report a new method for fabricating $MnFe_2O_4$ nanocrystals and their toxicity studies. Additionally, the possibility for a dual functional MRI contrast agent in T_1 and T_2 imaging will be presented. The cytotoxicity of manganese ferrite was examined on MCF-10A normal cells and various breast cancer cells (MDA-MB435S, MDA-MB 231 and MCF-7). Few reports have been published on cytotoxicity of manganese ferrite nanocrystals. The microscopy images showing the morphological changes indicated that two type cells were not damaged at concentrations between 0.1 mM and 1 mM.The magnetization value is much lower than those reported previously, which might be due to the small size and low crystallinity of the ferrite nanoparticles. Although the weak magnetic property could be regarded as a drawback, it was found that it can provide an opportunity for dual MRI contrast agents. Generally, manganese ferrite has a T_2 weighted effect because of its strong magnetic properties. However, the low r_2 value of ferrite by this method gives it a useful T_1 weighted effect.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Metal Coordination Polymeric Hydrogel from A Pyridine-Based Ligand

정성호, 이혜진, *J. J. Vittal, 정종화

*경상대 화학과 *National University of Singapore, Singapore*

Compound 1 was synthesized and its gelation ability was evaluated in the absence and the presence of transition metal ions such as Cu^{2+}, Zn^{2+}, Co^{2+}, Mn^{2+}, Fe^{3+}, and Cd^{2+} in organic solvents. Interestingly, 1 formed gel in the presence of Cu^{2+} ion without heating process. In addition, the rdination polymeric hydrogel 1 induced Cu^{2+} was evaluated by various anions such as NO_3^-, ClO_4^-, CH_3COO^-, SO_4^-, I^-, Br^-, and Cl^-. The coordination gel formation of 1 is independent anions. The gelation is attributed to the self-aggregation of 1D coordination polymers to form 3D nanostructures through non-covalent interactions to entrap solvent molecules. The freeze-dried organigel exhibits rod-like fiber structure with 40-50nm diameter. The fluorescence intensity of the coordination polymeric hydrogel 1 in the presence of Cu^{2+} decreased upon the addition of Cu^{2+} ion. According to DSC measurement, the coordination polymeric hydrogel 1 in the presence of 3 equivalent of Cu^{2+} ion was stable until 90 oC. Furthermore, mechanical ananlysis including dynamic oscillation on shear, steady shear, and creep testing have been performed to elucidate the supramolecular nature of 3D assembly. Together with the viscoelastic properties and biocompatibility, hydrogel may find utility as a novel soft material in biomedical and photochemistry fields.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis of Tetrazol-Based Coordination gelator and Its Gelation Fluorescent property

이혜진, 정성호, *J. J. Vittal, 정종화

*경상대 화학과 *National University of Singapore, Singapore*

Compound 1 was synthesized and its gelation ability was evaluated in the absence and the presence of transition metal ions such as Cu^{2+}, Zn^{2+}, Co^{2+}, Mn^{2+}, Fe^{3+}, and Cd^{2+} in organic solvents. Interestingly, 1 formed gel in the presence of Zn^{2+}, Cu^{2+} and Co^{2+} ions without heating process. In addition, the coordination polymeric gel 1 induced Zn^{2+} was evaluated by various anions such as NO_3^-, ClO_4^-, CH_3COO^-, SO_3^{2-}, I^-, Br^- and Cl^-. The coordination gel formation of 1 is independent anions. The gelation is attributed to the self-aggregation of 1D coordination polymers to form 3D nanostructures through non-covalent interactions to entrap solvent molecules. The freeze-dried organigel exhibits a fibrillar network structure. UV/vis absorption studies illustrate that the organogel displays a typical π - π* transition. The fluorescence intensity of the coordination polymeric gel 1 in the presence of Zn^{2+} is enhanced dramatically with a longer lifetime upon gel formation. In particular, the fluorescence intensity of the coordination polymeric gel 1 was highest in the presence of 3 equivalent of Cu^{2+}, ion. The results indicate that 1 forms the coordination polymeric gel by 1:3 stoichiometry. These results imply that the 1 forms the coordination polymeric gel is applicable as a novel soft material in biomedical and photochemistry fields.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Development of Volatile MetalAlkoxide Precursors for Transparent Conductive Oxides Thin Film.

민재기, 김창균, 정택모

한국화학연구원 화학소재연구단

Transparent conductive oxides (TCO) have been widely used as passive applications like transparent electrodes for liquid crystal display (LCD), organic light-emitting diodes (OLED), and solar cells. Recently, transparent oxides have attracted considerable attention asnovel candidates for channel materials of thin-film transistors (TFTs). Various kinds of oxide semiconductors have been reported in the last few years, such as ZnO, Mg-Zn-O, Zn–Sn–O (ZTO), In–Zn–O (IZO), SnO_2, Ga_2O_3, In–Ga–O (IGO), In_2O_3, In–Sn–O (ITO), TiO_2, single-crystalline $InGaO_3(ZnO)_5$ superlattice and amorphous In–Ga–Zn–O (a-InGaZnO).In this presentation, we will talk synthesis, structure, and properties of novel metal precursors, containing volatile donor-functionalized alkoxy derivatives for transparent conductive oxides.

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Synthesis of new alkylimido tantalum complexes with amino alcohol ligands; their thermal behaviour and application to tantalum containing thin film.

박용주, 성기환, 신수정, 이상경

테크노세미켐(주) 박막재료개발팀

Metal organic tantalum complexes have been attracted in the preparation of tantalum containing materials as precursors for MOCVD or ALD. In this presentation, we introduce the synthesis and characterization of novel alkylimido tantalum complexes with aminoalkoxide which are synthesized by the substitution reaction of amino alcohol with alkylamide of TBTDET (tert-butyltridiethylaminotantalum) in hexane. Amino alcohol ligands, as bidentate ligands, were introduced to stabilize the coordination sites of metal. Thermal behaviour of the compounds are presented and discussed by the results of NMR and TGA. We have prepared tantalum containing films on Si or SiO_2 substrates using new tantalum precursors with /without oxygen gas by MOCVD. The properties of deposited films in the various temperature were characterized by SEM, XPS and XRD.

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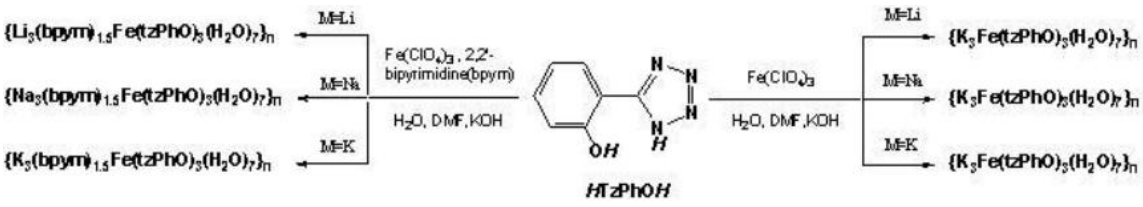
Fe – M Mixed Metal High Dimensional Coordination Polymers Containing Tetrazole (M = Li, Na, K)

이강문, *이준승, 도영규

*KAIST 화학과 *Department of Chemistry, University of Utah, U.S.A.*

From the aqueous reaction of iron perchlorate, MOH, 2,2'-bipyrimidine(bpym) and 5-(2-hydroxylphenyl)-1H-tetrazole (HtzPhOH) in 1 : 3 : 1.5 : 3, high dimensional coordination complexes, $[M_3(bpym)_{1.5}Fe(tzPhO)_3(H_2O)_7]_n$ (M = Li, 1; Na, 2; K, 3), have been synthesized and their structures were determined. All complexes bear $Fe(tzPhO)_3$ fragment of C_3 symmetry as building unit. By hydrogen bonding among alkali-metal cation hydrates, all complexes have 3-D structures. In addition, complexes 2 and 3 have quite short Fe – M distances. In the absence of bpym, the foregoing reaction system afforded high dimensional coordination complexes $[\{LiFe(tzPhO)_3(H_2O)\}_2\{Li(H_2O)_4\}_2\{Li_2(H_2O)_7\}(H_2O)_{4.5}]$ (1'), $[Na_3Fe(tzPhO)_3(H_2O)_3]$ (2') and $[K_3Fe(tzPhO)_3(H_2O)_7]$ (3'). X-ray analysis revealed that alkali metal ion was encapsulated in two pairs of $Fe(tzPhO)_3$ fragment via two κ^3-O binding in 2' and 3', resulting in the alternating arrangement of transition metal and alkali metal (M – Fe – M – Fe – M; M = Na, K). For 3', π-interaction of K and phenyl ring of tetrazole ligands was observed.



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Nanocomposite Borides based on $LiBH_4$and $Ca(BH_4)_2$ for Hydrogen Storage

이지연, 허남회

서강대 화학과

$LiBH_4$ is one of the promising candidates for hydrogen storage materials. However, dehydrogenation of $LiBH_4$ occurs above 400℃, which limits its use in its pristine form. In order to lower the dehydrogenation temperature, we have designed to make new composite materials simply by mixing with $Ca(BH_4)_2$. The underlying design principle of this composite system is on the basis of the recently proven reversibility of $6LiBH_4$+CaH_2 composite and $Ca(BH_4)_2$ itself. By a combination of differential scanning calorimeter and in-situ synchrotron XRD measurements, we have found that eutectic melting of $(1-x)H_4$ +$xCa(BH_4)_2$ takes place around 200 ℃ in a wide range of x. The decomposition characteristics and the hydrogen capacity of this composite are strongly dependent on the relative composition (x), and at a certain value of x we found that decomposition was finished below 400 ℃, showing more than 10 wt% hydrogen capacity. Reversibility of this system was also confirmed.

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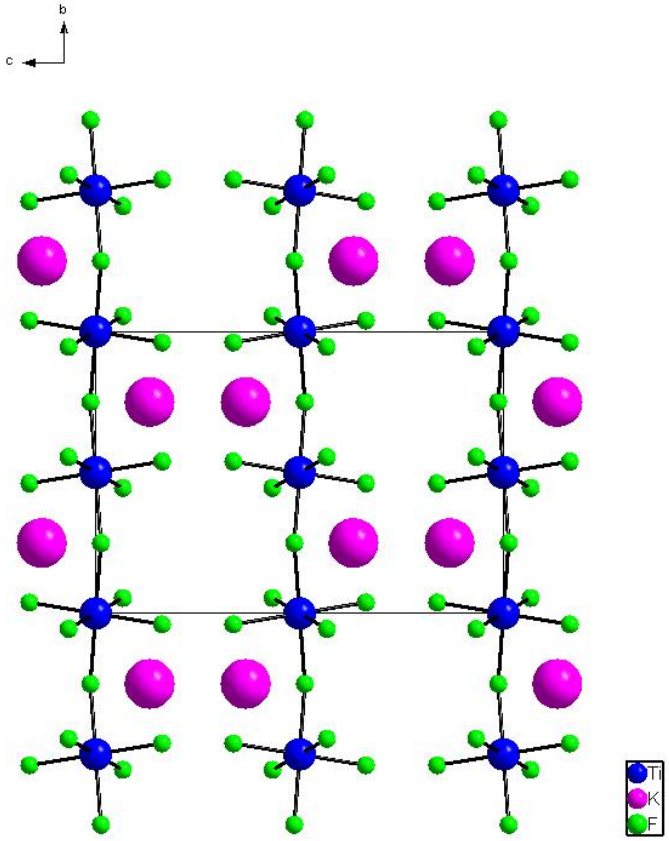
New 1D chain titanium fluoride materials : Synthesis, Structure, and Magnetic properties of K_2TiF_5 and $Rb_2TiF_5.H_2O$

조빛나, 김민경, 이동우, 옥강민

중앙대 화학과

Two new uni-dimensional chain comounds, K_2TiF_5 and $Rb_2TiF_5.H_2O$ have been synthesized by a mild hydrothermal reaction technique using TiO_2, KHF_2 (or RbF), N,N-dimethylformamide (DMF), and H_2O as reagents. The structure of the reported materials were determined by single crystal X-ray diffraction. K_2TiF_5 and $Rb_2TiF_5.H_2O$ exhibit similar 1D chain structures with corner-sharing Ti3+ O6 octahedra. Interestingly, the titanium metal cations have been reduced from Ti^{4+} to Ti^{3+} during the synthesis. Thus, both single crystal products show light violet. Powder X-ray diffraction, Infrared spectra, thermogravimetric analysis, and magnetic measurements are also presented.


b
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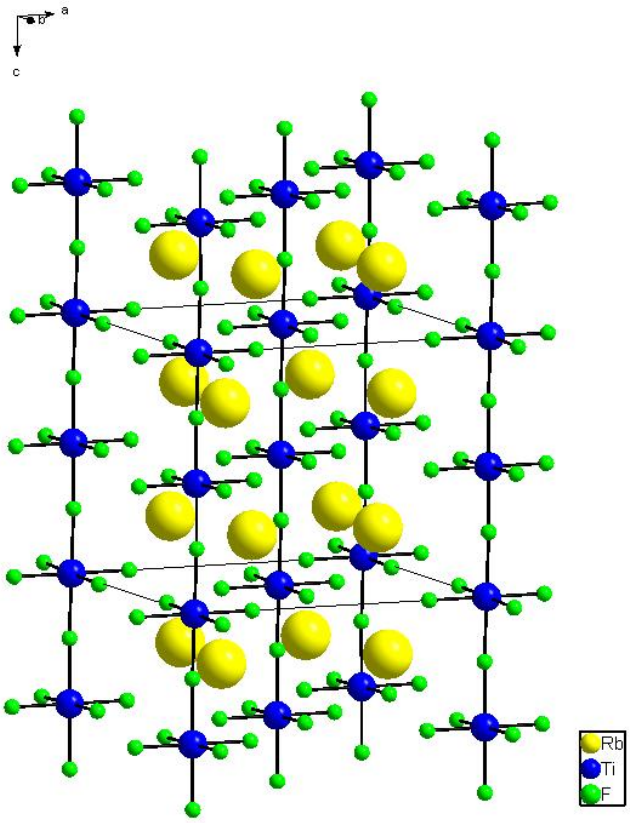
F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Anionic and Cationic recognition property of a new Luminescent molecular probe

정수희, **danielt, 이용일**

창원대 화학과

A new emissive molecular probe (1) derived from aminophenazine and aminothalazine have been synthesized and characterized by using standard analytical and spectroscopic techniques. Its sensor capability towards first-row transition metal cations and various anions was explored in organic solution. The receptor-anion/cation interaction, *via* hydrogen bonding or metal–ligand interactions distinctly modifies the emission of the luminophore. Titration experiments (Fluorescence, UV-absorption and ^{1}H NMR) and X-ray crystal studies shed light on the nature of the interactions between 1 and the anions and cations.

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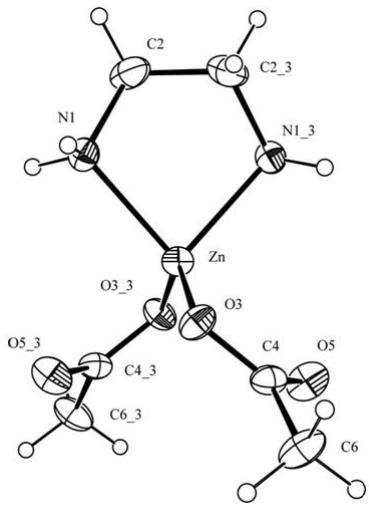
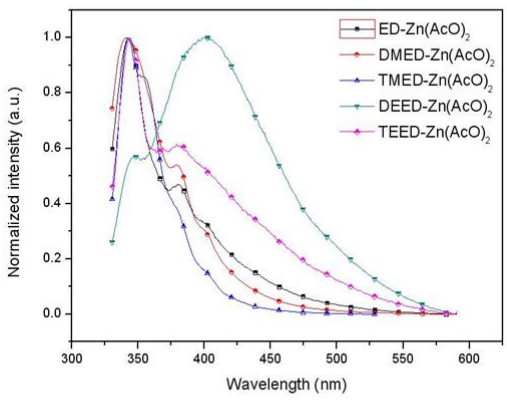
Structural and Luminescent Studies of Zinc Complexes with N,N-dialkylethylenediamine and N,N,N',N'-tetraalkylethylenediamine

윤선영, *서회주, **김지훈, ***강성권, 김영인

*부산대 화학교육과 *부산대 화학과 **부산대 첨단정보및디스플레이소재협동과정*
****충남대 화학과*

We synthesized luminescent Zn(Ⅱ) complexes containing N,N-dialkylethylenediamine, N,N,N',N'-tetraalkylethylenediamine(alkyl = H, CH_3, CH_2CH_3) by the direct reaction of $Zn(OAc)_2$ with ligands in ethanol. The structure of these complexes were determined by single-crystal X-ray diffraction analysis and showed a tetrahedral geometry around the Zn(Ⅱ) metal ion with a MN_2O_2 chromophore. The photoluminescenece spectra of these complexes showed emission from 350nm to 405nm, which is contributed from the intra-ligands charge transfer(ILCT). The quantum yield of these complexes is higher than the corresponding ligands, indicating that the zinc metal ion reduced the loss of energy by radiationless thermal vibrations resulting in stabilizing the ligand.





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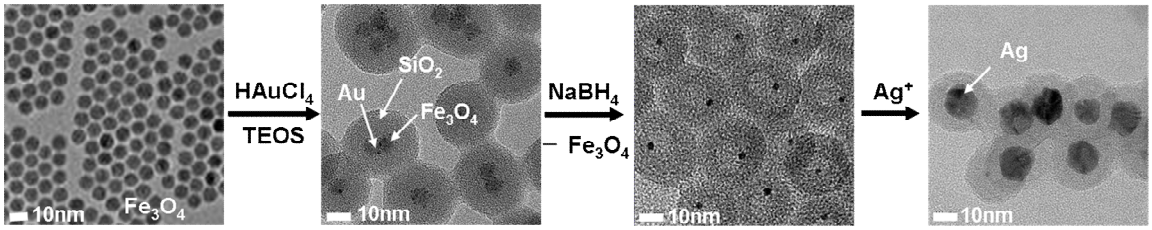
발표종류: 포스터, 발표일시: 목 12:30~14:30

Reductive Dissolution of Fe_3O_4 Facilitated by the Au Domain of a Fe_3O_4/Au Hybrid Nanocrystal: Formation of a Nanorattle Structure Composed of a Hollow Porous Silica Nanoshell and Entrapped Au Nanocrystal

여경민, 신종민, 이인수

경희대 응용화학과

The Fe_3O_4/Au hybrid nanocrystal was spontaneous generated during encapsulating Fe_3O_4 and Au^{3+} complexes with silica nanosphere. In the course of treating the hybrid nanocrystals with $NaBH_4$, it was found that Fe_3O_4 grain is rapidly and exclusively dissolved through the reductive process facilitated by the attached Au grain. The selective removal of Fe_3O_4 from the hybrid nanocrystal produced the nanorattle structure consisting of a hollow and porous silica nanoshell and an Au nanocrystal, which has the utility as a nanoreactor to template the growth of nanocrystals inside the cavity.



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A simple fluorescent "ON–OFF" receptor for biologically important anions based on urea moieties

윤성학, danielt, 이용일

창원대 화학과

A simple fluorescent anion sensor based on amide moieties, 1,1'-(naphthalene-1,8-diyl)bis(3-(9H-fluoren-9-one)urea) (1) have been designed, synthesized and characterized by IR, NMR (^{1}H and ^{13}C), ESI-MS and elemental analyses. The strong basic anions such as F^- and AcO^- resulted in significant decrease in fluorescent emission intensity of the compound 1, accompanied with a dramatic color change on irradiation at 300 nm. Anion binding studies were investigated by using fluorescence and ^{1}H NMR titration experiments.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Structure and Magnetic Properties of Closely Related Mono- and Di-Cu(II) Schiff Base Complexes: Water Clusters, Coordination Polymers, Hydrogen Bonded Networks

강지나, **Snehadri Khatua, D.G.Churchill**

KAIST 화학과

Three mononuclear complexes [Cu(rslysH)(OAc)]4.5H_2O (1), Na[Cu(rslys)(OAc)]3.5H_2O (3) and K[Cu(rslys)(OAc)]3.5H_2O (5) [rslys = 6-amino-2-{(2-hydroxybenzylidene) amino}hexanoate] have been prepared by way of an easy "one-pot" synthetic method in which the corresponding D/L-lysine derived Schiff base ligand is generated in situ. Further, three dinuclear acetate-bridged Cu(II) complexes, Li[Cu_2(rslys)$_2$(μ-OAc)]6H_2O (2), Na[Cu_2(rslys)$_2$(μ-OAc)]5H_2O (4) and K[Cu_2(rslys)$_2$(μ-OAc)]5H_2O (6) were obtained as minor products along with three mononuclear compounds from a "one pot" crystallization. These complexes have been characterized by various spectroscopic techniques and single-crystal X-ray diffraction. The molecular structures of 2, 4 and 6 confirm their dimeric nature with similar dicopper(II) phenolate and acetate-bridge environments, differing only in solid state molecular packing upon counter ion used. Variable-temperature magnetic analysis revealed a weak anti-ferromagnetic coupling interaction mediated through the phenolate- and acetate-bridged O atoms between the two Cu(II) centers. Large numbers of solvent water molecules are present in the lattices of the mononuclear compounds 1, 3 and 5. The carboxylate oxygen of the Schiff base ligand and terminal –NH_2 groups engage in intermolecular hydrogen bonding with solvent water molecules, giving 1-D, 2-D and 3-D network. The lattice water molecules form cyclic water clusters octamer and 1-D polymeric water cluster chains, which also assist the formation of 3-D hydrogen-bonded networks. In compounds 2 and 4, 2-D and 3-D hydrogen bonded networks are observed; but in 6, a 1-D helical $[K_1(H_2O)2]_\infty$chain is formed, allowing for the formation of an additional 2-D coordination polymer and finally a 3-D hydrogen-bonded network. The racemic D-/L-lysine used herein as a source of the Schiff base ligand led to racemic

hydrogen-bonding networks containing enantiomeric complexes of D- and L-lysine Schiff base ligands in all packing structures for compounds (1 - 6).

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Characterization of Novel Heavier Alkaline Earth Metal Complexes

윤혜정, 이선숙, *원종찬, 김창균, 정택모

*한국화학연구원 화학소재연구단 *한국화학연구원 화학소재연구단 정보전자폴리머연구센터*

The heavier group 2 elements are constituents in many important solid state materials, including high k dielectrics for dynamic random access memories (SrTiO3, (Sr,Ba)TiO3), ferroelectric phases for computer memory devices (BaTiO3, SrBi2Ta2O9), high-Tc superconductors (YBa2Cu3O7-x, La1-xCaxMnO3), electroluminescent devices (SrS:Ce, BaS:Ce), and nonlinear optical crystals (β-BaB2O4).In this presentation we will discuss synthesis of novel heavier alkaline earth metal complexes containing multidentate ligands which might stabilize the vacant sites of the large central metal. The synthesized compounds can be used as a source for the prepation of inorgnic/organic hybrid materials with polymer composites. We confirmed new group 2 complexes by 1H-NMR, IR spectroscopy, elemental analysis (EA), and thermogravimetric analysis (TGA).

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Characterization of Volatile Metal Precursors of Donor-founctionalized Alkoxy Derivatives for Transparent Oxide Thin Films

정인경, 김창균, 정택모

한국화학연구원 화학소재연구단

Over the past a few years, there has been an explosive growth of interest in both fundamental research and industrial applications of transparent conductive oxides (TCOs). This unique class of fascinating materials is entering a variety of cutting-edge applications, such as, solar cells, gas sensors, organic light-emitting diodes, liquid crystal and high definition displays, electrochromic and smart windows, as well as architectural coatings. Now a variety of transparent conductive oxide thin films including ZnO, In_2O_3, SnO_2, ZnO-In_2O_3 (ZIO), In_2O_3-SnO_2 (ITO), ZnO-SnO_2 (ZTO), and In_2O_3-Ga_2O_3-ZnO (IGZO) have been manufactured by several methods such as, reactive evaporation, solution growth, spray pyrolysis, sputtering, metal organic chemical vapor deposition (MOCVD), and pulsed laser deposition (PLD) using metal precursors. Most of the conventional metal precursors have big problems such as low volatility and films contamination by halide and carbon atoms. Therefore, we will present the design, synthesis, and characterization of volatile metal precursors of donor-founctionalized alkoxy derivatives which have high volatilities and good stabilities. Novel metal alkoxy complexes of nickel, indium and zinc were synthesized by the reaction of metal halide with donor-funtionalized alkoxy derivatives. New compounds have been characterized by NMR, FT-IR, mass spectroscopy, and elemental analysis. Thermal analysis has also been performed to qualitatively evaluate their volatility and thermal stability for potential use as transparent conducting oxides (TCOs).

일시: 2009년 10월 28~30일(수~금) 3일간
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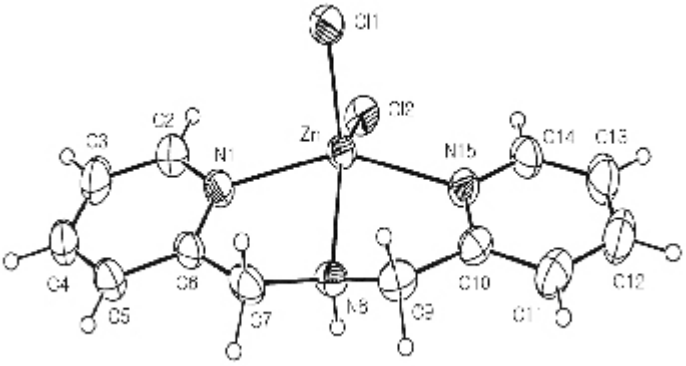
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Luminescent Zn(II) Complexes based on Pyridine Derivative Ligands

김지훈, *서회주, **진성호, **김영인

*부산대 첨단정보및디스플레이소재협동과정 *부산대 화학과 **부산대 화학교육과*

We synthesized luminescent Zn(II) complexes by direct reaction of $ZnCl_2$ with phenyl-N-(pyridine-2-yl) methaneamide (ppmma) (1), N-benzyl-N-2-pyridylmethylamine (bzp) (2) and di-(2-picolyl)amine (dpa) (3) in ethanol. The emission maximum peaks complexes in solution (DMF) were between 400 to 450 nm, which were contributed from the intra-ligand charge transfer (ILCT). Quantum efficiency of the complexes showed 5.2 (1), 2.5 (2) and 5.9 (3)%, respectively. The structure of $Zn(dpa)Cl_2$was 5-cordinated trigonal bipyramidal distorted geometry with a ZnN3Cl2 chromosphore. The calculated trigonality index, τ, of 0.21 is consistent with a distorted trigonal bipyramid.



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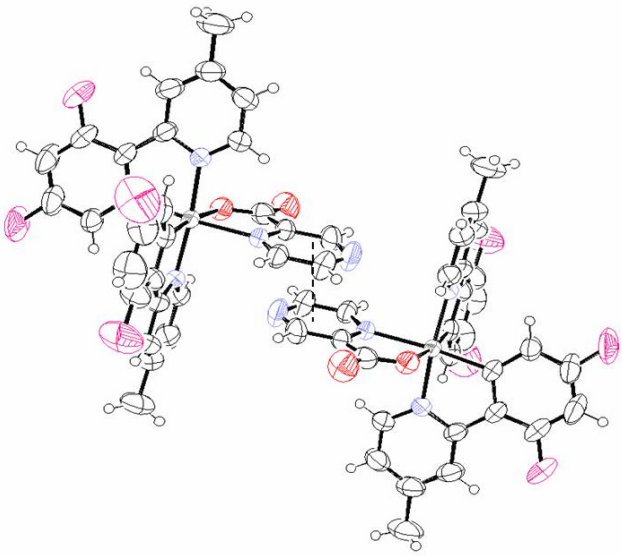
발표종류: 포스터, 발표일시: 목 12:30~14:30

Red Phosphorescent Ir(III) Complexes and Their Organic Light-emitting Diodes Applications

서희주, *김지훈, **진성호, **김영인

*부산대 화학과 *부산대 첨단정보및디스플레이소재협동과정 **부산대 화학교육과*

We prepared two heteroleptic cyclometalated Ir(III) complexes containing 2-(2,4-diflurophenyl)-4-methyl pyridine (dfpmpy) as the main ligand and ancillary ligands such as pyrazine-2-carboxylic acid (prz) and 5-methyl-pyrazine-2-carboxylic acid (przMe). The crystal structure of $(dfpmpy)_2Ir(prz)$ revealed that there is a π-π interaction (3.39 Å) between two pirazine ring of prz ligand. The emission peak of these complexes in solution showed at λ_{max} = 589 and 531 nm whereas those in film state (5 wt. % doped in PMMA) emitted at λ_{max} = 543 and 575 nm. Peak maximum of $(dfpmpy)_2Ir(prz)$ was observed at 492 nm and 553 nm at 15 % doping and showed a red-shift at high doping concentration. $(dfpmpy)_2Ir(prz)$ device showed a color index of (0.43, 0.53).



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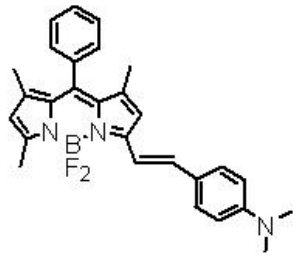
발표코드: **Ⅰ33P75포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Intramolecular Charge Transfer Processes in a BODIPY with Copper Ion

이혜영, 정종화

경상대 화학과

Boron dipyrromethene (BDP) chromophore has recently gained importance in the design of selective fluorescent chemosensor systems. We studied the synthesis and spectroscopic properties of the 3-dimethylaminostyryl substituted BDP 1. As part of our ongoing studies on the emission responses of various BDP derivatives, 3-dimethylaminostyryl substituted BDP 1 had an unexpected emission response. It was not sensitive to metal ions, but in the case of mixed solvent (ACN:H2O=3:1), only copper ion had made emission shift to shorter wavelength. Also, its color was changed from blue to pale yellow.



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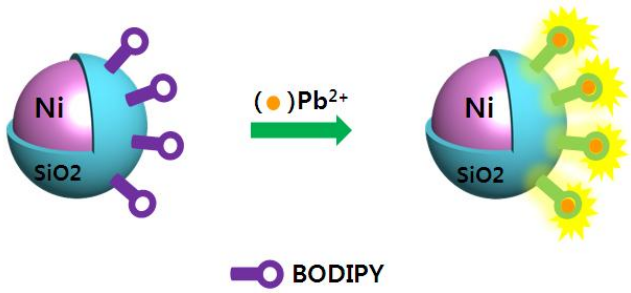
Chemosensor Based on BODIPY Derivative Immobilized Magnetic Silica Nanoparticles for Detection and Separation of Pb^{2+}

손현종, 이혜영, 정종화

경상대 화학과

The BODIPY derivative was synthesized of the benzoylchloride, 2,4-dimethylpyrrole, BF3-OEt2, and 3-(triethoxysilyl) propyl isocyanate. The BODIPY was immobilized onto magnetic silica nanoparticles by sol-gel reaction. The ability of 1 to sense metal ion was studied by addition of various metal ions. The fluorescence spectrum, free 1 exhibited an emission maximum at 704 nm. Addition of 20 equiv of Pb^{2+}ion results in an obviously enhanced fluorescence at 570 nm, while the other ions intensity was not changed. Upon addition of increasing Pb^{2+} concentrations, the intensity gradually increased. We will detail discuss on the synthesis of BODIPY fluorophore immobilized magnetic silica nanoparticle and its binding ability for heavy metal ion.



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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis, and Characterization of New Vanadium and Tungsten alkylidene Complexes, and Catalytic Activity for Ring Opening Metathesis Polymerization

Nayab Saira, *성익경, 정종화, **이효선

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

New vanadium and tungsten alkylidene complexes containing β-dikitimenate and related ligands have been synthesized with the starting materials, NArVCl3, WOCl4, and WCl6. Specifically, dialkyl complexes of WNArL(R2)OR'(PCy3) with bidentate ligand (L = N,N'-((Z)-1,3-diphenylprop-1-ene-1-yl-3-ylidene)dianiline, R = CH2Ph, Me, Ph, R' = alkyl or aromatic) and of vanadium complex with monodenate oxo-ligand V(L')NAr(R2), (L' = Diphenyl(1H-pyrazol-1-yl)methanolate) were prepared to get the alkylidene complex through α-Hydrogen elimination. In some occasion, the "alkylidene" complexes were obtained from by direct method such as "azide" in the presence of L ligands of complex. The synthesized complexes were characterized by various spectroscopic techniques and their catalytic activity in Ring Opening Metathesis Polymerization (ROMP) of cyclic olefins was studied.

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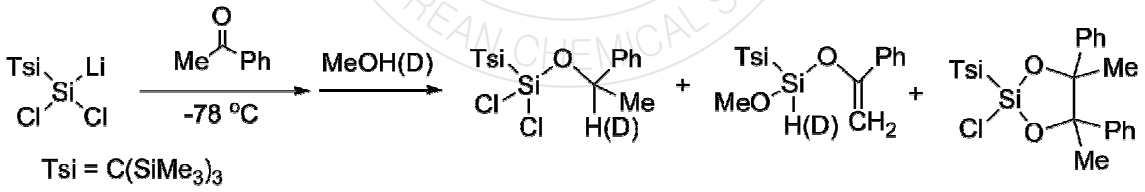
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Reactivities of Chlorosilylenoid with Ketones

윤수진, 임영묵, 이명의

연세대 화학과

Over the past decade, a few novel silylenoid has been the subject of the extensive study. Recently, we reported stable silylenoids, which are functionalized halosilylenoid stable at room temperature, and we indentified their existence through various trapping experiments. Also we observed some evidence for the reduction, substitution and transmetallation of halosilylenoids. As a part of this research, we wish to report some examples of the reactivity of chlorosilylenoid with ketones such as acetone, acetophenone, α-diketone and β-diketone to show an unique synthetic strategy for the syntheses of silaheterocycles. In this presentation, we will discuss the chemistry of chlorosilylenoid in more detail.



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Novel Synthetic Strategy of Silylenoid; From Bromodilithiosilane to Silylenoid

임영묵, 윤수진, 이명의

연세대 화학과

Recently, we reported the first functional dilithiosilanes having a halogen substituent, $TsiSiXLi_2$ ($Tsi=(Me_3Si)_3C$, X = Cl, Br) stable at room temperature. Dual functional moiety of halogen and lithium show unique reaction property compare to those of 1,1-dilithiosilanes. Not only dilithiosilanes but also silylenoids were very important reactive species in organosilicon chemistry. Generally, silylenoids were synthesized by the reduction of dihalosilanes. In this presentation, we wish to report new synthetic strategy of silylenoid from bromodilithiosilane, which showed the distinctive reactivity of bromodilithiosilane. The reaction of $TsiSiBrLi_2$, with Me_3SiCl gave new silylenoid, $Tsi(Me_3Si)SiBrLi$, which was moderately stable at room temperature. ^{29}Si NMR resonance of $Tsi(Me_3Si)SiBrLi$ represented the most shielded silylenoid among the reported stable silylenoid. From various intermolecular reactions, $Tsi(Me_3Si)SiBrLi$ show amphiphilic property of silylenoid. In this poster section, we will discuss in detail.

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Syntheses of Silanones having Intramolecular Donor-Atom

이수정, *임영묵, *이명의

*연세대 화학 *연세대 화학과*

Silanone ($R_2Si=O$), as the silicon analogy of ketone, is known as important intermediates of silane combustion and vacuum plating in microelectronics industry. For a long time, the isolation of stable silanones had not been successful until Driess group reported the first isolable silaformamide-borane complex with considerable silicon-oxygen double-bond character. Recently, we reported the syntheses of disilanols, 1,3-dihydroxy-1,3-bis[*o*-(*N*,*N*-dimethylaminomethyl)phenyl]-1,3-divinyldisiloxanes, bearing an intramolecular donor-atom, which could be promising precursors for silanones.The flow vacuum pyrolysis (FVP) of disilanols gave D_3 and D_4 products in high yields, which indicated that silanones were generated as an intermediate. The silanones were identified through various trapping experiments.In the extension of this research, we attempted to synthesize the stable silanone having intramolecular donor-atom and a bulky substituent, tris(trimethylsilyl)methyl group. In this presentation, this result will be discussed in detail.

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장소: 대전컨벤션센터
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발표분야: 무기화학
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Reactivities of Bromosilylenoid with Olefins

복경진, 임영묵, 이명의

연세대 화학과

Several halosilylenoids, having bulky substituent Tsi, tris(trimethylsilyl)methyl, have been synthesized by the reduction of the corresponding $TsiSiX_3$ (X=Cl, Br) with 2 equiv. of MNp (M=Li, Na, K). Among these halosilylenoids, bromosilylenoid is stable at room temperature. The reaction of silylenoids are often similar to those of silylenes. Reactions of silylenes with organic carbonyl compounds have been studied in detail by several research groups. Most of these reactions were carried out under photolytic or thermolytic conditions to generate the silylenes, making them difficult to determine the reaction mechanism. We recently observed evidence for the reduction, substitution and transmetalation of the silylenoid containing a halogen substituent. As a part of this research, we wish to report some unprecedented examples of the reactivity of the bromosilylenoid with olefins, such as styrene, *trans* and *cis*-2-butene, cyclopentene, cyclohexene and cyclohexadiene. These reactions of silylenoids can be used as new synthetic routes for silaheterocycles. Here, we will describe the reactivity of the bromosilylenoid toward styrene and various other olefins.

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장소: 대전컨벤션센터
발표코드: **Ⅲ33P5포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Electrochemical Assay of Adenosine Based on Guanine Bases of an Adenosine-sensitive Aptamer

최민선, Wu Qiong, 이성은, 김진홍

이화여대 나노과학부

Aptamers as the active sensing materials are synthetic oligonucleotides forming characteristic tertiary structures, such as G-quartet and hairpin, upon binding to specific proteins, small molecular targets, and metal ions. Up to now, various techniques, such as colorimetry, fluorescence, and electrochemistry, have been used for the detection of thrombin, adenosine, cocaine, and potassium ions as the targets using the corresponding aptamer probes. As a result of their high selectivity, stability, target versatility, and convenient regeneration and modification, aptamers hold great promise for various diagnostic applications. Recently, sensing of small molecules and ions coupling the attractive properties of aptamers has received considerable attention. Electrochemistry offers attarctive routes for interfacing aptamer interactions with the signal generating element in a simple, fast, and inexpensive manner. Modern electronic aptamer biosensors commonly rely on redox tags with conformational changes, or impedance detection to offer convenient measurements of nanomolar concentrations of target molecules. Further enhancement of the sensitivity of such devices is urgently needed for measuring ultra low levels of target agents. Recent studies to improve the sensitivity of aptamer-based biosensors and bioassays have lowered their detection limits to the picomolar level through the use of nanoparticle tags, binding-induced conformational changes, and label-free impedance detection. We herein present an electrochemical aptamer-based sensors with metal complexes as mediators utilizing a specific interaction between DNA and metal complex.

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Crystal Engineering of Anion-Controlled Endo/Exo-Cyclic Silver(I) Complexes of an S_2O_2 Macrocycle

이소영, *Jagadese J. Vittal, 김기환, 이심성

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

A 16-membered S_2O_2-macrocycle (L) with a dibenzo-subunit was synthesized and structurally characterized. Reactions of L with silver(I) salts (NO_3^-, ClO_4^-, $CF_3CO_2^-$, $CF_3SO_3^-$ and BF_4^-) afforded the respective anion-directed supramolecular complexes 1-5 with different topologies; 2-D square grid network $[Ag(L)NO_3]_n$ (1), double-stranded 1-D coordination polymer $[Ag(L)ClO_4]_n$ (2a), 2-D polymeric sheet $[Ag(L)X]_n$ (2b: X = ClO_4^-, 3: X = $CF_3CO_2^-$ and 4: X = $CF_3SO_3^-$) and cyclic tetramer with endo/exo-cyclic Ag(I) coordination network $[Ag_4(L)_4(BF_4)_2(CH_3OH)_2](BF_4)_2$. The formation of such discrete, 1-D and 2-D supramolecular complexes is discussed in terms of anion effect.

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Synthesis, crystal structure, and magnetic properties of iron(III) and cobalt(II) complexes with a chiral tridentate ligand.

로투산카라라오, 신종원, 이유경, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

There is currently active interest in the development of inorganic systems based on the interaction between transition metal ions and organic photoactivity ligands. Due to this interest, we have synthesized iron(III) and cobalt(II) complexes with a bis-pyridine tridentate chiral ligand, $\{[Fe^{III}(L^S)(NCS)_3]\bullet(CH_3OCH_3)(H_2O)$ (1)} and $\{[Co^{II}(L^S)(NCS)_2]\bullet H_2O$ (2)} from the reaction of $[Fe^{II}(H_2O)_6]\bullet(BF_4)_2/[Co^{II}(H_2O)_6]\bullet(ClO_4)2$, (S)-1-phenyl-N,N-bis(pyridine-2-ylmethylene)ethanamine (L^S), and NaSCN in methanol under aerobic conditions. The crystal structures of 1 and 2 have been determined by single-crystal x-ray analysis. The iron(III) in complex 1 showed a distorted octahedral geometry having a tridentate chiral ligand and three NCS anions, while the cobalt(II) ion in 2 displayed a distorted trigonal bipyramidal geometry binding a tridentate chiral ligand and two NCS anions. Unfortunately, both compounds do not show spin crossover behaviors. Here in the detailed preparation, crystal structure, magnetic properties, UV/Vis spectra and CD spectra will be described.

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장소: 대전컨벤션센터
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Supramolecular Chemistry of An 1,3-alt-Thiacalix[4]arene Bis(crown-5) Ethers: Endocyclic Dipotassium complex and Silver-Based Networking by Exo-Coordination

박선홍, *Jagadese J. Vittal, 이심성

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

Thiacalixarenes are modification of classic calixarenes in which methylene bribges between aromatic rings are substituted by sulfur atoms. Coupling reaction of thiacalix[4]arene with tetraethylene glycol ditosylates afforded 1,3-alt-Thiacalix[4]arene Bis(crown-5) Ethers (L). Self-assembled supramolecular networks (1-D and 2-D) were prepared by the reaction of thiacalix[4]arenes with silver salts (NO_3^- and ClO_4^-). Whereas, endocyclic dipotassium complex was obtained from the reaction of L with mixture of $KClO_4$ and $AgClO_4$.

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Synthesis of Phase-Pure Interpenetrated MOF-5 and Their Gas Sorption Properties

김현욱, Sunirban Das, 김기문

포항공과대 화학과

Metal-organic porous materials (MOPMs) have attracted great interests because of their well-defined and adjustable porous structure. MOF-5, one of the best known MOPMs, has been extensively investigated for gas storage for the past several years. Interpenetrated MOF-5 (int-MOF-5) was recently discovered, but phase-pure int-MOF-5 has not been synthesized. Here we present the synthesis of phase-pure, int-MOF-5 and their hydrogen sorption properties.We synthesized int-MOF-5 in pure phase by carrying out the reaction in presence of weak bases such as melamine and 2,4,6-tris(4-pyridyl)-1,3,5-triazine. Single-crystal X-ray diffraction analysis revealed that int-MOF-5 has the same cubic topology of MOF-5 with two fold interpenetration. The phase purity of the framework was confirmed by X-ray powder diffraction analysis on bulk samples. Interestingly, int-MOF-5 shows a higher hydrogen sorption capacity than MOF-5 at 77 K and 1 atm, even though it has a lower surface area. The higher hydrogen sorption capacity is presumably due to its higher enthalpy of adsorption. Details of the work will be presented.

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발표분야: 무기화학
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Reduction of Eu(III) to Eu(II) in Chloride Based Molten Salts by Variation of Temperature

임희정, 송규석

한국원자력연구원 원자력화학연구부

Both of Eu(II) fluorescence peak at around 425 nm and Eu(IIII) peaks at ca. 580 nm to 650 nm were observed when $EuCl_3$ was dissolved in LiCl-KCl or LiCl molten salt by increasing the temperature from room temperature to 683°C. It has been known that fluorescence of lanthanide ions generally decrease when temperature is increased possibly due to a quenching of the fluorescence. However, $EuCl_3$ dissolved in LiCl molten salt showed peculiar fluorescence behavior according to a changing temperature. The detailed results of in-situ fluorescence studies, self-reduction of Eu(III) to Eu(II), and estimated changes of the chemical properties of europium in chloride based molten salt according to a variation of the temperature will be discussed in this presentation.

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

Preparation of Silica Nanotubes Using Organogelator as Templates

오경지, *진종성, 정옥상

*부산대 화학과 *한국기초과학지원연구원 하이테크부품소재연구지원센터*

We synthesized gelators based on optical active or racemic 1,2-diphenylethylendiamine and prepared organogels with the synthesized gelators. After the calcinations of the gel prepared by adding tetraethylorthosilicate(TEOS) to the one to one mixture of neutral and ionic organogelator, we found that the helical silica nanotubes are produced, the neutral organogelator(G1) determines the shape of morphology, the ionic organogelator(G1N) covers neutral organogelator and the complex is polymerized by silica oxide compounds.We experimented in the same of ionic organogelator except using dodecyltrimethyammonium instead of ionic organogelator(G1N). The result was identical to ionic gelator, G1N.

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Synthesis and Crystal Structures of Di- and Tetra-Nuclear Dicarboxylate-Bridged Copper(II) Complexes

구본권, 김정숙

대구가톨릭대 화학과

Three new Cu(II) complexes, $[Cu_2(C_3H_2O_4)(phen)_2(H_2O)_3](NO_3)_2(H_2O)_2$ (1) ($C_3H_2O_4$ = malonate, phen = 1,10-phenanthroline), $[Cu_2(C_4H_4O_4)(phen)_2(H_2O)_2]$ $(NO_3)_2$ (2) ($C_4H_4O_4$ = succinate), and $\{[Cu_2(phen)_2(H_2O)(NO_3)]_2(C_5H_6O_4)_2\}(NO_3)_2$ (3) ($C_5H_6O_4$ = glutarate) have been synthesized and characterized by elemental analysis, infrared spectroscopy, thermo gravimetric analysis, and single crystal X-ray diffraction. Single crystal X-ray diffraction analyses reveal that both complexes of 1 and 2 are discrete dinuclear $[Cu_2(L)(phen)_2]$ (L = $C_3H_2O_4$ for 1 and $C_4H_4O_4$ for 2) motif and complex 3 presents a discrete tetranuclear $[Cu_4(L)_2(phen)_4]$ (L = $C_5H_6O_4$) core formed by two $[Cu_2(L)(phen)_2]$ units. In these complexes, it is notable that the dicarboxylates show a different coordination modes on complexation; malonate acts as chelating and bridging (1), succinate as monodentate (2), and glutarate as bridging (3).

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Structural and Spectral Properties of *s-cis*-[Cr(acac)(edda)]

최종하, *유건상, **이상학

*안동대 화학과 *안동대 응용화학과 **경북대 화학과*

The crystal structure of [Cr(acac)(edda)] (edda=ethylediamine-N,N'-diacetate; acac= acetylacetonato) has been determined by a single-crystal X-ray diffraction study at 150 K. The chromium ion is in a distorted octahedral environment coordinated by two N and two O atoms of chelating edda and two O atoms of acac, resulting in *sym-cis* configuration. The complex crystallizes in the space group $P2_1/c$ of the monoclinic system in a cell of dimensions a=10.2588(9), b=15.801(3), c=8.7015(11) Å, β = 101.201(9)° and Z=4. The mean Cr-N(edda), Cr-O(edda) and Cr-O(acac) bond distances are 2.0829(14), 1.9678(11) and 1.9477(11) Å while the angles O4-Cr-O6 of edda and O1-Cr-O2 of acac are 171.47(5) and 92.72(5)°, respectively. The crystal structure is stabilized by N-H…O hydrogen bonds. The visible electronic and IR spectral properties are also discussed.

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Discrimination Amine Cations from Uncharged Neutral Amines by trans-Dihydoroxo[(2-pyridyl)porphyrinato]tin(IV) complex

장헌정, 김희준

금오공과대 응용화학과

Tin(IV) porphyrins have drawn recent attention in the architectures of supramolecular porphyrin arrays because of their useful coordination properties conferred by the highly charged main group metal center. In particular, the ditopic porphyrins such as dihydroxotin(IV) pyridylporphyrins, possessing the cooperative binding sites in their axial and peripheral positions, have great potential in molecular recognition leading to the construction of functional multiporphyrin supramolecular arrays and nanostructures. Aiming at this goal, we have recently investigated molecular recognition by [(2-pyridyl)porphyrinato]tin(IV) complexes using cooperative interactions of axial ligands and peripheral functional groups. We here present the discrimination a series of amine cations from the uncharged neutral amines by the molecular recognition with dihydroxotin(IV) pyridylporphyrins.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Preparation of Nano Composite Materials with Porphyrin-Polyoxometalate

LICHANGHONG, 김희준

금오공과대 응용화학과

Porphyrins and metalloporphyrins are functional molecules that are used for a variety of applications and devices, such as sensors, luminescent devices, catalysts, solar energy harvesting systems, photonic materials, and therapeutics. On the other hand, polyoxometalates (POMs) are the inorganic equivalent of a porphyrin. POMs are discrete metal oxide clusters that are ca. 1 nm in diameter and can have a variety of compositions. Since the diverse chemical and physical properties of porphyrins and POMs are in many ways complementary rather than overlapping, a composite organic/inorganic nano-material formed by association of metalloporphyrins and POMs can show more efficient catalytic properties than the corresponding metalloporphyrins alone. Here we present that porphyrin nano-materials can be prepared by ionic self-assembly of porphyrin cations and polyoxometallates anions in aqueous solution.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication of carbon nanotube based transparent conductive film

황선나, *김희숙, **이현정

*연세대 화학공학과 *KIST **KIST 고분자하이브리드센타*

Carbon nanotubes due to superior mechanical, chemical and electrical properties are one of the candidate for transparent conductive film. In this study, we used carbon nanotubes (CNTs) and silver nanofibers to fabricate a transparent conductive films. The silver nanofibers have been produced by using a sol-gel solution consisting of silver nitrate (AgNO3) and polyvinylpyrrlidone (PVP). The formation mechanisms are discussed based on the redox reaction between AgNO3 and polymer matrix during heat treatment. Then, CNTs were deposited on silver nanofiber. Surface morphology was studied by scanning electron microscopy (SEM) and field-emission scanning electron microscopy (FE-SEM). The optical properties were studied using UV-visible absorption spectroscopy. X-ray diffraction (XRD) was used to confirm the presence of silver crystals. The electrical conductivity of the transparent conductive film was measured four-point probe method.

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Novel preparation of DSSCs using electrolyte_based pastes

김민아, *이현정

*고려대 화공생명공학과 *KIST 고분자하이브리드센타*

Dye-sensitized solar cells based on highly porous nanocrystalline TiO2 films have drawn much attention due to their high conversion efficiency and low production cost. Recently, various techniques have been employed to improve the performance of the DSSCs. Typical methods for DSSCs need usually a multi-step progress, a long preparation time and a high temperature treatment. In this study, we introduce a novel preparation using dye-coated TiO2 particles and electrolyte_based pastes. We prepared a paste material by mixing polymeric binders and TiO2 particles coated with dye molecules. In this case, a polymeric binders act also as an electrolyte in DSSCs. This fabrication method provides the process at the room temperature because it doesn't need a removal of polymeric binders in the paste at high temperature. It would save time, an effort and a cost in facilitating the manufacture.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Panchromatic Polymers based on Tin(IV) Porphyrins

박부배, 김희준

금오공과대 응용화학과

Dye-sensitized and organic solar cells have attracted much attention relevant to global environmental issues. Large π-aromatic molecules such as porphyrins are important classes of potential sensitizers for highly efficient solar cells, owing to their photostability and high light-harvesting capabilities. The efficiency of porphyrin molecule-sensitized solar cells could be improved significantly if the dyes with larger red and near-infrared absorption could be developed. Elongation of the π conjugation in porphyrins causes broadening and a red shift of the absorption bands together with an increasing intensity of the Q bands relative to that of the Soret band. In this context, we have recently synthesized tin(IV)-porphyrin polymers which are highly soluble and fully conjugated. Here we present panchromatic polymers based on tin(IV) porphyrins as a potential sensitizer for solar cell.

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Syntheses, Characterizations, and Crystal structures of MII(Ni, Cu) Macrocyclic Complexes Containing TTF derivative [TTF = Tetrathiafulvalene]

이주은, 이홍인, *나명수

*경북대 화학과 *한양대 응용화학과*

Charge-transfer complexes, composed of TTF and metal ions, exhibit interesting electric and magnetic properties. We synthesized Ni(Ⅱ) and Cu(Ⅱ) macrocycle - TTF complexes in which TTF is functionalized with two carboxylate groups, BCDT-TTF [Bis(4(5)-carboxy-1,3-dithiolidene)]. Single-crystal X-ray analyses determined the structures of the complexes. The Ni(Ⅱ)macrocycle - TTF complexes shows an expanded 1-D coordination polymer where Ni(Ⅱ)macrocycles play roles as beads and the TTF derivatives (BCDT-TTF) as linkers. In Cu(II)macrocycle - TTF compound, instead of forming a network, BCDT-TTF anions exist between the copper(II) macrocyclic complexes with H2O ligands. In this poster, we will present the detailed preparation procedures, crystal structures, and physical properties as well as interesting coordination chemistry of the complexes.

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The Modification Study of CGC and the Related Catalysts for Improving the Ethylene Polymerization

WU CHUN JI, *이효선

*경북대 화학과 *경북대 자연과학대학 화학과*

CGC (Constrained Geometry Catalyst), representatively, “[Me2Si(Me4C5)(NBut)]TiCl2” were commercially very successful due to the distinguished chemical properties and abnormally high activity and high thermal stability on the ethylene polymerization so far. We have prepared dimethysilyl bridged 3,4-dimethyl cyclopentadienyl/amido zirconocene and titanocene complexes, [Me2Si(Me2C5H2)(NBut)]TiCl2 and [Me2Si(Me2C5H2)(NBut)]ZrCl2 by using 2,3-dimethyl cyclopentadiene as a p-donor ligand. The catalytic activity of synthesized complexes [Me2Si(Me2C5H2)(NBut)]MCl2 (M = Ti,Zr) will be studied by comparison with standard CGC in ethylene polymerization in order to survey the influence of 3,4-Me2Cp on the reactivity. We further investigated the synthesis and catalytic activity of [Me2Si(Me2C5H2)(NBut)]MR2 (M = Ti, Zr, R = CH3, CH2Ph) derivatives.

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Novel Pd catalysts for polymerization of norbornene derivatives

이응준, 이익모

인하대 화학과

Various olefins has been polymerized by the Vinyl addition polymerization catalysts based on Ni & Pd catalysts. The resulting polyolefins showed some weakness such as high sensitivity to UV due to presence of double bonds. In order to improve this property, coordination polymerization of various olefins with group 10 metals containing β-ketoiminate ligands with high solubility in organic solvents has been carried out. These new complexs showing high activity towards olefins polymerization, are characterized by NMR and elemental analysis. The effects of several reaction factors were studied and the results will be presented.

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Microwave hydrothermal synthesis of titania nanostructure and its photocatalytic property

이한빈, 최민식, 이익모

인하대 화학과

Nanocrystalline TiO_2 of the anatase phase has been synthesized by means of microwave hydrothermal process. The mixture solution of tetrabuylammonium hydroxide (40wt% in water) and titanium tetraisopropoxide is treated by microwave irradiation at 200℃ for 6 hours. The obtained TiO_2 powder was characterized by UV-VIS reflectance, X-ray diffraction, scanning electron microscopy and transmission electron microscopy. Various morphologies of TiO_2 nanostructure have been found such as cube, rod, sphere, hollow sphere and hollow rod. The photocatalytic activity also was measured by GC. TiO_2 nanoparticles, found to have superior visible light photocatalytic activity were synthesized by addition of small amount of acid to the mixture solution.

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Synthesis Nanocrystalline TiO2 Was by Microwave Hydrothermal Reaction and Its Photocatalystic Property

최민식, 이한빈, 이익모

인하대 화학과

We reports a new synthetic process for controlling the structure shape and size of TiO_2. Nanocrystalline TiO_2 was synthesized by microwave hydrothermal reaction using tetramethylammonium hydroxide (TMAH), titanium isopropoxide (TTIP) in ethanol as starting materials. Each structure was selectively controlled by simply altering the concentration of TMAH. The overall procedure is simple, reproducible, and relatively inexpensive with the availability of scale-up.

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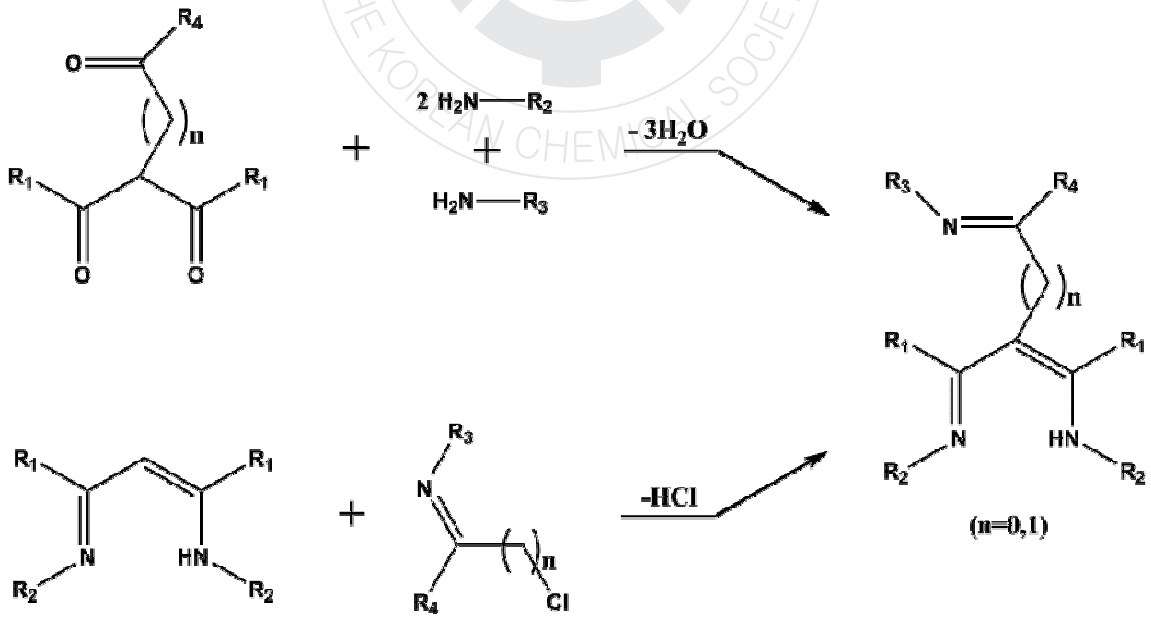
Synthesis of Triketimine as a Potential Multi-dentate Ligands

오인숙, 윤샛별, 이익모

인하대 화학과

As from the beginning of olefin polymerization by Ziegler-Natta catalysis, intensive search has been performed to find the organometallic compounds catalytically active in polymerization. One of examples is known to be a late metal complex containing a bidentate a-Diimine ligand. In this study, we have tried to synthesize a triketimine as a potential multi-dentate ligand to coordinate a metal compound as shown below.



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Synthesis of β-diketimine ligands by triethyloxonium tetrafluoroborate.

윤샛별, 양문규, 오인숙, 이익모

인하대 화학과

1,3-Diketimine compounds as bidentate chelating ligands have been reported versatile as ancillary ligands for various organometallic or inorganic compounds. Here, we report a convenient synthesis of 1,3-diketimines from 1,3-diketone moieties. 1,3-Diketone was treated by an amine in the presence of triethyloxonium tetrafluoroborate (Meerwein's salt) which is known as a strong alkylating reagent. The experiment was performed by microwave method (100-150 W, 100-120 ℃, 0.5-2hr) to give ca. 70 % of the corresponding 1,3-diketimine product.

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Syntheses, structures and physical properties of two Mn(II) complexes with Schiff base ligands

이유경, 신종원, 로투산카라라오, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

Multidentate Schiff base ligands have been interested for many years because of the important of coordination chemistry and their ability of readily forming complexes. Two manganese complexes were synthesized with the tetradentate Schiff base ligands derived from the reactions of 2-pyridinecarboxldehyde and amine in the 2:1 molar ratio. The complexes have been characterized by elemental analysis, FT-IR, X-ray crystallography. The magnetic property of the complex 2 are presented.

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Effect of polyelectrolyte multilayers on the growth and photoelectric properties of CdS/Cu2S nanoheterostructures for thin film photo-transistor application

구금애, 채강일, 한성환

한양대 화학과

The soft alkaline chemical route and to control the flow of anions and cations into surface of layer for growths of nanocrystals heterostructures are offering a convenient way to design the electronic thin film photo- transistors. The multilayer (PEI/PAA)n (n= 0.5 to 1.5) of polyethyleneimine (PEI) and polyacrylic acid (PAA), polyelectrolytes are playing a major role to protecting the cation exchanges in the formation of nanoheterojunction. The nanocrystalline heterostructures have been grown on ITO glass substrates, using, in alkaline medium at pH ~11. The annealed nanocomposite heterojunctions have mixed cubic (for CdS) and orthorhombic (for Cu2S) phases and nanoparticle sizes have been accelerated with increasing the number of (PEI/PAA)n layers from n=0.5 to 1.5. The surface morphology was observed that the annealed structures contain nano size crystallite grains of Cu2S (8 nm) connected with each other through grain boundaries of the porous CdS (25 nm) structures with the single (PEI/PAA)n (n=0.5) layer in between them. Whereas the Cu2S (30 nm) increasing sizes of nanoparticles were filled inside porous CdS (40 nm) structures and formed the smooth nanoparticles heterojunction with the multilayer (PEI/PAA)n (n=1.5).The higher optical absorption was found in the composite nanocrystalline layers, whereas, photoluminescence (PL) quenching was observed onto these structures. The higher photoconductivity behaviour was estimated by measuring the current voltage (I-V) characteristics, in the dark and under the light illumination (80mW/cm2. The two silver metal evaporated contacts (0.5 cm) at the end points of the heterostructures are working as a source and drain with virtual gate of illuminated portion (0.5 cm). The designated photo-transistors are representing their characteristics in visible light illumination.

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Liquid phase deposited cadimium selenide nanofiber on TiO2 electrodes for quantum dots-sensitized solar cells

이미선, 채강일, 황윤희, 길병호, **Ganesh**, 한성환

한양대 화학과

The crystalline CdSe quantum dots on TiO2 electrodes were prepared using electrodeposition and chemical bath deposition. Compared to chemically deposited CdSe quantum dots on TiO2 electrodes, electrodeposited CdSe quantum dots have high crystallinity. The electrodeposited CdSe quantum dots on TiO2 electrode showed power conversion efficiency of 0.5 %, which is 40% higher than that of chemically deposited CdSe quantum dots.

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Utilizing pH-dependent Ion Permeability due to Selective Swelling of Polyelectrolyte Multilayer Films

길병호, 채강일, 구금애, 한성환

한양대 화학과

The selective swelling behavior of polyelectrolyte multilayer (PEM) films prepared by layer-by-layer (L-b-L) assembly influences the ion-permeability in contrast to surface charge density of the films. The cation terminated polyethylene amine (PEI) and anion terminated polyacrylic acid (PAA) were dissolved in DI water, and the pH was adjusted to 10 and 4, respectively, exemplifies thick denser film with good layering structure. The layered polyelectrolyte films has selective swelling behavior at pH 4 (PEI) or pH 10 (PAA), influences the permeability of both Ru(NH3)62+ and Fe(CN)63- rather than surface charge character or film charge density. The swollen top most layer shows “on” character, whereas, shrunken top most layer shows “off” character for the ion-permeability. Such “on–off” character can be used for the pH-dependent switches based on surface morphology.

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Chemical bath deposited -Bi2O3/PANI Composite for Supercapacitor Applications

Ganesh, 채강일, 길병호, 한성환

한양대 화학과

Crystalline -Bi2O3 was synthesized through pH-dependent chemical bath deposition process, altering the morphology and evolution from nanoparticles (40 nm) at pH 9 to platelets (40 nm width and 0.8 m length) at pH 12. In-situ aniline nucleation and growth at less basic condition on the -Bi2O3 increased the surface area and specific capacitance of the device. The morphological change of -Bi2O3/PANI composite from nanoparticles to platelets like nanostructure facilitates higher specific capacitance from 210 to 430 F/g at a scan rate of 10 mV/s with enhanced ionic diffusion and retention of specific capacitance up to 84% at higher scan rates.

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Low bandgap chemical bath deposited polycrystalline CuInSe2 : An effective material for solar cells

황윤희, 이미선, 한성환

한양대 화학과

The thin films of nanocrystalline CuInSe2 were prepared on glass substrates using chemical bath deposition in acidic medium at room temperature. Thickness of the chemically deposited CuInSe2 thin films was ~ 100 nm. The films were composed of closely packed irregular grains of ~100–120 nm in diameter. The X-ray diffraction analysis and the selected area electron diffraction analysis revealed the deposited thin films were polycrystalline with highly (112) preferential orientation. The films exhibit pure faint black, and direct band gap energy was 0.96 eV.

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Modification of MnO2 Surface Morphology using Polyelectrolyte via Spray Pyrolysis Processes

채강일, 길병호, Ganesh, 한성환

한양대 화학과

Manganese oxides find application as cathodes in lithium ion batteries, oxidation catalysts, and selective adsorbents and exhibit giant or colossal magnetoresistance. With this motivation, in the present work we demonstrate the fabrication of MnO2 thin-film on ITO glass substrate with controlled morphology using spray pyrolysis approach. In this, varying composition ratio of the mixture of manganese salt (MnSO4) and polyacrylic acid (PAA) polyelectrolyte is sprayed over the heated substrate (300 oC) with deposition time of 15 min. It is observed that the swelling of the resultant films depend on the extent of Mn2+ ions associated with PAA polyelectrolyte1,2, which helps in controlling the morphology (Fig. 1). The MnO2 thin-films were further subjected to structural, morphological and electrical property characterization using X-ray diffraction, UV-Vis spectra, atomic force microscopy, scanning electronic microscopy and electrochemical impedance spectroscopy. It is noted that the morphology, crystallinity and the thickness of MnO2 thin-films could be controlled by varying the molar ratio of MnSO4 and PAA in the aqueous precursor solution. Interestingly, with increase in PAA concentration, rough and thicker films were produced. Furthermore, the structure and crystallinity is found to be significantly different with and without the PAA polyelectrolyte being used during spray pyrolysis. This approach can be extended for fabrication of thin films of different metal and metal oxides with selective controlled properties.

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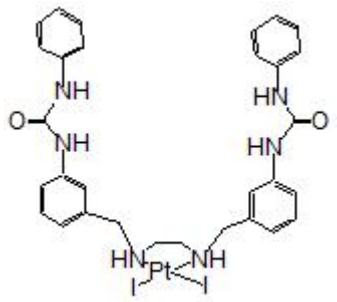
Conformational switching operating on platinum(II) coordination plane triggered selectively by oxalate anion

주리라, *김관묵

*이화여대 화학나노과학과 *이화여대 화학과*

The elaborate control of molecular motions is essential in developing molecular machines and sensors and is well realized in numerous biological systems. External stimulations such as a transition metal, a light, a redox reaction and a pH variation are used to disturb the thermodynamic equilibrium to take one conformation as major among the possible stereoisomers. N-Alkyl-substituted-ethylenediamine complexes of platinum(II) are well known to adopt syn and anti conformers which are inter-converted fast in aqueous solution. It is attractive to develop a conformational switching system by exploiting this behavior. We designed molecule 1 with two uryl groups that are well known to bind carboxylates. We expected that syn and anti conformer of 1 would be interconverted and suitable dicarboxylate anion would urge the conformation to syn form.



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Polymer을 이용한 macroporous TiO2의 합성과 염료감응 태양전지 (DSSC)로의 응용

이예지, 강미숙

영남대 화학과

현재 전 세계적으로 화석연료의 고갈과 화석연료가 야기하는 환경오염으로 인해 수소에너지나 태양에너지와 같은 신재생 에너지의 개발이 활발히 진행되고 있다. 이 중에서 태양에너지를 이용한 염료감응 태양전지(DSSC)의 경우 기존의 실리콘 태양전지에 비해 효율은 낮지만 가격이 저렴하고 많은 개발 가능성을 내재하고 있어 연구가 활발하다. 이러한 염료감응 태양전지의 효율을 높이기 위해서는 염료의 개발, 전해질 개발, TiO2 전극의 개발 등 많은 새로운 소재의 개발이 필수적이다. 본 연구에서는 염료감응 태양전지의 핵심 소재인 working 전극으로 사용되는 TiO2 를 polymer 를 사용하여 macroporous TiO2 를 개발하고자 하였다. 다공성을 가지는 TiO2 의 경우 기존의 TiO2 에 비해서 염료의 흡착량을 증가시키고 cell 내의 전자의 이동을 용이하게 하여 전자의 손실을 줄일 수 있어 염료감응 태양전지의 수명에도 영향을 미친다. Macroporous TiO2 를 pH 와 polymer 의 비율, 반응 온도, 시간에 따라 합성한 후 염료감응 태양전지의 working 전극으로 사용하여 가장 좋은 효율을 나타내는 조건을 알고자 하였다. 합성한 macroporous TiO2 는 SEM image 를 통하여 pore 의 크기를 확인하였으며 그 결과 5~10μm 크기의 pore 를 확인하였고, TiO2 아나타제의 구조는 XRD pattern 으로 확인하였다. 또한 염료의 흡착량의 차이는 FT-IR 을 통하여 확인하였다.

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Synthesis and characterization of new Pt(II) complexes with dithiocarbamate ligands

정현진, 이영아

전북대 화학과

A vast range of Platinum(II) metal dithiocarbamate complexes is known with examples finding use in applications as diverse as materials science, medicine and agriculture. We made a new series of complexes, $Pt(TC\text{-}1)_2$ and $Pt(TC\text{-}2)_2$ (Na(TC-1) = sodium bis(pyridin-2-ylmethyl)carbamodithioate Na(TC-2) = sodium ethyl(pyridin-4-ylmethyl)carbamodithioate). These complexes were characterized by IR, ^1H and ^{13}C NMR spectra. The Pt^{2+} in both complexes is located at the inversion centre and the PtS_4 moiety has a square-planar configuration. The complexes expected building block unit for supramolecular.

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Structural characterization of a novel thulium bis((cyclooctane-1,5-diyl)dihydroborate) complex $(THF)_3Tm\{(\mu\text{-}H)_2(BC_8H_{14})\}_3$

정장훈, 하성인, *강안수

*명지대 화학과 *명지대 화학공학과*

The thulium bis((cyclooctane-1,5-diyl)dihydroborate) complex $(THF)_3Tm\{(\mu\text{-}H)_2(BC_8H_{14})\}3$ including the hydrogen bridged Tm-H-B three-center, two electron bond was prepared in the metathesis reaction of 1:3 molar ratio of $TmCl_3$ with $K[H_2BC_8H_{14}]$ in THF at room temperature. The coordinated THF in the complex can not be removed under dynamic vacuum, remaining bound to Tm. From single-crystal X-ray analysis, the structure of the complex was shown to possess the coordination geometry around Tm atom consisting of a pseudo octahedral arrangement of three $(\mu\text{-}H)_2(BC_8H_{14})$ groups and three THF ligands. Each 9-BBN cyclic organohydroborate ligand is attached to Tm through Tm-H-B bridges. The distance of Tm to the α hydrogen is well beyond consideration for an agostic interaction. The crystal system is a monoclinic. R1 and wR2 are 0.0267 and 0.0481, respectively.

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Fabrication and Characterization of Biotin-functionalized and Germanium Nanoparticle-infused Porous Silicon Smart Particles

진성훈, *조성동, *손홍래

*조선대 화학과 *조선대 화학과*

Biotin-functionalized and germanium nanoparticle-infused porous silicon (PS) smart particles (SP) for the detection of biomolecules have been developed. PS sample was prepared by anodization of a highly doped P++-type Si wafer in ethanolic HF solution (3:1 (v/v) 48% aqueous HF/ethanol) using a platinum mesh counter electrode. In this work, PS is generated by electrochemically etching two discrete porous multilayered dielectric mirrors into Si, a top layer is referred to as the “DBR” multilayer, and a bottom layer is the “host” layer intended to contain Ge nanoparticles (NPs). The DBR layer is chemically further functionalized with biotin before the etching of the host layer. Resulting PS was removed from the Si substrate by an applying of electropolishing current. Prepared Ge-NPs were infused into the host layer of PS free-standing film. Samples were then made into particles by ultrasonic fracture in an organic solution. PSSP is used as biosensor for the detection of avidin. PSSP is characterized by FE-SEM, FT-IR, EDX, Fluorescence spectroscopy. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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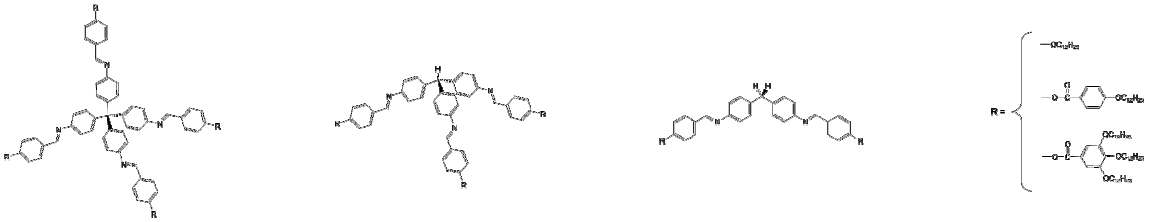
Structural variations, molecular geometry and liquid crystalline behavior of tertra-, tri-, and diphenylmethane derivatives.

나영준, Oleg Kadkin, *최문근

*연세대 화학과 *연세대 이과대학 화학과*

Liquid crystals (LC) have a great potential as dynamically functional materials for electrooptics, photonics, sensors, bio-active systems, etc. In this report LC molecules with tetra-, tri- and diphenylmethane derivatives have been synthesized using mono- and trialkyl substituted promesogenic building blocks. Three types of geometries can be obtained from these compounds. Tetraphenylmethane derivatives with a tetrahedratal shape show crystalline properties instead of liquid crystal properties. Triphenylmethane derivatives with a bowl shape exhibit the columnar mesophase when a triakyl substituted promesogenic building block is used. Bent shaped diphenylmethane derivatives show enantiotropic columnar mesophase, classified in terms of banana mesophase as B1. Dependence of the mesogenic properties on structural variations and quantity of terminal alkyl chains in the synthesized compounds will be discussed.



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발표코드: **Ⅲ33P39포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Three Dimensional CdSe/Single-walled Carbon Nanotubes Solar Cell with Reverse Field-Enhancement Effects

민선기, 이정우, 이휘건, 한성환

한양대 화학과

The field enhancement phenomena of SWNTs were applied to the design of 3-D CdSe solar cells. Fibrous CdSe was grown on the SWNTs/ITO surface by the electrodeposition, which has ideal shape for the 3-D solar cell system. The photovoltaics performance of the solar cell of 3-D CdSe/SWNTs/ITO showed 3.34% conversion efficiency under AM 1.5 condition (I = 100 mW/cm2), which is 50 % increase compared to the one without SWNTs layer. The improvement of cell performance is attributed to the reverse field enhancement effects of SWNTs. The reverse field enhancement factor of CdSe/SWNTs/ITO, β value, increased 380% with SWNTs layer with a texturized Si cathode

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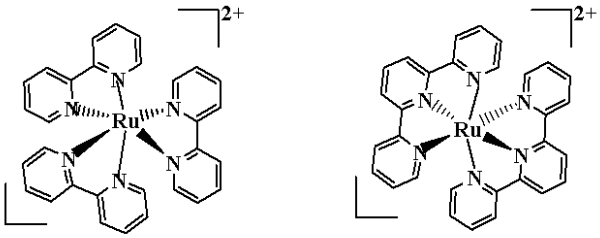
발표종류: 포스터, 발표일시: 금 10:30~12:30

Effect of differential geometry on the DNA binding behavior of the two Ru(II)-polypyridyl complexes

여가영, 이현미, 장윤정, 김석규, 조태섭

영남대 화학과

The $[Ru(tpy)_2]Cl_2$ (tpy : 2,2':6',2"-terpyridine, Ru(II)-tpy complex, Figure) complex was synthesized and its structure was confirmed by 1H NMR and elemental analysis(EA). The binding mode of this Ru(II) complex toward DNA was compared with well-known $[Ru(bpy)_3]Cl_2$ (bpy : 2,2-bipyridyl, Ru(II)-bpy complex, Figure) using various spectroscopic methods including isotropic absorption, linear dichroism(LD), circular dichroism(CD) and fluorescence. The Ru(II)-bpy complex exhibited some fluorescence when it was excited at the MLCT band which remained in the presence of DNA, while Ru(II)-tpy did not produce any fluorescence whether DNA is present or not. Very small change in the absorption pattern, especially in the MLCT band, was observed upon binding to DNA for both complexes. One the other hand, significant difference was observed in LD spectrum: a strong positive LD signal in the ligand absorption region was apparent for the Ru(II)-tpy complex which is in contrast with the Ru(II)-bpy case. Observed spectral properties led us to conclude that the interaction between ligands and DNA-base is negligible although both complexes bound to DNA. This conclusion implies that both complexes bind to the surface of DNA, probably to negatively charged phosphate groups via a simple electrostatic interaction thereby they orient to exhibit LD signal.



Ru-bpy Ru-tpy

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Detection of Biomolecules besed on surface-modified DBR Porous Silicon Interferometer

정경선, 조성동, 손홍래

조선대 화학과

Porous silicon obtained by chemical or electrochemical dissolution of c-Si has shown a great quantity of applications and extensive works on this material has been reported both in the scientific and technological areas. The visible photoluminescence at room temperature of this material reported in 1990 by Cangam has attracted considerable interest due to the possibility of manufacture an integrated optical device on Si. Porous silicon multilayers, sometimes also called porous silicon superlattices, improve the feasibility of optical components realized from this interesting material : distributed Bragg reflectors(DBR) and Fabry-Perot interferential filters, Rugate filters, microcavities with controlled spontaneous emission properties, waveguides, colour-sensitive photodiodes, and resonant cavity light emitting diodes are some of them. By adjusting the electrochemical etching conditions such as alternating current densities, time, and HF concentration, the morphology and porosity of PSi can be easily controlled.Distributed Bragg reflector (DBR) PSi exhibits unique optical properties. DBR PSi has been typically prepared by an applying a computer generated pseudo-square current waveform to the etch cell which results two distinct indices and exhibits photonic structure of Bragg filters. The study of random dielectric multilayers is of interest in the field of one dimensional light localization.-This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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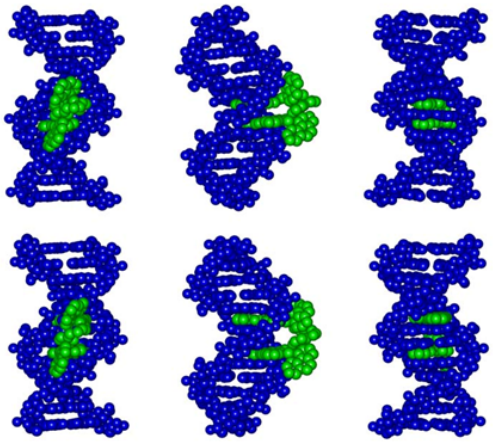
Binding mode of a New bis-Ru(II) Complex between DNA Base Pairs: Violation of the Nearest Neighbouring Site Exclusion

김은미, 이현미, *정맹준, 김석규, 장윤정

*영남대 화학과 *경북대 나노소재공학부*

The *bis*-[dipyrido[3,2-a:2',3'-c]phenazine)$_2$(1,10-phenantheroline)$_2$Ru$_2$]$^{2+}$ complexes (*bis*-Ru(II) complex) tethered by linker with proper length were synthesized and their binding property to DNA was investigated by normal absorption and linear dichroism spectrum, and fluorescence techniques in this study. Both the dipyrido[3,2-a:2',3'-c]phenazine ligands of a newly synthesized (*bis*-Ru(II) complex were intercalated between DNA base pairs with a binding stoichiometry corresponding to 1 ligand per 3 DNA bases, effectively violating the nearest neighbouring site exclusion model for classical DNA intercalation.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Application of Organic Light-emitting diodes based on Silafluorene

이성기, 조성동, 손홍래

조선대 화학과

1,1-dimethyl-1-silafluorene and 1,1-methylhydro-1-silafluorene are synthe-sized and characterized. These compounds are of interest as light emissive layers, as they prossess relatively low LUMO energy levels while maimtaining high HOMO-LUMO optical gaps. Differential scanning calorimetry measurements revel that these silafluorene compounds have advanteges of thermal stability above room temperature regions. Organic light-emitting diodes have been fabricated using thermal evaporation technique which emit violet-blue light with an excellent diode behavior under the foward bias. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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Fabrication of Optically Multi-functionalized Rugate Porous Silicon and Their Biosensor Application

조보민, 조성동, 손홍래

조선대 화학과

Optically Multi-functionalized rugate porous silicon (RPSi) for biosensor was developed to specify the biomolecules. RPSi was generated by an electrochemical etching of silicon wafer in aqueous ethanolic HF solution. RPSi prepared by using etching conditions showed that many sharp spectral lines can be obtained in the optical reflectivity spectrum. Multi-funtionalized RPSi with biotinylated silole groups has been characterized by FT-IR, Ocean optics 2000 spectrometer, and fluorescence spectroscopy. The RPSi with biotinylated silole groups was exposed to change of the effective optical thickness according to step by step addition of protein A and human Ig G. Optical Charactristics such as reflectivity and photoluminescence were observed. Further in details will be presented. -This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation-

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Optical Chracterization of borole compounds Based on Silafluorene

양진석, 손홍래

조선대 화학과

To explore their suitability for applications in molecular optoelectronics and as detector materials, novel boron compounds have been synthesized and their reactivity and properties investigated. Depending on the electronic nature of the boron center, the materials exhibit distinctive optoelectronic properties suggesting that the borole system may be useful as detector material.-This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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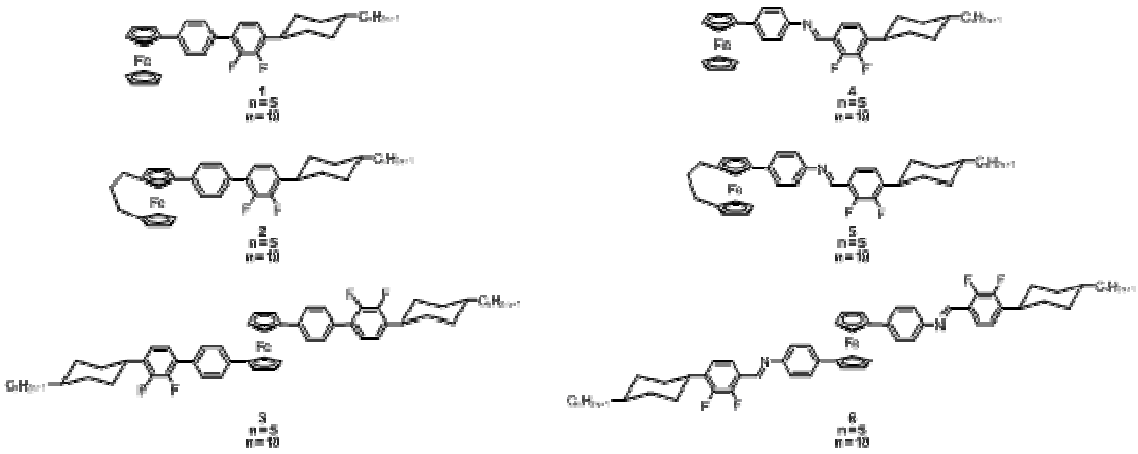
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and liquid crystal properties of a novel series of mono- and bis- substituted ferrocene derivatives containing cyclohexane units

김소연, 김은호, 나영준, **Oleg Kadkin**, *최문근

*연세대 화학과 *연세대 이과대학 화학과*

Most of the known metallomesogen compounds have a major disadvantage connected with high transition temperatures limiting their use in technologies. It is well-established that incorporation of the cyclohexyl units in the rigid core of mesogens allows to achieve lower transition temperatures and broader mesophases. The main purpose of the present work was the molecular design and synthesis of ferrocene derivatives containing the cyclohexyl unit instead of the traditional aromatic rings. As result a series of mono- and bis substituted ferrocene derivatives has been synthesized and fully characterized. Compounds of the structure 3 exhibit enantiotropic mesophases identified by POM, DSC and XRD methods as columnar, tetrahedratic smectic and tetrahedratic nematic. Compounds of the structures 4 and 5 show nematic, and 6 both smectic and nematic mesophases. However, compounds of structures 1 and 2 do not show mesogenic properties.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication of Chemosensors Based on Fluorescent Thiophene Cavitys Polymer Films

한정민, 조성동, 손홍래

조선대 화학과

The synthesis, spectroscopy, and fluorescence quenching behavior of thiophene pentiptycene-derived phenyleneethynylene polymers. The incorporation of rigid three-dimensional pentiptycene moieties into conjugated polymer backbones offers several design advantages for solid-state (thin film) fluorescent sensory materials. The fluorescence attenuation (quenching) of polymer films upon exposure to analytes depends on several factors, including the exergonicity of electron transfer from excited polymer to analytes, the binding strength (polymer-analyte interactions), the vapor pressure of the analyte, and the rates of diffusion of the analytes in the polymer films. In short, thinner films show a larger response to nitro-aromatic compounds, but show a lower response to quinones. Such differences are explained in terms of polymer-analyte interactions, which appear to be electrostatic in nature. The rapid fluorescence response (quenching) of the spin-cast films of porous polymer to nitro-containing compounds qualifies these materials as promising nitroaromtic compounds chemosensory materials.-This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Core/Shell 타입의 NiFe2O4/TixOy 나노 광촉매 소재 합성 및 수소 제조

채진호, 강미숙

영남대 화학과

광촉매를 이용하여 물이나 저급 알콜류를 분해하여 수소를 제조하는 연구는 친 환경적인 방법으로 국제적으로도 그 중요도가 매우 증가하고 있다. 하지만, TiO2 와 같이 일원 메탈로 이루어진 광촉매 반도체는 광에 의해 여기된 전자와 정공의 빠른 재결합에 의해 야기되는 비활성화 때문에 열 촉매를 이용한 steam reforming 이나 partial oxidation 에 의해 발생하는 수소 제조량에 비해 그 양이 매우 미소하다. 따라서 고 활성의 새로운 광촉매 시스템 개발이 절실하다. 본 연구는 자성체인 NiFe2O4 에 광촉매인 TiO2 가 Core/Shell 형태로 혼합된 복합 나노 광촉매 시스템을 디자인하여 전자의 흐름을 용이하게 하여 광촉매의 활성을 배가시켜 저급알코올과 물 분해에 의한 수소 제조량을 개선하는데 그 목적을 두고 있다. TEM 분석결과, NiFe2O4 Core 의 크기는 20-50nm 였으며, Ti shell 을 입힌 후 Core/Shell 크기는 100nm 임을 확인하였다. 또한 XRD, UV, PL 을 통하여 합성한 NiFe2O4/TixOy 결정체의 구조와 광학 물성을 분석하였다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication of anti-CRP Modified DBR Porous Silicon Interferometer for detected CRP

최태은, 손홍래

조선대 화학과

A biosensor was described an optical interferometric transducer scheme based on inexpensive and readily available optically flat thin films of Distributed Bragg reflector (DBR) porous silicon (PSi). Porous silicon films displaying a distribution of pore dimensions can be generated by electrochemically etching silicon in aqueous ethanolic HF using an asymmetric electrode configuration. The median pore size and breadth of the size-distribution in the film can be set by adjusting the HF concentration, current density, and position of counter electrode relative to the silicon electrode. Multi-arrayed DBR PSi exhibiting unique reflectivity was successfully obtained by an electrochemical etching of silicon wafer using square current waveform. The sensor system studied consisted of a muliti-layer of porous silicon modified with anti-C-reactive protein(anti-CRP). The system was probed with various fragments of an aqueous C-reactive protein(CRP) analyte. The sensor operated by measurement of the reflection peak in the white light reflection spectrum from the porous silicon layer. Molecular binding was detected as a shift in wavelength of reflection peaks. This research was financially supported by the Ministry of Coomerce, Industry and Energy (MOCIE) and Korea Industrial Technology Foundation (KOTEF) through the Human Resource Training Project for Regional Innovation.

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

Synthesis and Characterization of benzo annulated silafluorene

엄성용, 조성동, 손홍래

조선대 화학과

In recent years, containing silole unit has been a topic of interest because of the wide range of optical, electrical and luminescent properties. In previous work, we synthesized 6,7-dibromo-1,4-dihydronaphthalene-1,4-epoxide from the reaction of 1,4-dibromobenzene and bromine. characteristics of the [1',2']Benzeno-5,14-dihydropentacene investigated by ^{1}H-and ^{13}C-NMR spectroscopy

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A Metal-Organic Framework Based on a 1D Columnar Structure

정세현, 오민학, 나명수

한양대 응용화학과

A new microporous 3D metal-organic framework (MOF), $[Mn_3(2,7\text{-ndc})_3(DMF)_2]_n$, based on a linear trinuclear manganese cluster as a secondary building unit (SBU) was prepared, where 2,7-naphthalene dicarboxylic acid ($H_2$2,7-ndc) served as a rigid bent ditopic ligand. The SBU is connected to two adjacent SBUs by two bridging μ_2-carboxylates, which leads to an infinite 1D columnar structure. The 1D columns are further connected through the naphthalene moiety of 2,7-ndc to four adjacent 1D columns to form the microporous 3D MOF with 1D channels along the crystallographic [011] direction. The structural feature of the MOF and other properties such as gas sorption behavior will be discussed in the presentation.

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발표분야: 무기화학
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TiO2 나노튜브의 합성과 DSSC로서의 성능 평가

김지은, 강미숙

영남대 화학과

인류의 에너지 사용 증가에 의해 화석연료의 고갈과 유가가 계속 올라감에 따라 탄소 이외의 다른 원소로 구성된 3 차원 나노튜브구조는 환경 분야와 에너지 분야 등 수많은 곳에 적용할 수 있기 때문에 많은 연구가 진행되고 있다. 그 중 길이가 수 마이크로에 달하는 TiO2 나노튜브는 튜브 내부로 전자의 원활한 이동을 제공함과 아울러 빛을 효율적으로 이용하기 위한 넓은 표면적을 제공하므로 염료감응태양전지의 효율을 상승시킨다. 본 연구에서는 Electrochemical Method 을 이용하여 시간과 전압에 따른 TiO2 나노튜브를 합성하여 나노튜브구조를 scanning electron microscopy(SEM)로 확인하고 ,입자의 결정구조를 X-ray diffraction(XRD)을 통해 확인하였다. 또, 광에 수직으로 배열된 나노튜브와의 상호작용을 최적화시킴으로서 태양에너지를 전기에너지로 효율적으로 변환시키는 DSSC 의 재료로서 성능을 평가할 것이다.

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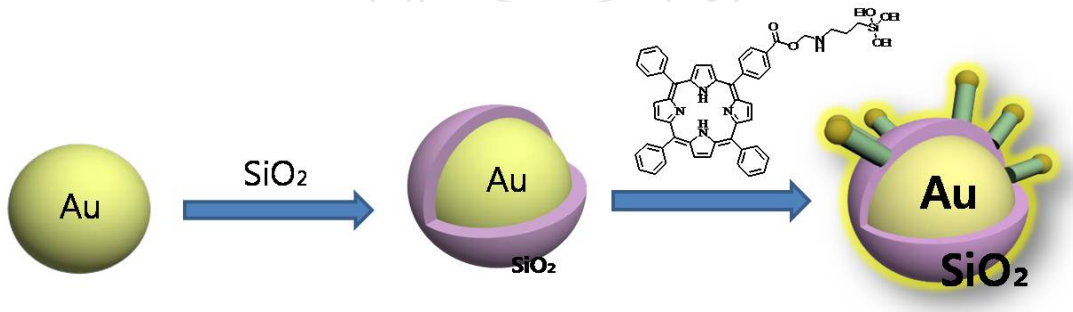
Synthesis of Porphyrin Immobilized Silica Gold Nanopaticles as Efficient Chemosensor for Heavy Metal Ion

조영제, 정종화

경상대 화학과

The porphyrin derivative(2) having triethoxy silane moiety was prepared. Au@SiO_2 nanoparticle was also prepared as supporting material. To fabricate inorganic-organic hybrid nanoparticle, we attached 2 onto the surface of Au@SiO_2 by sol-gel reaction. The porphyrin immobilized silica gold nanopaticle(1) was prepared by sol-gel reaction and characterized by SEM, TEM, FT-IR and TGA. In addition, we observed adsorption capacity and color change of PSGNP for several heavy metals in aqueous solution. We will detail discuss the color changes and adsorption capacity of 1 for toxic heavy metal ions.



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장소: 대전컨벤션센터
발표코드: **Ⅲ33P54포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, Structure and Chemical Properties of New Late Transition Metal Complexes, [bpmta]MCl2 and [bpmpa]MCl2 (M = Co, Cu, Zn) and Their Derivatives

양민규, Nayab Saira, 정종화, *이효선

*경북대 화학과 *경북대 자연과학대학 화학과*

In previous study, we have found that namely, ligands [bpmta] and [bpmpa] which is composed of N,N-Pyrazolylaniline moiety as an role of handle, have been successfully coordinated to the cobalt metal. Thus to study chemical effect of these ligands to the late transition metal in more detail, we have prepared new complexes, [bpmta]MCl2 (M = Co, Cu, Zn) {bpmta= N,N-Bis{(1-pyrazolyl)methyl}-2,4,6-trimethylaniline}, [bpmpa]MCl2 (M = Co, Cu, Zn) {bpmpa= N,N-Bis{(1-pyrazolyl)methyl}-2,6-diisopropylaniline} and their derivatives. Including characterizations and their chemical reactivity such as binding mode of the ligand to these metals, the possibility of cationic olefin oligomerization and acrylate polymerization of their derivatives are surveyed.

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Syntheses and Crystal Structures of Metal Organic Frameworks Composed of Tricarboxylate Type Ligands and Manganese

심수연, 조장훈, *나명수, 이홍인

*경북대 화학과 *한양대 응용화학과*

We obtained new metal organic frameworks (MOFs) from the reaction of $MnCl_2 \cdot 4H_2O$ and 1,3,5-benzenetricarboxylic acid (1,3,5-BTC) in DMF and 1,4-dioxane at 120℃. X-ray crystallographic study revealed that the compound has a 3-D network structure consisting of di-nuclear Mn centers, in which two manganese ions are bridged by three carboxylate groups with d(M-M) = 3.84Å. Each Mn center is working as a node with three paddle wheels of 1,3,5-BTCs. Thermal decomposition of the compound occurs at 350℃. We also synthesized new network compounds by using Mn(Ⅱ) and 1,3,5-cyclohexanetricarboxylic acid at different experimental conditions. This will be also presented.

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Synthesis and Characterization of $[Au(TC\text{-}3)]_2$

한세미, 이영아

전북대 화학과

최근의 gold(Ⅰ) 화합물들은 luminescence 성질을 이용하여 luminescent swich 나 sensor 로 사용이 되고 있다. 본 연구에서는 $Au(SMe_2)Cl$ 에 Sodium methyl(2-(pyridin-2-yl)ethyl)carbamodithioate(Na(TC-3)•EtOH)를 반응시켜 $[Au(TC\text{-}3)]_2$ 를 합성하였다. 화합물의 특징으로는 luminescence 가 최대 emission 값이 552 nm (λ_{ex} : 366 nm) 에서 측정되었다. 이 화합물은 ditopic metalloligand 로 분자의 양 끝에 다른 금속이나 유기산과 결합 할 수 있는 피리딘의 질소원자가 존재하며 분자 내에서 Au(Ⅰ)-Au(Ⅰ) 상호작용을 가질 것으로 예상된다. FT-IR 과 NMR, 그리고 Spectrofluorometer 를 사용하여 합성된 화합물의 구조와 형광성질을 살펴 보았다. 이 화합물을 dicarboxylic acid 와 반응시키면 dicarboxylic acid 의 종류에 따라서 구조적 변화에 의해 luminescence 가 사라지는 것을 확인 할 수 있다. 이 성질을 이용하여 스위치 on-off system 에서의 활용이 기대된다.

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A Double-walled Triangular Metal-Organic Macrocycle and a [2+2] Parallel and Inclined Interpentrating Metal-Organic Framework

Song xiaokai, Liu Xinfang, 오민학, 나명수

한양대 응용화학과

A double-walled triangular metal-organic macrocycle (MOM), $[Cu_6L_6(DMF)_2(H_2O)_4]$, has been synthesized by a solvothermal reaction of $Cu(NO_3)_2$•$2.5H_2O$ with 3,3'[1,4-benzenediyldi(ethynyl)]dibenzoic acid (H_2L) as a long and rigid dicarboxylate ligand in dimethylformamide (DMF) at 85 °C for 1 day. X-ray diffraction study of a sinlge crystal revealed that the pseudo-C_3 symmetric triangular MOM was composed based on three Cu paddle-wheel SBUs doubly connected by dicarboxylate ligands to form a finite cyclic structure. A similar solvothermal reaction of the ligand with $Zn(NO_3)_2$•$6H_2O$ but in presence of dabco at 120 °C for 2 days gave pale yellow block-shaped crystals, $[Zn_2L_2(dabco)_2]$, which was a 3D metal-organic framework (MOF). The MOF, based on a Zn-paddle-wheel secondary building unit, has [2+2] parallel and inclined interpenetrating 2D sheets interconnected by dabco to a 3D network. The structural features of the MOM and MOF and other properties will be discussed in the presentation.

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수소 제조를 위한 저온 활성 Sn 함유 촉매 개발

강미숙, *이준성

*영남대 화학과 *영남대 이과대학 화학과*

최근 전 세계적으로 대체 에너지에 대한 관심이 집중되고 있고, 화석연료로 인한 환경오염 방지와 에너지 효율의 향상 및 새로운 에너지원 창출에 온 전력을 기울이고 있다. 특히 수소에너지는 미래의 청정에너지원 가운데 가장 손꼽히는 신재생에너지의 하나이다. 최근 들어 ethanol steam reforming 에 의한 수소 제조 연구가 활발히 이루어지고 있는데 Al2O3 담채에 귀금속을 담지 시킨 촉매들을 대부분 사용하고 있다. 이 촉매들은 고온에서 높은 수소 전환율을 나타내고 있어 차세대 성공적인 수소경제 시스템으로 전환하기 위해서는 새로운 저온활성 촉매의 개발이 시급하다. 본 연구에서는 새로운 촉매인 Sn/Al2O3 촉매를 합성한 ethanol reforming 반응을 행하여 수소를 생산하고자 하였다.

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Synthesis, Crystal Structure and Magnetic Properties of Cyano-Bridged $Mn^{III}_2Mn^{II}$ Trimer Constructed from $[Mn^{III}(CN)_6]^{3-}$ Precursor

최상엽, 이진욱, 홍창섭

고려대 화학과

$\{[Mn(3MeO\text{-}salpn)]_2[Mn(CN)_6]\}[Mn(3MeO\text{-}salpn)(H_2O)_2]\cdot ClO_4\cdot 4H_2O$ (1) [salpn = N,N'-bis(salicylidene)-1,3-diaminopropane] was prepared by self-assembling the molecular precursor $[Mn(CN)_6]^{3-}$ and the tetradentate Schiff base. The crystal structure contains the trinuclear molecule constructed from $Mn^{III}Mn^{II}$ repeating unit linked by cyanide bridges and an isolated Mn^{III} moiety. It is worth noting that intermolecular contacts such as H-bonding or π-π stacking interaction exist between the trimeric unit and the isolated MnIII molecule. Detailed structural and magnetic studies will be given in the presentation.

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Syntheses, structural and physical characterizations of cyanide-bridged bimetallic $[W(CN)_6(bpy)][MnL]$ compounds

이진욱, 유인영, 윤정희, 홍창섭

고려대 화학과

The title compounds were prepared by self-assembly between $[W(CN)(bpy)]^-$ and MnL ($MnL_1=[Mn^{III}(F\text{-}salen)]^+$, $MnL_2=[Mn^{II}(N_3O_3\text{-macrocycle})]^{2+}$) in a stoichiometric ratio. The molecular precursor, which contains six CN groups and a bidendate blocking ligand, was utilized to prevent molecular structures from extending to high dimensions. But, this precursor tends to reduce the oxidation state of W. Compound 1 is a one-dimensional bimetallic W-Mn molecules in a identical pattern. Compound 2 is a bimetallic W-Mn dimer. Structural characterizations for these compounds will be described with some physical properties.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Two chiral Co-Cu bimetallic coordination polymers with permanent porosity: structure, magnetic and sorption properties

유대원, 이진욱, 홍창섭

고려대 화학과

Two three-dimensional porous materials, $[Co(Tt)_2Cu_4((1R,3S)\text{-}(+)\text{-camphorate})_4]\cdot DMF\cdot 5H_2O$ (1) and $[Co(Tt)_2Cu_4((1S,3R)\text{-}(-)\text{-camphorate})_4]\cdot DMF\cdot 5H_2O$ (2), have been synthesized by a solvothermal reaction of (1R,3S)-(+)-camphoric acid or (1S,3R)-(-)-camphoric acid, Cu(II) ions and $Co(Tt)_2$ (Tt=tris(1,2,4-triazolyl)borate) in mixed solvent of DMF, H_2O, and MeOH. X-ray crystallography reveals 2D sheet containing copper paddle-wheel secondary building unit (SBU) and, left or right handed rotating camphorates. $Co(Tt)_2$ that has six binding sites is connected to axial position of four SBUs. We will show the structure, sorption and magnetic properties in the presentation.

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

Synthesis, X-ray structures and magnetic properties of the cyano-bridged Fe_2Mn_2 tetramers

조경진, 이진욱, 홍창섭

고려대 화학과

Using an anionic precursor $[(Tp^{me,mt3}Fe^{III}(CN)_3]^-$, cyanide-linked Fe-Mn assemblies $[Mn^{III}_2(hadp)_2Fe^{III}_2(Tp^{me,mt3}_2(CN)_6]$ have been synthesized and characterized by means of X-ray, IR, elemental analysis, and magnetic property. This compound shows a tetranuclear Fe_2Mn_2 entity bridged by cyanides of the precursor and phenoxides of the Schiff base. In this tetramer, the angle of Fe(Ⅲ)-C-N is 178.323° and the angle of C-N-Mn(Ⅲ) is 154.995°. The distance between Mn(Ⅲ)-Mn(Ⅲ) is 3.45Å. Magnetic characteristics of the present compound will be discussed in a more detail.

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Cyanide-Bridged One-Dimensional Fe(Ⅲ)-Mn(Ⅲ) Complexes with Conflicting Magnetic Behaviors

유인영, 이진욱, 윤정희, 홍창섭

고려대 화학과

Low-dimensional molecule-based magnetic materials with magnetic anisotropy are of high interest due to their unusual physical properties applicable to information storage. A molecular precursor $[Fe(iqcq)(CN)_3]^-$ with a low-spin Fe^{III} center (S_{Fe} = 1/2) and Mn^{III} Schiff bases have been used in the construction of anisotropic magnetic systems of two one-dimensional linear chains, $[Fe(iqcq)(CN)_3][Mn(salen)]\cdot MeCN\cdot H_2O$ (1) and $[Fe(iqcq)(CN)_3][Mn(F\text{-}salen)]\cdot MeOH\cdot H_2O$ (2). Each Fe center of the complexes adopts a distorted octahedral environment consisting of three N atoms from a planar iqcq and three terminal CN groups. The axial elongation around Mn(III) accounts for the existence of the well-known Jahn-Teller effect on an octahedral high-spin Mn(Ⅲ) ion. Both complexes are almost structurally identical. However the magnetic behaviors are so different: ferromagnetic couplings via the cyanide-bridged occur in 1 whereas antiferromagnetic interactions are operating in 2. Detailed structural and magnetic studies will be given in the presentation.

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Structures, sorption, and luminescence properties of porous heterometallic coordination polymers containing both lanthanide and zinc ions.

이우람, 홍창섭

고려대 화학과

Porous three-dimensional bimtallic networks (Tb-Zn (1), Eu-Zn (2)) were synthesized via solvothermal condition by reacting H_3TPO (tris-(4-carboxylphenyl)phosphine oxide), respective Ln nitrate, and zinc nitrate in DMF solvent. The structures of (1) and (2) contain heterometallic SBU (Ln and Zn ions). The luminescence of (1) displays selective detection of Eu^{2+} ions. When (1) was immersed in DMF solution of $Eu(NO_3)_3$ for 24 h at 100 ^oC, Tb(III) ions in (1) were exchanged by Eu(III) ions in the wake of changing luminescent properties. Single crystal X-ray structures and sorption properties of the title compounds will be presented in detail.

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Cation-dependent magnetic variations of one-dimensional Mn(III) compounds bridged by a single end-to-end azide

윤정희, 이진욱, 유대원, 홍창섭

고려대 화학과

Single chain magnets (SCMs) are of importance due to their unusal physical properties and potential applications in information storage. Three new compounds with the general formula [Mn(3-MeO-salpn)(N_3)]•0.5AClO_4 [A^+ = Na^+(1), K^+(2), Rb^+(3); salpn = N,N'-bis(salicylidene)-1,3-diaminopropane] have been successfully obtained and structurally characterized. Compound 3 shows a field-induced metamagnetic transition, whereas compounds 1 and 2 exhibit SCM behaviors with slow relaxation of the magnetization. Interestingly, a spin-canted antiferromagnetism and a field-induced two-step magnetic phase transition are observed simultaneously in 1. Detailed structural and magnetic studies will be given in the presentation.

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A 3D metal-organic framework from a silicon-centered tetrahedral ligand

방원주, 이우람, 유대원, 홍창섭

고려대 화학과

Metal-organic frameworks have attracted great attention because of their unique properties as permanently microporous materials. We have synthesized a 3D metal-organic framework from cadmium nitrate and tetrahedral ligand, tetrakis(4-carboxyphenyl)silane, which contains 1D chains. We have found that the 1D chains consist of two kinds of six-coordinated cadmiums which are bridged through oxygens from carboxyl groups. One has distorted six-coordinated structure with carboxyl groups, and the other is bound by four oxygens from carboxyl groups and two oxygens from H_2O molecules. The framework is robust and thermally stable up to 400 ℃. We will also present the gas sorption study with this framework.

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Metal-Organic Frameworks Based on Covalently Interconnected Metal-Organic Cuboctahedra

김동욱, 오민학, **Liu Xinfang**, 나명수

한양대 응용화학과

Rational design of novel metal-organic frameworks (MOFs) is of great interest because the topology of the framework could be manipulated to influence the properties and functions of the materials. The common strategy for the construction of MOFs relies on the proper programming of building blocks made up of simple metal ions and organic ligands for the spontaneous self-assembly of a well-defined structural entity. We have reported a construction of 3D MOFs using zinc metal-organic cuboctahedra (MOCs) as supramolecular building blocks (SBBs). Highly porous MOFs based on MOCs covalently interconnected could be prepared through the linkage at the edges the MOCs using C_3 symmetric ligands having predesigned organic linker moieties. The metal ions could be extended from zinc(II) ion to other M^{2+} ions such as cobalt(II) and copper(II) ions which have some degree of preference for paddle-wheel secondary building units with carboxylate groups. Details of the structural features and other properties including sorption behaviors of the MOFs will be presented.

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Structures and Characterization of Eu(III) Complexes

이태우, 강성권

충남대 화학과

In this research, structures and properties of Eu(III) complexes combined with 2,6-pyridinedicarboxylic acid, 2,3-pyridinedicarboxylic acid, 3-methyldicarboxylic are investigated by the methods of PL spectrum, FT-IR, and X-ray diffractometer.

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Titanium complexes containing new dianionic Salan-type tetradentate [ONNO]-type ligands with benzyl substituents on bridging nitrogen atoms: Syntheses and catalytic activities in ring opening polymerization of lactide

윤성우

충북대 화학과

The ring opening polymerization (ROP) of lactide (LA) with a wide variety of catalytic systems based on tin, aluminum, zinc, magnesium, iron, lanthanide and lithium organometallic complexes containing initiating groups such as amides, carboxylates, and alkoxides has been intensively studied over the past few decades. Despite the fact that some excellent initiators have been reported for the polymerization of LA in the literature. Here we report a synthesis of new titanium isopropoxide complexes containing tetradentate dianionic Salan-type [ONNO]-type ligands with benzyl groups on two bridging nitrogens and their very efficient catalytic behavior both under the bulk and in solution ROP condition of LA.

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센서활용을 위한 다양한 모폴로지의 SnO2 나노입자 합성

김영미, 강미숙

영남대 화학과

산업사회의 급속한 발전으로 생산현장에서부터 가정에 이르기까지 각종 가스의 사용이 증폭하고, 그 종류도 날로 다양해지고 있다. 또한 생산과정에서 여러 종류의 가스가 발생되고 있어 보다 효율적인 가스활용 문제와 이에 따른 안전관리가 심각한 문제로 대두되고 있다. 특히 유독성의 폭발성 가스는 누설 전에 이를 감지하여 대처하는 것이 무엇보다도 중요하다. 가스센서는 빠른 응답속도, 안정성, 고감도, 재현성, 선택성 및 경제성 등의 기대되는 성능과 목적이 충족되어야 하며, 이와 같은 조건들을 만족하는 소자를 얻기 위해 그 제조와 응용기술이 연구되고 있다. 따라서 본 연구에서는 SnO2 모폴로지에 따른 가스센서활용능력을 평가하고자 하였다. Solvothermal method 를 이용하여 SnO2 를 합성하고 온도에 따라 모폴로지를 제어하였다. 그 결과 cube type 과 Hexagonal type 의 SnO2 를 얻을 수 있었고 TEM 을 통해 모폴로지와 입자크기를 확인하였으며 결정 구조는 XRD 를 통하여 확인하였다. 합성되어진 SnO2 를 이용하여 가스센서로써 적합성을 확인해보고자 한다.

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Construction of Cd(II) Compounds with a Chelating Ligand 2,2'-Dipyridiylamine (Hdpa): Anion Effect and Catalytic Activities

엄근희, 이주훈, 박현민, *김진훈, **김철, ***김영미, ****김성진

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Six new structures of Cd(II) complexes containing Hdpa ligands have been shown to study anion effects. With chloride and bromide, Cd(II) ions produce halide-bridged dinuclear units 1 and 2 while CdI2 produces mononuclear unit 3 without halide-bridging. Cd(II) produces different types of structures: with chelating benzoate, Cd(II) produces mono-Hdpa complex 4; with coordinating anions, Cd(II) does di-Hdpa complex 5; with non-coordinating anions, Cd(II) does tri-Hdpa complexes 6 and 7. These results indicate that an anion effect is very important for construction of Cd(II) complexes containing chelating Hdpa ligands, and intermolecular hydrogen bonds are also very important roles for construction of polymeric crystal structures. We have also shown that the homogeneous catalyst 4, 5, and 6 catalyzed efficiently the transesterification of a variety of esters with different alcohols, while 1, 2, 3 and 7 has displayed a very slow conversion. Importantly, the transesterification reaction catalyzed by the catalyst 6 is the best among the catalytic systems reported previously in Cd-containing coordination and polymeric compounds, to our best knowledge.

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Metal-Organic Polyhedra Decorated Using a Square Paddle-wheel Secondary Building Unit

Prakash, 오민학, **Liu Xinfang**, 나명수

한양대 응용화학과

A general strategy for the self-assembly of metal-organic polyhedra (MOPs) having C_4 symmetric Cu(II) paddle-wheel as a secondary building unit was developed using C_3-symmetric tricarboxylic ligand as a facial component and C_2 symmetric dicarboxylic ligand as a pincer-type edge component. While a metal-organic octahedron augmented via a Cu(II) paddle-wheel secondary building unit at its octahedral corners was prepared using a C_3 symmetric tricarboxylic ligand as a facial componet, a metal-organic tetragon augmented via the same paddle-wheel unit at its two square faces was prepared using a C_2 symmetric dicarboxylic ligand as an edge component.

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Selective synthesis of monomeric or dimeric titanatranes via fine tuning in triethanolateamine ligand

문정희

충북대 화학과

The use of triethanolamine ligand in the chemistry of atrane, which has high stability of the five-membered tricyclic frameworks, has expanded its application across the periodic table. Previous works have shown that the steric bulk of the substituent trans to the triethanolateamino N of a titanatrane complex has a significant influence of its solid state structure. However, no examples for the solid state structures of monomeric titanatranes based on tetradentate triethanolateamine and a small O-i-Pr axial ligand have to our knowledge been reported. Here we report a selective synthesis and characterization of monomeric or dimeric titanatranes via fine tuning in triethanolateamine ligands.

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Cutting Ultrathin Gallium Oxide Nanoribbons into Nanoplates having Single Unit-Cell Thickness

juanxu, 장권호, 손성욱

성균관대 화학과

Inorganic nanomaterials having two-dimensional (2D) structural motifs have attracted the continuous attention of material scientists due to their promising electrical and physical properties and have been applied as electrodes, sensing materials, and mechanical lubricants. For fundamental studies or practical applications of 2D nanomaterials, the shape-controlled synthesis is crucial as their properties are quite dependent on shape. However, the most studied synthetic route for 2D nanomaterials is high temperature (600-1300°C) chemical vapor deposition of a precursor having a layer-structural motif. Moreover, as far as the authors are aware, there is no report on the shape-conversion of nanoribbons into plates in solution. Our research group has made continuous efforts to prepare ultrathin two-dimensional nanomaterials via colloidal chemical synthesis at relatively low temperature. In this work, we report the wet-chemical synthesis of gallium oxide (Ga_2O_3) nanoribbons and their cutting into ultrathin nanoplates having a single-unit cell thickness by treatment with a sulfur solution.

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Hydrocarbon Oxidation of Two Novel Tetrarhenium Cluster-Supported Mn Compounds : [{Mn(Saloph)H2O}4Re4Q4(CN)12]•4CH3OH•8H2O (Q = Te, Se)

유승만, *김수현, *구효근, **이정아, 김철, ***김성진, ****김영미

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

Two new tetranuclear chalcocyanide cluster compounds, [{Mn(Saloph)H2O}4Re4Q4(CN)12]•4CH3OH•8H2O (Q = Se (1-Se), Te (2-Te)) have been synthesized by diffusion of methanol solution of [PPh4]4[Re4Q4(CN)12] (Q = Te or Se) in a methanol solution of Mn(Saloph). Compound 1 was characterized by X-ray crystallography. The compound 2-Te crystallizes in the tetragonal space group P42/n with two formulas in unit cell of dimensions a = 19.220(9) Å, c = 14.420(14) Å; V = 5327(6) Å3. These clusters (1-Se and 2-Te) catalyze olefin epoxidation upon treatment with MCPBA. Olefin epoxidation by these catalysts was proposed to involve an Mn(V)-oxo species which is formed upon heterolytic O-O bond cleavage of an Mn-acylperoxo intermediate (Mn-OOC(O)R). Evidence for this Mn(V)-oxo species was derived from H218O-exchange experiments, the product analysis and a mechanistic probe PPAA.

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DNA cleavage by autoxidation of Fe ions

박보라미, 윤효영, 김석규, 김종문

영남대 화학과

Iron ions are ubiquitous and critical in the cell metabolism, but it has been proposed that they can damage to various biological components including DNA. The well-known mechanism for iron-induced DNA cleavage reaction is “Fenton reaction” in which Fe(II) reacts with H_2O_2 to produce highly reactive •OH and related oxidants. Subsequently, •OH induces DNA cleavage by proton subtraction via attacking sugar or by hydroxylation to the DNA base. Alternatively, another pathway of iron-induced cleavage has been proposed that iron ions alone can generate DNA cleavage in the absence of H_2O_2. In this study, we are investigating the properties and the mechanism of iron ions induced DNA cleavage reaction. First, we compared the cleavage reaction with Fe(II) and Fe(III) ions. Fe(III) ion also exhibited plasmid DNA degradation although the efficiency was much lower than that by Fe(II). However, it seemed that Fe(II) and Fe(III) may follow different mechanism according to the pH dependent cleavage reaction. N_2 bubbling diminished the Fe(II)-induced plasmid cleavage efficiency, indicating that Fe(II) may use oxygen molecules to produce reactive molecular species. In the compare of the Fe(II)-induced reaction in the presence and absence of H_2O_2, the cleavage efficiency was much higher with Fe(II) alone than that in the presence of H_2O_2. On the other hand, decrease of cleavage ability of Fe(II) upon increase of H2O2 indicates that there might be a competition for Fe(II) to oxygen molecules and $H_2O_2$2. In the experiment with various radical scavengers, it seems that several radical species such as singlet oxygen, superoxide radical as well as •OH participate in the iron ions induced DNA cleavage reaction.

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Solvothermal 법에 의한 Sn-티타니아 나노 반도체 촉매의 합성 및 광분해 성능평가

강혜미, 심은희, 성윤경, 박혜진, *류시경, **김영미, **김지연, **김지은, **강미숙

*경산과학고 2학년 *경산과학고 과학부 **영남대 화학과*

최근 새로 지은 주택이나 리모델링하는 기존 주택의 벽지에서 발생되는 톨루엔이나 인체 유해화학물질인 휘발성 유기 화합물(Volatile Organic Compounds) 등으로 인하여 실내의 공기가 오염되어 일시적 또는 만성적인 두통, 눈·코·목 등의 이상, 구토, 어지러움, 가려움증 등 거주자의 건강에 이상을 일으키는 증세(새집증후군)가 발생하고 있다. 새집증후군에 따른 유해 유기화합물 제거 기술로서 여러 가지 연구들이 활발히 진행되고 있으나 그 중 광촉매를 이용하는 방법이 가장 각광받고 있다. 본 연구에서는 solvothermal 법을 이용한 Sn-TiO_2를 합성하고 새집증후군의 대표적인 발생물질인 톨루엔의 광산화 분해반응을 실시하였다. 기존의 티타니아가 초기 활성은 좋으나 홀과 전자와의 재결합으로 인한 광분해 성능 저하가 발생됨에 따라 본 연구에서는 밴드갭이 큰 Sn 을 티타니아 골격에 삽입하여 밴드갭을 늘림으로써 기존 티타니아가 가지고 있던 홀과 전자와의 재결합을 최소화 하여 광분해 성능을 향상 시켰다. 그 결과 500ppm 톨루엔을 분해 하였을 때 TiO_2 보다 Sn-TiO_2 1 시간 30 분가량 더 빠른 분해성능을 나타내었다.

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Synthesis of Gallium-hematoporphyrin dimethyl ester (Ga-HP-Me)

이은선, *박정훈, *김상욱, *허민구, **김인종, **최상무, *양승대, 유국현

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***한국원자력연구소 방사선공업환경연구부*

헤마토포피린 (Hematoporphyrin, HP)은 포피린 (porphyrin)의 구조를 가진 화합물로 암세포에 선택적으로 축적이 된다고 보고되어 있다. 최근 연구에서 헤마토포피린과 Ga 을 킬레이트한 복합체가 종양치료에 효과적이라고 보고되었다. Gallium (Ga)은 DNA 의 복제, 단백질의 합성, 그리고 효소 등을 저해하여 항암적인 효과를 나타낸다. 따라서 양전자 방출핵종 Ga-68 을 헤마토포피린에 킬레이팅을 한 ^{68}Ga-HP 복합체는 PET 용 암영상 진단 시약으로서 응용이 가능하다. 본 연구에서는 PET 용 암영상 시약의 개발에 대한 선행연구로 Gallium-hematoporphyrin dimethyl ester (Ga-HP-Me)를 합성하였다. 먼저 헤마토포피린 (~50%) 카르복시기의 에스터화 반응을 수행하여 hematoporphyrin dimethyl ester (HP-Me)를 43%의 수율로 합성하였다. HP-Me 에 염화갈륨 3 당량을 넣고 30 분동안 환류하여 TLC 확인 후 column chromatography 를 통해 분리 . 정제하여 Ga-HP-Me 을 21% 수율로 얻었다. ^{1}H NMR 를 통해 포피린 -NH 의 -4.00 peak 사라짐과 UV-Vis spectroscopy 의 최대흡수파장이 400nm 에서 405nm 로 이동한 것을 통하여 확인하였다.

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Electroparamagnetic study of Mo(V) ion species incorporated into aluminosilicate nanospheres with solidcore/mesoporous shell structure

백건호, *유종성

*창원대 화학과 *고려대 신소재화학과*

Silica spheres with sub-micrometer sized solid core and mesoporous shell (SCMS) structure were synthesized,and aluminum was incorporated into the mesoporous shell framework by impregnation method to generateSCMS aluminosilicate (AlSCMS) nanospheres. The impregnation of aluminum into the SCMS spheresgenerates the acid sites on the framework due to the presence of Al3+ ions. The AlSCMS was then used tosupport molybdenum ion species on the mesoporous shell framework. A solid-state reaction of MoO3 withAlSCMS followed by thermal reduction generated paramagnetic Mo(V) species. The dehydration produceda Mo(V) species that is characterized by electron spin resonance with g e > g ⊥ > g ‖. The structuralproperties of active sites in the AlSCMS were characterized by means of XRD, UV−Vis, 27Al MAS NMR,FT-IR, and energy dispersive X-ray spectrometric measurements. Upon O2 adsorption, the Mo(V) ESR signalintensity decreased, and a new O2 − radical was generated. The Mo species in the dehydrated Mo-AlSCMSis found to exist as oxo-molybdenum species, (MoO2)+ or (MoO)3+. Since the AlSCMS has a low frameworknegative charge, the MoO2 + with a low positive charge can be easily stabilized and thus seems to be moreprobable in the AlSCMS framework.

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Core/Shell type의 TiO2/WxOy 촉매 제조 및 광전기화학적 물분해에 의한 수소제조

김지연, 강미숙

영남대 화학과

화석 연료의 고갈로 인한 원유 값의 폭등과 석유 자원의 사용으로 발생된 CO2 로 지구 온난화가 심각한 문제로 대두되고 있다. 따라서 지속적이며 깨끗한 신·재생에너지에 대한 관심이 높아졌으며 그에 따라 많은 연구가 이루어지고 있다. 대표적으로 광전기화학적 방법을 이용하여 물을 분해하는 수소 제조 연구가 가장 활발히 진행되고 있다. 이는 태양광으로부터 물을 분해하여 수소와 산소를 제조하는 방법으로 가장 깨끗한 방법으로 수소를 제조할 수 있다. 기존 광전기화학적 물분해에 사용되어 오던 전극소재인 WO3 는 태양광-수소 변환 효율이 낮고 소재 가격이 높은 단점을 보였다. 본 연구에서는 광촉매 활성종으로 많이 사용되는 TiO2 micro 촉매에 W 을 입혔다. 이 촉매는 기존의 전극소재보다 표면 활성을 좋고 소재 가격을 낮출 수 있다는 점에서 장점을 가질 것으로 예상된다. 또한 합성한 TiO2/WxOy Core/Shell 촉매를 음극 촉매로 사용하고 상대극으로 순수 TiO2 를 이용하여 혼합형 수소제조 시스템을 디자인하여 수소제조 성능을 개선하고자 한다. TiO2/WxOy 촉매의 Core/Shell 구조 및 형상은 XRD 와 TEM 으로 확인하였다.

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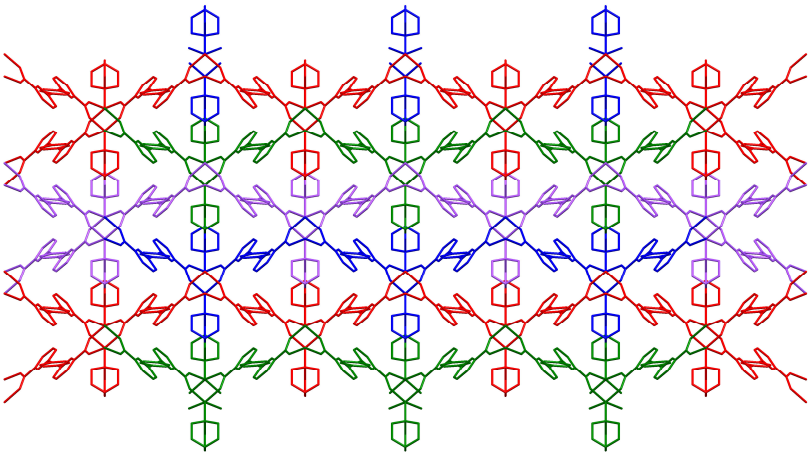
Metal-Organic Frameworks Bearing a Terphenyl Dicarboxylate Linker with a C_{2h} Symmetry

허성, 구자민

한국외국어대 화학과

In pursuit of new topologically interesting metal-organic frameworks (MOFs), we synthesized a new organic linker with a C_{2h} symmetry, 3,3''-dicarboxy-1,1':4',1''-terphenyl (1), through Suzuki coupling. Due to the lower symmetry of the new linker than conventional D_{2h} symmetry linkers, the MOFs obtained by using 1 as an organic linker molecule have shown unique structural features. For instance, a reaction between Zn(II) ions with an equimolar amount of 1 in the presence of 1,4-diazabicyclo[2,2,2]octane (DABCO) afforded colorless crystals. The crystal structure analysis of the Zn-based MOF revealed a new topology, 9-connected uninodal net with a Schläfli symbol of $3^{12}\cdot4^{24}$. The structure consists of a three-dimensional framework. Disordered DMF solvates occupy the one-dimensional channels of the framework. Interestingly, DABCO coordinates a Zn(II) ion by using one nitrogen donor atom. Therefore, another nitrogen atom remains intact.



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Preparation of Hollow and Non-Hollow $In_2O_3$with Pre-Defined Morphology

조원, 이희정, 오문현

연세대 화학과

Semiconductor particles have been widely studied due to their unique properties and resulting many useful applications including optoelectronic devices and gas sensors. Among them, indium oxide (In_2O_3) is an extremely wide-bandgap oxide material and is known for its unique electronic and optical properties. It has been widely used in solar cells, gas sensors, optoelectronic devices, and photocatalysis. Several methodologies have been developed for the preparation of In_2O_3 with a variety of morphologies and dimensions. However, a synthetic method for creating In_2O_3 materials with complicated structures is still essential and significant. Herein we report a novel methodology for the preparation of variously shaped In_2O_3 particles. The simple calcination of indium-containing coordination polymer particles (CPPs) produces In_2O_3 particles while maintaining the original shape of the CPPs.

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Biomimetic Hydrocarbon Oxidations by Nonheme Manganese(III) Complexes with m-CPBA

송영주, *풍정인, **김은영, **이태금, 장승표, **이홍규, **조영단, 김철

서울산업대 정밀화학과 친환경소재제품센터
**서울산업대 생무기화학 실험실 **서울산업대 정밀화학과*

Two mononuclear nonheme manganese(III) complexes of tetradentate ligands containing two deprotonated amide moieties, [Mn(Me2bpb)Cl(H2O)] (1) and [Mn(bpc)Cl(H2O)] (2), were prepared and characterized by IR and elemental analysis. Complex 2 has also been characterized by X-ray crystallography. These nonheme Mn(III) complexes (1 and 2) catalyze olefin epoxidation and alcohol oxidation upon treatment with m-CPBA as an oxidant. Hydrocarbon oxidation by these catalysts was proposed to involve an adduct LMn-OC(O)Ph species which is found to be a reactive intermediate. Evidence for this LMn-OC(O)Ph species was derived from Hammett studies and the concentration effect of substrate. Our results suggest that an M-OOR (M = Mn) moiety can form in a system wherein the supporting chelate ligand is comprised of a mixture of neutral and anionic nitrogen donors.

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Synthesis and characterization of Cd(II) and Zn(II) complexes with dithiocarbamate ligands

한아름, 이영아

전북대 화학과

Dithiocarbamate 의 구조를 기초로 하는 리간드인 Na(TC-2)와 Na(TC-3)를 합성하고 이를 전이금속과 반응시켜 전이금속 착물인 $M(TC\text{-}2)_n$ 와 $M(TC\text{-}3)_n$ (n = 2, 3 ; M = Zn(II), Cd(II) ; Na(TC-2) = sodium ethyl(pyridine-4-ylmethyl)carbamodithioate, Na(TC-3) = sodium methyl(2-pyridine-2-yl)ethyl)carbamodithioate)을 합성하였다. 새롭게 합성한 전이금속 착물을 FT-IR 과 ^{1}H NMR 로 분석하였다.

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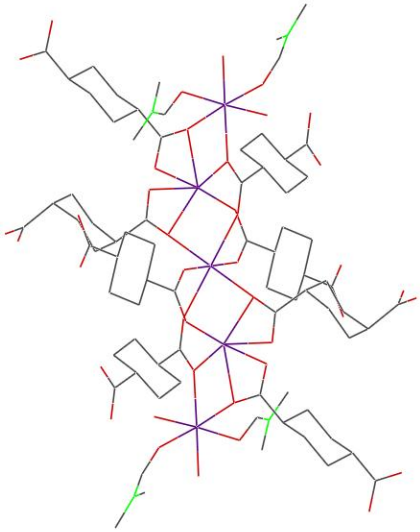
A New Cd(II) 1-D network constructed based on 1,4-cyclohexanedicarboxylates.

박경세, 구수연, 유수창, *윤민영, *김기문

*군산대 화학과 *포항공과대 화학과*

An one-dimensional metal-organic framework, $[Cd_2(chdc)_2(DMF)]$ (1) (1,4-chdc = 1,4-cyclohexanedicarboxylates and DMF = *N,N*-dimethylforamide), has been synthesized and characterized by X-ray crystallography. The title compound crystallizes in the momoclinic group *C2/c* with unit cell parameters of a = 14.134(3), b = 18.697(4), and c = 17,205(3) Å, α, γ = 90 °, β = 98.84 (3) °, V = 4492.6 (2) $Å^3$, and Z = 8. An asymmetric unit of 1 contains three different Cd(II) metal centers, $Cd(II)_1$, $Cd(II)_2$, and $Cd(II)_3$. The coordination spheres of $Cd(II)_1$ and $Cd(II)_3$3 are described as a slightly distorted octahedral, however, that of $Cd(II)_2$ is a highly distorted octahedtal. Interestingly, asymmetric unit of 1 contains two different ligand conformations. One of four 1,4-chdc has axial conformation and the others have equatorial conformations.



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One dimensional hybrid nanomaterials with Te nanowire core and SiO_2 shell

비노드, 김진권

공주대 화학과

Core-shell nanostructures attract intense attention due to their enhanced physical and chemical properties over their individual component counterparts. This aspect is of pivotal importance in a large variety of applications such as electronics, magnetism, optics etc. Te nanowires and other one dimensional structures has been a topic of extensive research because of their peculiar properties and potential uses. We prepared Te nanowires through the reduction of ammoniumsulftellurite with sodium sulfite in presence of sodium dodecylbenzenesulfonic acid (SDBS) and poly (sodium 4-styrenesulfonate) (PSS). The surface charge of nanowires was altered consecutively by layer by layer coating of polyallylamine hydrochloride (PAA) and polyvinylpyrrolidone (PVP). Growth of silica shell was obtained over PVP-coated nanowires through the hydrolysis of tetraethylorthosilicate (TEOS) with ammonia. The core-shell structures obtained were characterized with transmission electron microscopy. Te@SiO_2 hybrid materials are expected to have promising applications in various areas.

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Preparation and Characterization of In - Doped CdTe Nanorods

마문, 김진권

공주대 화학과

Negative charged water-soluble In-doped CdTe nanorods were prepared by wet chemical process in presence of thioglycolic acid (TGA) as capping ligands. One-dimensional (1D) nanorods assemblies by spontaneous self-organization of nanoparticles into nanorods occurred when partially removal of the surfactant. The X-ray diffraction (XRD) patterns of the In-doped samples retained alike crystal structure as the CdTe nanocrystals, indicating no 2nd phase formation while incorporating of In- ions into CdTe lattice. TEM images showed that the diameter of the nanocrystals varied when the dopant concentration increased. The interplaner spacing (d-spacing) of doped CdTe nanorods were of 0.215 nm, which corresponds to the value for the (220) plane of the zinc-blende structure of CdTe, was in good agreement with the value obtained from XRD analysis. The synthesis, self-assembly and characterization of the as prepared nanocrystals will be presented.

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Enhanced Water Miscibility of Ruthenium-Complex-Sensitized TiO2 Derived from Hydrophilic Group Substitution and Its Photocatalytic Activity on Water-Splitting Hydrogen Generation under Visible Light Irradiation

전지송, *한중규, 민경태, 손호진, 고재중, 강상욱

*고려대 소재화학과 *고려대 신소재화학과*

Various of Ru-based photocatalytic systems for hydrogen generation have reported chronic decrease of photoreactivity due to indigenous unstability of Ru-sensitizer in aqueous solvents. In an effort to overcome the limitation, we synthesized two Ru sensitized Pt/TiO2 photocatalysts (Pt/TiO2/RuLX2 1 or Ru(NCS)2LX 2), where X and L consists of 4,4'-di(2,5,8,11-tetraoxadodecyl)-2,2'-bipyridine and 2,2'-bipyridine-4,4'-dicarboxylic acid, respectively. Indeed, the hydrophilicity and bulkiness of the substituted ligand X induced the water miscibility and stability in water of 1 and 2. The durable photoreactivity of 1 and 2 was found in a standard photo-induced hydrogen production system.

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Bipyridyl Ligand 시스템의 Band-Gap 조절을 통한 Heteroleptic 루세늄 화합물의 광활성 특성 최적화

한중규, *손호진, **조대원, ***박종진, *고재중, *강상욱

*고려대 신소재화학과 *고려대 소재화학과 **고려대 광전자신소재연구소 ***삼성종합기술원 FRL*

Bipyridine 리간드를 포함하는 새로운 5 개의 heteroleptic Ru 화합물들이 합성되고 연구되어졌다. 준비된 Ru(NCS)2L(N^N-ArX) 형태의 루세늄 화합물들은 2,2'-bipyridine 리간드의 4,4'알릴 para 위치에 각각 NMe2, OMe, H, F, 그리고 CN 작용기들이 치환되어졌으며 그 체계적인 전자밀도조절로 인한 그 전자구조 변화가 광학적 전기화학적 분석을 통해 확인되어졌다. 일반적으로 Ru 화합물의 LUMO 는 pyridyl 리간드에 주로 분포하고 있기 때문에 그 LUMO 의 변화가 기대되어진다. 실제로 전자를 당기는 작용기가 최환된 화합물 (Ru-CN, F)의 경우, 상대적으로 작아진 band gap 가 함께 낮은 LUMO 준위를 보여주었으며 반대로 전자주게작용기가 치환된 화합물(Ru-OMe, NMe2)의 경우에는 증가된 band gap 가 함께 상대적으로 높은 LUMO 준위를 보여 주었다. 하지만 HOMO 에너지 준위의 경우 역시 그 치환기 변화에 따른 상당한 감소폭을 보여 주었다. 특히, 준비된 화합물을 이용한 DSSC 소자실험은 그 전자밀도의 변화가 소자와 광변환효율과 큰 상관관계가 있음을 보여주었는데 이는 화합물 자체가 가지는 에너지 준위 및 작용기들이 소자의 효율을 결정하는 Jsc 와 Voc 값에 크게 영향을 미친 것이다. 관련 실험결과에 대한 정확한 원인을 규명하기위한 시분해 흡수/발광 스펙트럼 분석 및 impedance 실험이 부가적으로 진행되었다.

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Efficient Organic Sensitizers in Dye-Sensitized Solar Cells (DSSCs)

강영진, *지희선, *김진호, **고재중

*강원대 과학교육과 *강원대 화학과 **고려대 소재화학과*

In designing metal-free sensitizer, it is important to escape from π-π stacking of adsorbent sensitizer at the TiO2 surface. Better morphological stability of the amorphous phase is often noted for metal-free sensitizer. However, strongly conjugated sensitizers should have wide absorption range in visible region which leads to wide light harvesting properties and consequently ensure high electron-transfer rate. Spacer controlled organic dyes have attracted attention because they show high open circuit voltage and high photon to current efficiency. The structural modification, such as control of spacer moiety, and its efficiency in DSSC performance will be discussed.

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Concomitant Formation of N-Heterocyclic Carbene-Copper Complexes within a Supramolecular Network in the Self-Assembly of Imidazolium Dicarboxylate with Metal Ions

천지슬, 정일구, 손성욱

성균관대 화학과

Recently, we designed and synthesized a new building block bearing imidazolium moiety. Using the diverse metals salts as connector, the corresponding supramolecular networks were prepared. When Cd^{2+} was used, 1D-network having inner space was obtained. The most interesting structure was obtained through assembly between Cu^{2+} and the new building block. Two kind of copper speices were observed in this supramolecular network. First, Cu(II) played a role of connector of building block by coordination with two carboxylates. Second, Cu(I) coordinated to central N-heterocyclic carbene coordination mode which was formed through abstraction of central proton in experimental conditions. In this presentation, we will discuss the formation mechanism and potential applications of NHC-copper decorated supramolecular networks.

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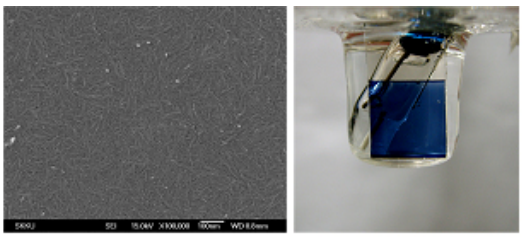
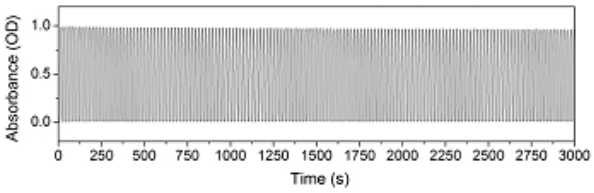
Colloidal approach for tungsten oxide nanorod-based electrochromic systems with highly improved response times and color efficiencies.

박소연, 손성욱

성균관대 화학과

Electrochromism-based displays have been expected as alternatives to liquid crystals or LED based ones. However, more efforts are required for improvement of their properties, including stability, color efficiency (CE), color diversity and response time.Tungsten oxide is famous inorganic electrochromic materials. The reduction of tungsten oxide induces the migration of cations such as proton or lithium and results in display of blue color. It has been reported that amorphous tungsten oxides have higher coloration efficiencies than crystalline ones. However, amorphous ones have poor durability in acidic electrolyte solution due to the dissolution of materials. In this regards, tungsten oxide nanocrystalline materials are very promising as electrochromic materials because they have not only much amorphous surface but also crystalline properties. In this presentation, we will discuss on the preparation of high quality tungsten oxide films in wide area by colloidal approach. They showed much improved response times and color efficiency, compared with conventional tungsten oxide elelctrochromic systems.





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Target-Cell-Specific Magnetic Nanoparticles for Simultaneous Molecular Imaging and siRNA Delivery

최은주, 천진우

연세대 화학과

It is known that synthetic small interfering RNA (siRNA) can inhibit specific protein expression by suppressing a target gene selectively at the posttranscriptional mRNA level by a mechanism called RNA interference (RNAi). siRNAs have been studied extensively to treat various genetic diseases, including cardiovascular diseases and various cancers. The development of appropriate carrier systems is crucial for practical applications of siRNAs as therapeutics. A number of inorganic nanocrystalline materials have been emerging as potential siRNA carriers in systems devised for simultaneous imaging and therapeutic purposes. Magnetic nanoparticles are highly attractive platform materials for siRNA delivery owing to their unique properties which include uniform size, biocompatibility, superior imaging characteristics, and facile surface modification. Cell-specific targeting strategies for high-performance magnetic nanoparticles with dual (diagnostic and therapeutic) functions also include the immobilization of various target-specific moieties, such as antibodies, small peptides that can be recognized by cells, and aptamers. Our magnetic nanoparticle probes were conjugated with siRNAs, cancer-cell-specific targeting moieties, and fluorescent dyes. Our purpose in designing the multifunctional nanoprobe was to enable highly accurate imaging to be carried out simultaneously with the delivery of therapeutics. It can minimizeinvasiveness and deleterious side effects. As a result of the ability of the probes to target specific cells, siRNAs will be unloaded only inside targeted cells with certain receptors; the disulfide linkages between siRNAs and the nanoparticles should be cleaved inside the cells. In principle, it is possible to monitor where the probes with therapeutics are located in the targeted areas.

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Catalytic Reactions on Coordinatively Unsaturated Metal Centers of Porous Frameworks

윤민지, 박상지, 김진홍

이화여대 나노과학부

Porous metal-organic hybrid materials, are currently of great interest and importance due to their novel coordination structures, diverse topologies, and potential applications including gas storage, separation, catalysis, and drug delivery. Although catalysis is one of the most important areas in these materials, their catalytic properties have been largely unexplored as compared with recent interest in porous hybrid solids with zeolitic guest-binding properties. The introduction or incorporation of coordinatively unsaturated metal sites (CUS) into porous hybrids is very beneficial since CUS can strongly interact with guest molecules such as gases and organic molecules in adsorption and catalysis. Li et al. have previously presented an example of how CUS can be achieved in the copolymerization of 1,4-benzenedicarboxylate with zinc(II), to give a 3-D metal-organic porous framework. Chui et al. reported that the channel linings of a porous metal coordination polymer HKUST-1 can be chemically functionalized, indicating the potential utilization of unsaturated copper sites. Indeed, it is believed that CUS can offer a promising tool in catalysis because regular arrangements and well-understood surrounding environments of metal centers in the pore channels induce regioselectivity and shape- or size-selectivity towards guest molecules or reaction intermediates. These characteristics are advantageous over other porous materials such as inorganic zeolites and mesoporous materials.

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Gold Nanoparticles Protected with a Cyclic Tetraaminethiol Compound: High Concentration and Stability

Wu Qiong, 김진홍

이화여대 나노과학부

Nanometer-sized colloidal Au nanopaprticles (AuNPs) has received a great deal of attention in recent years for their diverse chemical and physical properties. Gold nanoparticles present fascinating aspects such as their assembly into multiple types for applications in materials science, showing properties potentially relevant to nano-scale electronic and optic devices, magnetic metirals, multifunctional catalysts, chemical recognition, and biosensors. Several approaches have been developed to prepare monolayer protected clusters which are stabilized by a covalently attached shell of ligand molecules. While alkanethiolate-proteted nanoparticles are soluble in nonpolar organic solvents, the nanoparticles readily soluble in aqueous media that do not aggregate non-specifically due to electrostatic interactions are required for most biological or biomedical applications. In order to prepare stable, water-soluble gold nanoparticles, a number of different stabilizers such as tiopronin, glutathione, mercaptosuccinic acid, sulfonic acid, and ammonium ions have been used to result in the nanoparticles that are readily dispersible in water. However, gold nanoparticles protected with arylthiolates bearing OH, NH_2, COOH functional groups were found to be soluble only in polar organic solvents but not in water. A general synthetic method producing new water-soluble gold nanoparticles has been developed using a thioethyl-pendant cyclic tetraammine, 1- thioethyl-4, 8, 11-trimethylcyclam as a capping molecule. A single-phase synthetic route of Au nanoparticles can be performed in a high concentration and partly control their quantum size.

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Magnetic properties of Co Core/CoO Shell and Hollow CoO NPs

김상현, 김기섭

충주대 화공생물공학과

We present a magnetic properties on the magnetic structure of exchange biased Co core/CoO shell and hollos nanoparticles. Transmission electron microscopy measurements reveal that oxidation creates a Co core/CoO shell and hollos interface which is highly directional and epitaxial in quality. Neutron diffraction measurements find that below a Neel temperature of ~ 230 K the magnetization of the CoO shell is modulated by two different wave vectors, q1=(½ ½ ½) 2π/a and q2=(100) 2π/a. The large magnitude of the latter, relative to bulk CoO, is consistent with the presence of a tetragonally distorted interface region in the CoO shell, where the distortion magnitude and the related induced moment both increase with oxidation. We propose that the large exchange bias effect results from the highly ordered nature of the interface between the Co core and CoO shell, and by the enhanced core-shell coupling enabled by the uncompensated interface moment.

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흡수식 열펌프에 사용되는 작동유체 개발

김상현, 김기섭

충주대 화공생물공학과

1-Butyl-3-methylimidazolium tetrafluoroborate ([BMIm][BF4])+ 2,2,2-trifluoroethanol (TFE) and 1-butyl-3-methylimidazolium bromide([BMIm][Br]) + TFE mixtures exhibit properties which render them suitable as candidates for working fluids in absorption heat pumps or chillers. Refractive indices and heat capacities of each pure ionic liquid were investigated in the temperature range of 298.2–323.2 K. Vapor pressures were measured by using the boiling point method in the concentration range of 40.0–90.0 mass% of ionic liquid and were correlated with an Antoine-type equation. The average absolute deviations between experimental and calculated values were 0.6% for the [BMIm][BF4] + TFE and 0.4% for the [BMIm][Br] + TFE system, respectively.

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Effects of La^{3+} and B^{3+} on Luminescence Properties of Green Oxynitride Phosphors for Light-Emitting Device

오성일, 강준길

충남대 화학과

We prepared green $(Ba_{1-X}A_X)_aB_bSi_cO_dN_e:Eu^{2+},Cl^-$ phosphors (A: divalent cation, B = La^{3+}, B^{3+}). And investigated their luminescence properties for white light-emitting diode (LED). These phosphors were synthesized by low-temperature solid-state reaction under a NH_3 gas condition. Under 460 nm excitation, the phosphors produced green luminescence. The addition of B (La^{3+} or B^{3+}) greatly improved green luminescence. The peak position varied in the 510 ~ 530 nm region, depending on the mole fraction of B. The optimized phosphor was determined as producing the maximum luminescence intensity upon a 460-nm excitation. Furthermore, the optimized phosphors were fabricated with blue GaN LED and the chromaticity index of the phosphor-formulated GaN LED was investigated as a function of the wt % of the optimized phosphor.

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Effect of In_2O_3 coatings on enhanced characterization of phosphors for Field Emission Display.

오성일, 이효성, 강준길

충남대 화학과

The phosphors of $Y_2O_3:Eu^{3+},Tb^{3+}$, $ZnS:Cu^{+},Al^{3+}$ and $ZnS:Ag^{+},Al^{3+},Cl^{-}$ have been used in field emission display (FED) as red, green and blue phosphors, respectively. In this study, the phosphors (R, G, B) were coated by In_2O_3, using a sol-gel method to improve luminescence efficiency, resistance to current saturation and chemical stability. The coating effect on the cathodoluminescence (CL) properties was investigated as a function of applied voltage. For the $ZnS:Cu^{+},Al^{3+}$ and $ZnS:Ag^{+},Al^{3+},Cl^{-}$ phorsphors coated with more than 10 wt% In_2O_3, the CL aging was markedly improved at voltages higher than 10 keV. For the $Y_2O_3:Eu^{3+},Tb^{3+}$ phosphor, the coating of In_2O_3 nanoparticles was found to be very effective in the improvement of the cathodoluminescence efficiency. For the 7 wt% In_2O_3-coated red phosphor, the CL intensity was increased more than 10 %, compared with that of the uncoated phosphor at voltages higher than 13 keV.

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Transient Absorption Spectroscopy of 2,2'-Diamino-7,7'-nitrospirobifluorene: Elucidation of Triplet-triplet Absorption

부봉현, *E. C. Lim

*충남대 화학과 *Department of Chemistry, University of Akron*

We have studied spectral properties of singlet and triplet excited states of 2,2'-diamino-7,7'-dinitrospirobifluorene (ANSF) by means of nanosecond time-resolved transient absorption spectroscopy. Transient absorption spectra of ANSF were measured by a ns flash photolysis technique. Two transient absorptions are shown to occur at about 400nm and in the region of 450-750nm presumably due to the triplet-triplet absorptions. The first triplet excited state is shown to have a lifetime 3.98 ns. The second triplet excited state is observed to have a lifetime 2.95 ns.

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Dissociative Double Ionization Following Inner Shell Photoexcitation of $Br_2$and I_2 by Electron-Ion and Ion-Ion Coincidence Methods in the Range 88 –1000 eV

부봉현, *이재광

*충남대 화학과 *Department of Chemistry, University of Akron*

Dissociative multiple photoionization processes of Br_2 and I_2 have been investigated in the valence and inner shell photoexcitation/ photoionization regions by time-of-flight (TOF) mass spectrometry coupled to synchrotron radiation. Several discrete resonances are observed below thresholds of some specific core levels. Also slow rises in the total yield curve are observed beyond the threshold regions. This is caused by centrifugal barrier effects which are increasingly important with increasing angular momentum quantum number *l* involved. In the whole molecules, various multiply charged ions are detected along with monocations in the whole energy range. For I_2 molecule, multiply charged ions of I^{n+} (n=1-3) are observed in the range above 150 eV (above the 4p threshold). Above 650 eV (above the 3d threshold), I^{n+} (n = 4-5) ions begin to play an important role in the total ion yield. Various ion pairs I^+-I^+, I^{2+}-I^{2+}, I^{2+}-I^+, I^{3+}-I^{2+}, I^{3+}-I^+, and I^{4+}-I^{2+} are observed, showing that the PIPICO ratios depend significantly on the core excitation energy involved.

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Coulomb Explosion Decomposition Following Inner Shell Photoexcitation of MX_4 (M=C, Si, Ge, X=Cl, Br) by Electron-Ion and Ion-Ion Coincidence Methods in the Range 88 –1000 eV

부봉현, *이재광

*충남대 화학과 *Department of Chemistry, University of Akron*

Dissociative multiple photoionization processes of MX_4 (M=C, Si, Ge, X=Cl, Br) have been investigated in the valence and inner shell photoexcitation/ photoionization regions by time-of-flight (TOF) mass spectrometry coupled to synchrotron radiation. Several discrete resonances are observed below thresholds of some specific core levels. We have calculated the discrete resonance energies using the equivalent ionic core approximation method at the HF/6-311++G(d) level. The slow rises may correspond to the delayed onset phenomena in the atomic photoabsorption and photoionization. This is caused by centrifugal barrier effects which are increasingly important with increasing angular momentum quantum number *l* involved. For CBr_4, contrast to the Br(3d) core excitation, the Br(3p,3s) core excitation led to the detection of ion pair Br^{2+} - Br^{+}, and C^{+} -Br^{+} in significant yields. This indicates that local multiple ionization of the specifically excited bare Br atom follows fast dissociation of the bond between the central carbon atom and the core-excited Br atom.

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Theoretical study on the energy stabilization of iron according to the atomic environment

양혁, 이억균, *이영주, **김상원

*KAIST 화학과 *포항산업과학연구원 부품신소재연구본부 **포항산업과학연구원 원천소재연구본부*

The electronic and magnetic properties of bulk metallic iron have been studied for recent decades. Most of the experimental and theoretical studies found that the ground state of bulk iron is body-centered cubic(bcc) phase. While some early studies revealed the transition metals show consistent behavior as the d bands become progressively occupied, and the half-filled d band elements prefers hcp structure. Moreover, in the concept of bond-cutting model for the transition metal said that the energy gain from atomic bonding is proportional to the square-root of the coordination number. In this study, we analyze the stability of the bcc Fe in NM and FM configuration with the first principle calculation and reveal energy decomposition and electron population lead the bcc ferromagnetic is stable configuration in bulk Fe.

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First principle study on the elonagation of Fe grain boundary structure with boron

양혁, 이억균, *이영주, **김상원

*KAIST 화학과 *포항산업과학연구원 부품신소재연구본부 **포항산업과학연구원 원천소재연구본부*

The mechanical properties of nano-size materials depend on the lattice dislocations such as grain boundaries(GBs) and the interaction between grains depends on the geometry of grain boundary. The dislocation is investigated by tunneling electron microscopy(TEM), model analysis, or molecular dynamics simulations. But the clear evidence of trace element effect on the nano-size material strength. We investigate the stress-strain characteristic for various grain boundary conditions according to the locations of interstitial boron. We use density functional theory(DFT) to obtain stable geometry and accurate grain boundary enery.

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Synthesis and Crystallographic Studies of Highly NH_4^+-exchanged, Fully Deaminated, and Fully Tl^+-exchanged Zeolite Y (FAU, Si/Al = 1.56)

서성만, 임우택

안동대 응용화학과

Single crystals of zeolite Y, $|Na_{75}|[Si_{117}Al_{75}O_{384}]$-FAU, with diameters up to 0.30 mm were grown from gels; Si/Al = 1.56. They were ion exchanged and fully dehydrated to generate $|(NH_4)_{67}H_5Na_3|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 1, partially deaminated), $|H_{72}Na_3|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 2, fully deaminated at 473 K) and $|Tl_{75}|[Si_{117}Al_{75}O_{384}]$-FAU (crystal 3). Their structures were determined crystallographically at 294 K using synchrotron X-radiation in the cubic space group *Fd*3-*m*. They were refined to the final error indices R_1/wR_2 = 0.037/0.126, 0.055/0.190, and 0.044/0.121 using 884, 723, and 851 reflections with $F_o > 4\sigma(F_o)$ for crystals 1, 2, and 3, respectively. In crystal 1, 67 NH_4^+ and 3 Na^+ ions per unit cell are found at four different crystallographic sites. Six NH_4^+ ions were found at the centers of double 6-rings (site I; N···O = 2.888(3) Å). Filling site I' are 32 NH_4^+ ions (N···O = 2.774(5) Å); each is recessed 1.59 Å into the sodalite cavity from the plane of the three oxygens to which it bonds. Filling site II in the supercages are 29 NH_4^+ and 3 Na^+ ions, each of which extends 1.69 Å and 1.10 Å, respectively, into the supercage from its 3-oxygen plane (N···O = 2.818(5) Å, Na-O = 2.512(19) Å). The remaining 5 of the 72 NH_4^+ ions originally present per unit cell have apparently been deaminated by vacuum dehydration at 294 K. NH_4^+ ions simultaneously occupy sites I and I' as K^+ ions did in $|K_{71}|[Si_{121}Al_{71}O_{384}]$-FAU; the internitrogen distance is 3.36 Å. In crystal 2, three Na^+ ions per unit cell are found at site I' (Na-O = 2.207(13) Å); no other cations were found so the deamination of NH_4^+ is complete at 473 K. In crystal 3, 30, 30, 9, 4, and 2 Tl^+ ions were found at sites I', II, and three sites III' per unit cell, respectively. The total, 75, agrees with the results of EDX analysis to establish the framework composition (the Si/Al ratio) of these crystals.

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Crystal Structure Showing the Dehydration, Deamination, and Dealumination of Partially NH_4^+-exchanged Zeolite Y (FAU), $|Na_{33}H_{26}(Al_5O_4)|[Si_{126}Al_{66}O_{384}]$-FAU

서성만, 김후식, *김경화, 이오석, 임우택

*안동대 응용화학과 *포항가속기연구소 빔라인부 엑스선운영2팀*

A single crystal of zeolite Y, $|Na_{71}|[Si_{121}Al_{71}O_{384}]$-FAU, was ion exchanged to generate $|(NH_4)_{38}Na_{33}|[Si_{121}Al_{71}O_{384}]$-FAU. This was then vacuum dehydrated at 673 K, and, without re-exposure to the atmosphere, its structure was determined crystallographically using synchrotron X-radiation in the cubic space group *Fd*3-*m* at 294 K. It was refined to the final error index $R_1 = 0.0532$ with 522 reflections for which $F_o > 4\sigma(F_o)$. The composition (best integers) is determined to be $|Na_{33}H_{26}(Al_5O_4)|[Si_{126}Al_{66}O_{384}]$-FAU which means fully dehydration, deamination, and dealumination were achieved. The 33 Na^+ ions per unit cell were found at two crystallographically distinct positions: nine at site I (in the centers of the D6Rs) and 24 at site II (in supercages opposite S6Rs). The 2.5 sodalite units contained a dimeric tetrahedral aluminate cation (Al-O = 1.40(8) and 1.60(8) Å) at its center. Each $[Al_5O_4]^{7+}$ cation coordinates to framework oxygen of D6Rs with tetrahedral manner. This work demonstrates that it is possible to obtain large amount of dealuminated species within the H-Y zeolite framework which should enhance the acidity of adjacent sites for higher catalytic activity.

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ZnO Nanocrystals Grown by Chemical Vapor Transport : Temperature Dependence and Photoluminescence Studies

이슬기, *송재규

*경상대 화학과 *경희대 화학과*

We present the ZnO nanocrystals grown by chemical vapor transport (CVT) methods onto the ZnO nanofilms spin coated by sol-gel methods. ZnO nanocrystals were grown on Si wafer at different positions in a four zone furnace, a temperature range of 610-770℃. Different shapes of ZnO nanocrystals were identified with different temperature conditions by SEM. Temperature dependent ZnO nanocrystals, giving rise to different shapes, were investigated with SEM, UV-vis and photoluminescence.

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A Vibrational Transition Moment Angle Study of Several Iso-cytosine Tautomers using ab Initio and DFT Calculations

이슬기

경상대 화학과

Iso-cytosine, an isomer of cytosine, is one of the unnatural nucleic acid bases such as isoguanine having a pyrimidine backbone. Due to the similarity of guanine, it is of interest to investigate the structural information of iso-cytosine, the three lowest energy amino tautomers were chosen for the vibrational transition moment angle (VTMA) studies. We have conducted ab initio and DFT calculations to obtain the angles between permanent and transition dipole moments of several iso-cytosine tautomers. The VTMAs of each tautomer are investigated as function of several dihedral angles associated with the amino (NH2) group. By brute forcing the dihedral angles of the amino group while fully relaxing the other atoms in the molecule, the structural information of the tautomers is well denoted in the corresponding VTMAs. In the near future, we intend to study the nonplanarity of iso-cytosine by comparing the experimental VTMAs obtained from 0.37K superfluid helium nanodroplets and those from this study.

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Computational approaches on the thermodynamic properties of possible secondary structures by using the polyalanine model

홍주연, 함시현

숙명여대 화학과

Quantitative prediction of the possible secondary structures is important to understand the function of proteins at the molecular level. One of the most interesting secondary structures, the α-sheet has been received a great attention because it was proposed as the possible intermediate conformation to form the beta-sheet fibrils in the aggregation process. Including the α-sheet conformation, the eight possible secondary was investigated by using the density functional theory and molecular dynamics simulation to estimate the thermodynamic properties of the secondary structures. The relative thermodynamic properties are discussed in terms of the thermodynamic stability, gibb's free energy, enthalpy, entropy, dipole moment, and the charge separation.

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Dynamics of the HIV-1 Nucleocapsid Protein : A Molecular Dynamics Study

홍주연, 함시현

숙명여대 화학과

The HIV-1 nucleocapsid protein (NCp7) is a highly conserved protein generated by processing of the Gag polyproteins during retrovirus maturation. It has been widely studied that NCp7 protein was regarded as a potential target for the development of antiviral drugs. The two CCHC-type zinc knuckle domains of the NCp7 were known as the critical parts for the NCp7 function. Consequently, Zn^{2+} ejecting agents that disrupt the zinc knuckle domains were proposed to result noninfectious viruses. Herein, we present the molecular dynamics studies to understand the dynamical properties of the NCp7 in the aqueous phase. These theoretical approaches provide the insight of the critical role of the zinc knuckle in relation to the control of NCp7 functions at a molecular level.

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Vertical Epitaxial Co_5Ge_7 Nanowires and Nanobelts Arrays on a Thin Graphitic Layer for Flexible FED

윤하나, 서관용, 인준호, 김봉수

KAIST 화학과

We have successfully synthesized vertically aligned single-crystalline Co_5Ge_7 NWs on a curved thin graphite layer as well as on a very thin graphite layer. Vertical Co_5Ge_7 nanobelts are also synthesized on a graphite substrate. The vertical Co_5Ge_7 nanobelt arrays or Co_5Ge_7 NW arrays have been selectively grown on a graphite substrate depending on the experimental conditions. As grown Co_5Ge_7 NW arrays satisfy most requirements for the ideal emitters of field emission displays (FEDs), such as sharp tips, superb electrical conductivity, thermal and chemical stability, and vertical alignment to the substrate. The vertical Co_5Ge_7 NW arrays showed very efficient FE properties comparable to those of CNTs because of their optimum morphology. The NW emitter arrays on the curved graphite layer could be used for future flexible FEDs. Since the crystal structure of thin HOPG is close to that of graphene layers, our results could be extended to the epitaxial growth of Co_5Ge_7 NWs and nanobelts on graphene.

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Synthesis and Characterization of Manganese Silicide Nanowires

서관용, 윤하나, 김봉수

KAIST 화학과

Transition metal silicides can be used as ohmic or schottky barrier contacts and low resistance interconnects in electronic devices. Compared with other metal silicides, chemical compositions of manganese silicides can vary more flexibly and thus manganese silicides are expected to possess richer physical properties. For example, $MnSi_{\sim 1.7}$ is semiconducting and a promising material for silicon-based optoelectronic devices as well as a thermoelectric material operating at high temperatures. Mn_5Si_3 and MnSi compounds are metallic in bulk and MnSi is ferromagnetic with a Curie temperature of 30 K, which may find application in the developing field of "spintronics". Among the various manganese silicides, MnSi has attracted great interest because it continues to provide surprise in the area of metal physics. We report here synthesis of single-crystalline MnSi nanowires via a simple vapor transport method. Free-standing MnSi nanowires are grown on a Si substrate with no catalyst. We have studied the crystal structure of the MnSi nanowires. Transmission electron microscopy studies confirm the single crystalline nature of the simple cubic MnSi nanowires. The typical size of the MnSi nanowire is several micrometers in length and 70-150 nm in diameter.

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Femtosecond Transient Absorption of Distyrylbenzene in Vesicle: High Energy Absorption and Electron Transfer Efficiency in Comparison with Carotene Dyes

양일승, V. Ramanathan, *강준희, **박주현, ***김성근

*서울대 화학부 *서울대 생물물리 및 화학생물학 **중앙대 화학신소재공학부*
****서울대 화학부 & 서울대 생물물리 및 화학생물학*

Study of energy transfer in photosystems is important for fundamental understanding and practical applications of hydrogen storage device, hydrogen fuel cell, and solar cell. In natural photosynthesis, photosynthetic pigment such as carotene dyes absorbs light and transfers the light energy to the reaction center. We found that distyrylbenzene shows stronger light absorption as well as higher electron transfer efficiency in comparison with carotene dyes. In order to understand these potentially useful properties of distyrylbenzene in a spatially confined environment, we carried out a comparative study for the photophysics of distyrylbenzene and carotene in lipid vesicle by using femtosecond transient absorption spectroscopy.

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Excited State Dynamics of Curcumin Studied byFemtosecond Transient Absorption Spectroscopy

양일승, **V. Ramanathan,** *강준희, **김성근

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Curcumin has antioxidant, anti-inflammatory, antiviral and antifungal functions. Recent studies have shown that it may help stimulate the immune system to clear the brain of beta amyloid, which aggregates to form the plaques in Alzheimer's disease. Since it is known that excited-state intramolecular hydrogen atom transfer of curcumin is related to its medical antioxidant mechanism, we investigated its excited state dynamics by using femtosecond transient absorption spectroscopy in an effort to understand the molecule's therapeutic effect in terms of its photophysics and photochemistry.

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Theoretical Study of Ion Pair M+XO4- (M=Li, Na, K and X=F, Cl, Br, I) Structures:

Mohammad Harun, 최철호

경북대 화학과

We have investigated the structures and energetics of M+XO4- salt ion pairs (M=Li, Na, K and X=F, Cl, Br, I) using density functional theory (DFT) and ab initio calculations. The calculated all M+XO4- species have a bidentate and tridentate ground state structure and there have a general trend observed in their stability. The calculations showed that the (1) Molecular structure of alkaline metal perfluorate, M+FO4- [M=Li, Na, K] favors the tridentate structure with bidentate isomer higher in energy (2) M+ClO4-, M+BrO4- and M+IO4- ion pairs while M=Li and Na, favors the bidentate structure with tridentate association higher in energy (3) K+ClO4-, K+BrO4- molecule exists as bidentate and tridentate forms having almost similar energies and K+IO4- has only bidentate isomer. As a general trend for M+XO4- (M=Li, Na, K and X=Cl, Br, I) ion pairs we conclude, as the cation size decreases and anion size increases the bidentate structure favors with tridentate association higher in energy. The most interesting dual minima structure exists in NaClO4 and NaFO4 molecule cases. Both have four possible isomeric forms, two are bidentate and two are tridentate like and each bidentate and tridentate structure posses the dual minima (covalent and ionic type) which is a new invention. Bidenate and tridentate are almost isoenergetic, bidentate structure favours only 1 kcal/mol over tridentate one but the energy differences between this two respective dual minima of NaClO4 structures are about 35 kcal/mol by MP2/aug-cc-pVTZ and 41 kcal/mol by CCSD(T) which is quite high. Surprisingly DFT calculations with various functionals were seriously failed to predict the structures from Möller-Plesset second-order perturbation (MP2) theory and the most reliable coupled cluster theory with single, double, and perturbative triple excitations [CCSD(T)].

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The Onset of Ion-Pair Dissociation of NaClO4 in Water Clusters: A Microscopic Study

Mohammad Harun, 최철호

경북대 화학과

NaClO4(H2O)n (n = 0-4) clusters have been generated in the gas phase as model systems to simulate the ion pair dissociation of perchlorate salts in water.The dissociation is examined using DFT, HF and Moller plesset theory to second order (MP2). MP2 calculation shows NaClO4 with only one water which is a manifestation of initial steps of dissolution can significantly dissociates the contact ion-pair (CIP) and by the n=2, complete dissolution has occurred which eventually leads to the formation of solvent separated ion pair (SSIP). The calculation also shows CIP and SSIP coexist in the clusters for n=2. Interestingly, with n=3&4, ion pair recouples and exist as CIP, predominates over the all clusters.

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Synthesis and characterization of the Zn1-xCoxO obtained by sol-gel method

김재욱, 지명진, 김종규

단국대 화학과

We synthesized diluted magnetic semiconductor(Zn1-xCoxO) nanoparticles. The formation of diluted magnetic semiconductor(DMS) has been confirmed by thermogravimetry (TGA), X-ray powder diffraction (XRD), differential scanning calorimetry (DSC) and UV/Visible spectrometer (UV). The particle size of about 5 nm has been measured by transmission electron microscope (TEM) and Scanning electron microscope (SEM). The kinetic parameters such as activation energy (Ea) and pre-exponential factor for each compound were found by means of the Kissinger method and Arrhenius method. The thermodynamic parameters (ΔG#, ΔH# and ΔS#) for decomposition of DMS compound was determined.

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Conformational Preferences of the Aib-Pro Peptide

변병진, 강영기

충북대 화학과

A conformational study on *N*-acetyl-*N'*-methylamide of Aib-Pro peptide (Ac-Aib-Pro-NHMe) is carried out using density functional methods with the self-consistent reaction field method to explore its backbone conformational preferences and cis-trans isomerization in the gas phase and in solution. The Aib-Pro sequence serves an essential function as a “hinge” in peptaibol peptides that form voltage-gated transmembrane ion channels, although Aib is one of the naturally occurring rare amino acids. Our results based on the ΔG values show that the backbone conformations with the lowest free energies at the B3LYP/6-311++G(d,p) level of theory in the gas phase and at the B3LYP/6-311++G(d,p)//CPCM B3LYP/6-31+G(d) level of theory in chloroform and water are $E^{*}C$, AA, and EF with the trans prolyl peptide bond, respectively. It is also found that the up-puckered conformations are more preferred than the down-pucker conformations for the proline residue of the Aib-Pro peptide in water, in contrast to that found for Ac-Pro-NHMe. 이 연구는 2009 년 교육과학기술부의 지원 받아 수행된 연구임 (지역거점연구단육성사업 / 충북 BIT 연구중심대학육성사업단).

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천연물의 항산화력을 간편히 측정하는 방법

이현주, 곽소연, 김성호

순천향대 화학과

비색정량법은 검출시료에 발색시약을 첨가할 때 발생하는 흡광도의 변화를 측정하는 방법이다. 사용자의 편의를 위하여 상용화된 검출키트와 발색시약이 널리 보급되어 있다.DPPH 를 이용한 항산화법도 천연물의 항산화력 측정에 사용되는 방법으로 검출키트의 사용이 보편화되어있다. 그러나 이 키트는 고가이며, 별도의 전용장치를 필요로 한다. 발색시약의 형태로 제공되기도 하나 보관 및 이동에 불편함이 수반된다.본 연구에서는 이와 같은 단점을 보완하기 위하여 발색시약을 펠렛 형태로 제조하고 일반적인 UV-VIS spectrometer 를 사용하여 분석하는 방법을 확립하였다.

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Effect of Ion Size on Polyelectrolyte Diode using the Grand-Canonical Monte Carlo Simulation Study

이언지, 장락우, *한지형, *정택동

*광운대 화학과 *서울대 화학부*

We have performed grand canonical Monte Carlo (GCMC) simulations to understand the working mechanism of polyelectrolyte diodes, which are fabricated by directly attaching oppositely charged polyelectrolyte gels on a micro-chip. Polyelectrolyte gels are modeled as melts of freely-jointed chains with charged monomers. We applied positive voltage and negative voltage and observed that counter ions move. These simulations were in good agreement with experimental results. We also examined the effects of ion size. When ion size is smaller, mobility is very fast. As applied positive voltage (forward state), small ions start moving across the gel to generate electric current flow. On the other hand, negative voltage (reverse) no current flow is observed. We also examined the effects of applied voltage, gel structure, ion concentration.

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Molecular Dynamics Simulation Study of One-Dimensional Shock Waves Propagating in Inert Gases

이지혜, 황현석, 권찬호, 김홍래

강원대 화학과

A nonequilibrium molecular dynamics(NEMD) simulation method is applied to study shock waves propagating through argon and xenon gases. In this simulation method, shock waves are generated by pushing a piston at a constant speed from one side of the simulation box filled with argon or xenon molecules. Through this simulation, a linear relationship between piston speeds and shock speeds is observed. Density, temperature and pressure of the equilibrium regions which are before and after the generation of shock waves are obtained. These results are compared with the well-known Rankine-Hugoniot equations based on ideal gases. It is concluded that the conducted NEMD simulation results are well matched with the Rankine-Hugoniot theory.

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Photodissociation dynamics of propiolic acid at 212 nm

신명숙, 권찬호, 황현석, 김홍래

강원대 화학과

Photodissociation dynamics of propiolic acid at 212 nm has been investigated by measuring rotationally resolved laser induced fluorescence spectra of OH fragments produced in the ground electronic state. From the spectra, internal energy distribution of OH and the center of mass translational energy release of the fragments have been obtained. UV absorption spectrum of propiolic acid was measured in the gas phase and ab initio quantum chemical molecular orbital calculations have been carried out to assign the molecular orbitals responsible for the absorption. In addition, potential energy curves along the reaction coordinate have been calculated in the excited electronic state of propiolic acid. The dissociation dynamics will be discussed on the basis of the observed energy distribution and the potential energy curves

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Dispersion and stabilization of TiO_2 nanoparticles in aqueous solution

이노아, *송남웅, 윤민중

*충남대 화학과 *한국표준과학연구원 미래융합기술부 나노바이오융합연구단*

TiO_2 nanoparticles have been largely investigated in view of dispersibility and suspension stability since they easily aggregate in water. It is needed to stabilize the TiO_2 NP dispersion in aqueous solution to assess toxicity of the NPs. Thus we tried to disperse TiO_2 NPs in aqueous solution as small as possible and stabilize the suspension. Dispersion and stability of TiO_2 NPs in aqueous solutions were observed in acidic, neutral and basic conditions. Positive and negative surface ligands of cetrimonium bromide (CTAB) and citrate were also used to stabilize the dispersed NPs in aqueous solution. To observe the dispersibility and suspension stability in the aqueous solution, dynamic light scattering (DLS) size and UV/Vis absorption spectra were measured. The primary particle size was observed by using scanning electron microscopy (SEM) imaging.

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DNA Length-dependent in vitro Study for Telomere T-loop by ALEX-FRET

정지원, 이상학, 김성근

서울대 화학부

Telomeres constitute terminal regions of the gene. To protect the telomere from various kinds of unwanted modification, the gene changes its structure to a closed-ring form, often called the T-loop, which is enabled by a group of proteins called shelterin. By changing the concentration of shelterin, we studied the dynamics of T-loop formation using the ALEX-FRET (alternating laser excitation - fluorescence resonance energy transfer) technique. We also changed the length of the gene at otherwise constant conditions to determine the minimum length of the gene for the T-loop formation.

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The Effect of Analgesics on SNARE-mediated Vesicle Fusion

임영빈, *김지아, *이상학, **김성근

*서울대 생물물리 및 화학생물 *서울대 화학부*
***서울대 화학부 & 서울대 생물물리 및 화학생물과*

The typical working mechanism for analgesic agents is to block the pain signal by working on the ion channel of cell membrane. However, the effect of analgesic on the neuronal system is poorly understood at both the molecular and cellular level. In this study, we applied the fluorescence resonance energy transfer technique to SNARE-mediated vesicle fusion in order to observe the effect of analgesics such as lidocaine, acetaminophen, and fentanyl, in view of the fact that SNARE proteins play an essential role in membrane fusion at neuronal synapses.

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Interfacial Electronic Structures of Heterojunction Photovoltaics

박주연, *김성근

*서울대 화학부 *서울대 화학부, 서울대 생물물리 및 화학생물학과*

Primary step in heterojunction photovoltaics is charge separation at interface that generates photocurrent. Optimization of interfacial electronic structures is important in realizing high-efficiency photovoltaic, including band alignment, coupling strength across the interface, and dynamics of charge transfer. Here we employed a diamond thin film deposited on Ag(111) as a model heterojunction in our attempt to study, by time- and angle-resolved photoelectron spectroscopy, ultrafast charge carrier dynamics of heterojunction at interface. A particular attention was paid to the effect of diamond modification bonded to metal and added layers of electron acceptor such as C60.

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Interaction of Methanol with ZnO (0001) Single Crystal Surfaces

도원희, 프로비르찬드라로이, 김창민

경북대 화학과

Surface interaction of Methanol with ZnO (0001) single crystal surfaces have been investigated using the Temperature Programmed Desorption (TPD) in the range of 100 ~ 750 K. Multilayer is formed when the methanol is dosed over 0.5 L on the ZnO surfaces at 110 K. Desorption of multilayer of methanol is observed at around 200 K. Desorption of formaldehyde and hydrogen molecules are observed at around 500 K. We propose that the monolayer of methanol on the ZnO surfaces is formed by dissociative adsorption. It is cleaved into hydrogen and methoxy group. And most amount of monolayer is desorbed as formaldehyde at 500 K.

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Interaction of Molecular and Atomic Hydrogen with the ZnO (0001) Surfaces

프로비르찬드라로이, 도원희, 김창민

경북대 화학과

Surface reactions and bulk-diffusion of atomic hydrogen and ZnO (0001) have been investigated using the Temperature Programmed Desorption (TPD) in the temperature range of 100 ~ 800 K. Atomic hydrogen is produced by the self-designed hydrogen atom source. The hydrogen molecules do not react with the ZnO surface. But when the ZnO surface is dosed with atomic hydrogen, desorption of H_2 is observed at around 500 K and 750 K. The high temperature peak is continuously increased as the amount of atomic hydrogen dosing increases. We propose that the low-temperature desorption peak is from hydrogen of sub-surface range and the high-temperature desorption peak is the hydrogen in the bulk.

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Atomic Structure and binding Energies of Cerium, Oxygen , and Benzen

이지현, 이기학, 서영선

원광대 화학과

Atomic cation–π interactions involving benzene have been receiving growing attention in structural chemistry and chemical biology.biochemistry.Benzene is a prototype aromatic molecule in the study of cation–π interactions which mimic the structures of biomolecules.Recently benzene in circumstellar environments is detected, which also should show the importance of the organometallics of benzene in the interstellar gas if it could be a sink for metal ions. Ion structures, reaction enthalpies, and reaction free energies are computed for the binding of Cerium with benzene. Computations are performed using Gaussian 03. The hybrid density functional method denoted as B3LYP consisting of Becke's three-parameter exchange functional combined with the correlation functional of Lee, Yang and Parr was utilized.

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Production and NMR Structural Studies of the Second Transmembrane Domain from Human Wild-type and Mutant Melanocortin-4 Receptor

강가애, 박태준, 김용애

한국외국어대 화학과

The melanocortin receptor family belongs to the superfamilly of G protein-coupled receptors (GPCRs) which activate the adenylate cyclase signal transduction pathway. Recently, it has been suggested that normal melanocortin 4 receptor among five subtypes (MC1R-MC5R) increases energy expenditure and decreases food intake, and genetic disruption of MC4R causes obesity. Hence, MC4 receptors may be ideal pharmacological targets for treating disorders such as obesity and anorexia. MC4R is membrane-bound protein that transverse the lipid bilayers of the cell membrane, so it is difficult to express and characterize the membrane-bound three-dimensional structure by using conventional solution NMR and X-ray crystallography. In this study, we expressed and purified the wild-type TM2 and mutant TM2 peptides of MC4R. We successfully cloned and optimized the expression condition and purified the wild-type TM2 and mutant TM2 peptide of MC4R. In here, we present the methods how can we obtained milligram quantities of isotopically labeled peptide. Approximately, the yield was about 200mg/1L growth with a fusion partner. The two recombinant peptides were characterized by tris-tricine PAGE and mass spectroscopy. In addition, their initial structural data was obtained and compared with solution NMR spectroscopy in the membrane-like environments.

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Characterization of conducting polyaniline-alginate/titanium Dioxide nanocomposite films

김나리, pierson, C. Basavaraja, 허도성

인제대 화학과

Polyaniline-alginate/titanium dioxide (PAT) nanocomposite films were chemically synthesized, characterized, and studied for their electrical behavior. Characterization of the composite samples by Fourier transform infrared (FT-IR), UV-vis spectra (UV), and X-ray diffraction (XRD) and morphology analysis by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) indicated the formation of PAT composites. Furthermore, the temperature-dependent DC conductivity of the polyaniline-alginate (PA) and PAT composites fell within the range of $300 \leq T \leq 500^{\circ}$ K. These studies indicated that PAT composites were influenced by TiO2 nanoparticles in the composites.

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Synthesis and characterization of Ce/Au doped flower-like titanium dioxide (TiO_2) nanosheet for enhanced photoactivity

국지은, *김혜영, 이영식

*경희대 화학과 *경희대 응용화학과*

Titanium dioxide (TiO_2), widely known as photocatatlyst, is needed higher surface area and wider absorption both in the UV and visible region of solar radiation for its enhanced photocatalytic activity. In the present work, high surface area of flower-like TiO_2 nanosheet were synthesized by hydrothermal method, and then various wt% of Ce, Au metal were doped on the surface of TiO_2 nanosheet by solvothemal process. Photocatalytic activity was monitored by UV-induced degradation of Congo-Red dye dissolved in the aqueous suspension of each sample. The morphology and physico-chemical characteristics of the metal-doped TiO_2nanosheet were examined by BET surface area, scanning electron microscopy (SEM), X-ray diffraction (XRD), and transmission electron microscopy (TEM).

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Synthesis of berry-like titania(TiO_2)hollow microspheres for enhanced phtocatalytic activity

국지은, *박다위, *김지은, 이영식

*경희대 화학과 *경희대 응용화학과*

In the present work, crystalline berry-like titania (TiO_2) hollow microspheres were synthesized in distilled water by using SiO_2 microspheres as templates and TiF_2 as the precursor. For enhanced photocatalytic activity, various metal doped on berry-like titania hollow microspheres. Photocatalytic activity was monitored by UV-induced degradation of Congo-Red dye dissolved in the aqueous suspension of each sample. The morphology and physico-chemical characteristics of the metal-doped TiO_2 hollow were examined by BET surface area,SEM,XRD,and TEM. The effect of photoactivity of berry-like TiO_2 will be discussed.

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A Theoretical Study on the Photophysical Properties of Zn-tetraarylporphyrin Analogues for Solar Cells

Mannix Balanay, 김세미, 이상희, 김동희

군산대 화학과

The photophysical properties of β-substituted Zn–tetraarylporphyrin (ZnTAP) analogues used as dyes in dye-sensitized solar cells were studied using density functional theory (DFT). Singlet-excitation energy calculations of ZnTAP analogues were performed using time-dependent DFT with B3LYP, B3PW91,PBE0 exchange–correlation functionals at 6-31G(d) and 6-31+G(d) basis sets using B3LYP/6-31G(d) geometries. The PBE0 functional at 6-31+G(d) basis set provided a better correlation with the experimental data for both B- and Q-bands. The inclusion of solvation effect in the calculations provided a good agreement in terms of B:Qave ratio of the oscillator strengths for both analogues with the experimental values. Analogue 2 has a higher and a more balanced charge-carrier transport rates than analogue 1. In general, the addition of an electron-donating group in the meso-substituent (analogue 2) resulted in a narrower band gap, higher oscillator strength, a more red-shifted absorption spectra, and better charge-transfer characteristics than analogue 1.

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Time-resolved IR study of cytcCN

김주영, 임만호, 박재홍, 이태곤, 김혜림

부산대 화학과

Cytochrome c is chemically modified that is available to bind external ligands. It termed carboxymethyl cytochrome c(Ccytc). Rebinding dynamics of CN Ccytc in D_2O at 283 K was studied using femtosecond vibrational spectroscopy. The stretching mode of CN bound to Ccytc showed two bands near 2120 cm^{-1}, which can be modeled with two Gaussians. Rebinding kinetics are well described by the stretched exponential function and revealed slight dependence on the band position with average time constants of 2-3 ps. It is faster rebinding of CN to Ccytc than that to myoglobin(3-4 ps).

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Rebinding dynamics of CO to GdnHCl-denatured cytochrome c

김혜림, 임만호, 박재홍, 김주영, 이태곤

부산대 화학과

Cytochrome c, a small electron-transfer protein, has been utilized in the comparative study of CO rebinding. Since cytochrome c does not have heme pocket that is proposed to have functionally significant role and existing in hemoglobin and myoglobin, comparing rebinding characteristics of cytochrome c with that of myoglobin can provide various implications on the functional role of heme pocket. Previously we chemically modified cytochrome c which has no extra site for ligand to bind so that ligand can bind 6th coordination site of Fe. Here we unfolded cytochrome c using GdnHCl denaturant to have it bind CO and characterized its rebinding dynamics. We will compare the results with that of myoglobin and discuss its implication to the structure of heme pocket.

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Reaction Dynamics of photodissociated ICN in $CHCl_3$

이태곤, 임만호, 박재홍, 김주영, 김혜림

부산대 화학과

Chemical reaction in gas phase is well studied but condensed phase is not identified. Bimolecular reaction is a one of fundamental reaction to study chemical reactions and pump-probe system is a one of method to study chemical reaction in condensed phase. Time-resolved spectroscopy can investigate how fast reaction occurs and its pathway; abstraction, substitution reaction and recombination. Photodissociated ICN produces CN radical, and it abstracts H or Cl from CHCl3 and produces HCN and ClCN. HCN and ClCN is positioned at 3265 cm^{-1} (H-CN), 2093 cm^{-1} (HC-N), and 2205 cm^{-1} (ClC-N). Vibrationally excited state was observed at 3160 cm^{-1} (H-CN, v=0→1) and 2067 cm^{-1} (HC-N, v=0→1). Not only abstraction reaction, but substitution reaction and recombination can occur. We tried to search other products ($CHCl_2CN$, INC, and etc.) but we couldn't find.

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Kinetics and Mechanism of the Anilinolysis of Diethyl Phosphinic Chloride and Dimethyl Thiophosphinic Chloride with Anilines

Nilay Kumar Dey, 김찬경, 이해황

인하대 화학과

The reactions of diethyl phosphinic chloride (1) and dimethyl thiophosphinic chloride (2) with X-anilines and -deuterated anilines have been studied kinetically in acetonitrile at 50.0 and 55.0 ^{o}C. The obtained DKIEs for 1 (k_H/k_D = 0.828–0.974 < 1) and 2 (k_H/k_D = 0.740–0.945 < 1) are secondary inverse. The relatively large secondary inverse DKIEs involving deuterated aniline nucleophiles indicate that the aniline nucleophile attacks backside toward the reaction center P atom through a trigonal bipyramidal pentacoordinate TS.

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Kinetic Investigations of the Pyridinolysis of R,R′ Isothiocyanophosphates in Acetonitrile

Adhikary Keshab Kumar, 김찬경, *이본수, 이해황

*인하대 화학과 *인하대 총장실*

The mechanistic interpretation mostly depends on the kinetic investigations which are largely important for the interpreting characteristics of the organo-phosphorus compounds. The organo-phosphorus compounds are appearing as an interesting, informative and challenging recently in the field of physical organic chemistry specially to understand the potency in the biochemical activities in life. In the incessant of the progress of the search we have investigated the kinetics and concern physical factors of the pyridinolysis of RR′ isothiocyanophosphates in acetonitrile at 55.0^{o}C where R and R′ are MeO, EtO, PhO and their combinations. A biphasic Hammett plot indicates the mechanistic alteration during the course of reaction. The deuterium kinetic isotope effects, respective activation parameters and obtained selectivity parameters were used for interpretation of mechanistic behavior of the present system. Where we especially endeavor to introduce the frontal and backward attack of nucleophiles through the usual phenomena of nucleophilic substitution reactions and which are generally observed for the phosphate and phosphinic systems.

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Molecular Assembly and Structure of Pentafluorobenzenethiol and Pentachlorobenzenethiol on Au(111)

강훈구, 박태성, 최인창, 이남석, 노재근

한양대 화학과

Self-assembled monolayers (SAMs) prepared by aromatic thiols on gold surfaces have been often used for the fabrication of electronic device applications due to their electronic properties. In this study, the formation and structures of SAMs prepared by pentafluorobenzenethiol (PFBT) and pentachlorobenzenethiol (PCBT) on Au(111) were examined using scanning tunneling microscopy. It was found that the immersion temperature and concentration of the solution play a major roll in the formation of two-dimensional (2D) ordered SAMs. We clearly demonstrated that PFBT molecules on Au(111) at 75 °C can form 2D ordered SAMs, which can be described as a $(2 \times 2\sqrt{22})R30°$ structure, whereas PCBT SAMs have a $(4 \times \sqrt{3})R45°$ packing structure.

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Femtosecond Transient Absorption Study on MeH-PPV in Solution: Probing the Charge Transfer Efficiency

양일승, *강준희, V. Ramanathan, **김성근

*서울대 화학부 *서울대 생물물리 및 화학생물학*
***서울대 화학부 & 서울대 생물물리 및 화학생물학*

MEH-PPV, poly(2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene-vinylene), is an electroluminescent polymer used in LEDs and photonic devices. Especially in polymer solar cell MEH-PPV acts as electron donor and fullerene derivative (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) as electron acceptor. With the photophysical information about photo induced electron transfer we can elucidate the efficiency of polymer solar cell. We studied transient dynamics of photoexcited carriers in MEH-PPV, PCBM and their blend in solution and in composite film by using femtosecond transient absorption spectroscopy. We investigated photo induced electron transfer from conjugated polymer to fullerene system by changing the composition ratio of MEH-PPV/PCBM and addressed the overall dynamics in this system.

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Characterization and magnetic properties of conducing Poly-N-vinylcarbazole - capped Fe2O3 nanocomposite Langmuir-Schaefer films

조은애, C. Basavaraja, pierson, 김나리, 허도성

인제대 화학과

Capped magnetite nanoparticles (1, 2 and 3 %) were functionalized via oxidative polymerization of 3-3´(vinylcarbazole). Thin films of PVK-functionalized Capped magnetite nanoparticles were fabricated by the Langmuir–Schaefer (LS) technique and characterized by spectroscopic and microscopic techniques. The magnetization data exhibit a small hysteresis loop at room temperature.

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Microstructure properties of Conducting Poly-N-isopropylacrylamide - N-vinylcarbazole Copolymers

pierson, 김나리, C. Basavaraja, 조은애, 허도성

인제대 화학과

Conducting poly-N-isopropylacrylamide-N-vinyl carbazole (PNI–nvc) copolymers were synthesized via in situ deposition technique by dissolving different weight percentages of N-vinyl carbazole (10, 20, 30, and 40%). The structure and morphology of the polymer matrix were identified by UV-visible, fluorescence spectra, and atomic force microscope (AFM). Further, the electrical conductivity in the temperature range of 300-500 K showed a semiconducting behavior with a negative temperature coefficient of resistivity (TCR). In addition, the conductivity data were characterized by three different regions with increasing temperature.

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Synthesis of zinc oxide nanoparticles by pulsed laser ablation in aqueous media

Arif Ahmed, 송재규, 박승민

경희대 화학과

At room temperature and 1 atm pressure, zinc oxide nanoparticles have been fabricated using pulsed laser ablation (PLA) of a zinc target in aqueous media and their properties were found to be susceptible to the applied laser power and ablation time as well as pH, concentration of SDS(sodium dodecyl sulfate). The particle morphology, nanostructure, and optical properties of these zinc oxide nanoparticles were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), photoluminescence (PL) spectroscopy, and UV-visible spectroscopy. The relative intensity of exciton emission increased while the green emission related to the defects decreased, with increase in the laser power and ablation time. Possible mechanisms for the formation of ZnO nanoparticles and defects are presented.

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Effect of Plasma Gas Ratio on Zirconium Nitride Thin Films Deposited by RF Magnetron Sputtering

박주연, 허진국, 조준모, 강용철

부경대 화학과

Zirconium nitride thin films deposited on the n-type Si(100) substrates by Radio-Frequency (RF) reactive magnetron sputtering with different plasma gas ratios have been studied by using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and spectroscopic ellipsometry (SE). The deposition of the films was monitored by the nitrogen and argon gas ratio which has been increased from 0 to 100 %. We studied the effects of Ar/N_2 plasma gas ratio on the surface of films by investigating the surface crystallinity, morphology, and the thickness of the zirconium nitride thin films. The oxidation states of Zr, N, and O and the atomic ratio of the surface were analyzed by XPS analysis.

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Theoretical investigation for the molecular structures and interaction energy for complexes of $C_6H_6^+$-$(H_2O)_n$ (n=1-4)

김시조, 김승준

한남대 화학과

The intermolecular interaction between aromatic molecules and water plays a key role for many biophysical phenomena. The benzene-water has been well known that π electrons on a conjugated system can accept hydrogen to form a weak hydrogen bond, that is, so called π-hydrogen bond. The benzene-water cation complex is mainly bound by charge-dipole interaction. The global minimum structures of the benzene-water cation complex have been investigated using ab initio and density functional theory(DFT) with large basis sets. The highest levels of theory employed in this study are B3LYP/aug-cc-pVTZ for geometry optimization and MP2/aug-cc-pVTZ for interaction energy. The harmonic vibrational frequencies and IR intensities are also determined at the B3LYP/aug-cc-pVTZ level of theory to confirm whether the structure of water complexes is affected by the presence of benzene.

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Quantum mechanical investigation of the reaction mechanisms for the formation of $C_7H_7^+$ from *o*-, *m*-, and *p*-iodotoluene radical cations

이주영, 김승준

한남대 화학과

The formation of $C_7H_7^+$ from the dissocation of *o*-, *m*-, and *p*-halotoluene radical cations is one of the most interesting and challenging reactions that has been studied in mass spectrometry. This dissociation is known to have two competing pathways. The reaction pathways to $C_7H_7^+$ (tolyl, benzyl, and tropylium) from *o*-, *m*-, and *p*-iodotoluene radical cations have been studied at the B3LYP level of theory using the 6-311G** basis set. The equilibrium structures and relative energies for the local minima and transition states have been fully optimized and the harmonic vibrational frequencies have been evaluated to differentiate the local minimum and the transition state. The lowest barrier rearrangement pathway is the formation of the benzyl cation for all three isomers, corroborating the recent experimental findings of Kim and Shin. This benzyl channel involves [1,3] α-hydrogen migration at the entrance and the activation energy is calculated to be 42.5, 46.1, and 46.2 kcal mol^{-1} for the *o*-, *m*-, and *p*-isomer, respectively. The other competing rearrangement pathway involves [1,2] α-hydrogen migration at the entrance, which leads to the tropylium ion, and the activation barrier is predicted to be 48.0, 51.3, and 56.4 kcal mol^{-1} for the *o*-, *m*-, and *p*-isomer, respectively. The highest barrier process involves direct C-I bond cleavage that yields the tolyl cation with a 0K dissociation energy of 51.5, 57.5, and 62.4 kcal mol^{-1} for the *o*-, *m*-, and *p*-isomer, respectively.

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Photodynamics of XYO (X, Y = Cl, Br) systems by semiclassical AIMD and wavepacket method

이근혜, 백경구

강릉대 화학과

The photochemical processes of halo-oxides(Cl_xO_y, Br_xO_y) play an important role in the depletion of the ozone layer in the stratosphere. Recent experiments observed the isomerizations among ClBrO, BrClO, and ClOBr by the light between 317 and 870 nm, as well as similar isomerization between ClOCl and ClClO by the light between 320 and 428 nm, and the change between BrOBr and BrBrO by the light between 350 and 400 nm. The isomerisations could take place either by the direct isomerisation along their excited potential energy surfaces (PESs) or by the two-step process, the recombination after the photo-dissociation. In order to study the detail dynamics of the processes, PESs of the dissociation and direct isomerization processes as well as the spectroscopic properties of low-lying excited electronic states of the isomers are computed by using EOM-CCSD/TZV2d method. The transition states (TS) connecting the stationary structures of the states are investigated too. Then the details photodynamic of XYO are studied by applying the semi-classical ab initio molecular dynamics method (AIMD) as well as full-quantum numerical wavepacket propagation method. Similarities and differences of the above three systems are discussed in terms of dynamical viewpoints. The differences between results by the AIMD and the wavepacket methods are also analyzed, and its meanings are discussed.

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Pylene End-Capped Oligoacene as Organic Semiconducting Materials for Organic Field-Effect Transistors: the Relationship between Molecular Packing and Charge Transport

홍정표, 권종철, 홍종인, 이성훈

서울대 화학부

In the past few decades, organic electronics materials have been widely studied due to their use as organic semiconductors for the realization of devices such as organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), organic photovoltaic cells (OPVCs). Here, we report the synthesis and characterization of pylene end-capped oligoacene as organic semiconducting materials for OFETs. In order to establish the fundamental understanding of the effect of molecular packing on the charge transport of the pylene end-capped oligoacene, single crystals were grown using the physical vapor transport (PVT) method and characterized by XRD. In addition, the value of intermolecular reorganization energy that governs charge transport in the pylene end-capped oligoacene was determined by performing the density functional calculation with the B3LYP functional and a 6-31g** basis set

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Variation of CD_3CN vibrational spectra caused by solvation of $AgClO_4$ and $AgNO_3$

이주현, 조한국

인천대 화학과

The vibrational characteristics of acetonitrile show large variation upon solvation of silver salts. Especially large blue shifts of the υ_2 CN and υ_4 CC stretching bands are observed in the CD_3CN spectra. Electrophilic coordination of the Lewis acid (Ag^+) to the lone electron pair of the nitrogen end alleviates the anti-bonding character in the bonds along the molecular axis, which provided by the electron pair. While the extent of the blue shifts reflect the strength of the donor-acceptor interaction, the Raman intensity ratio between the new and original bands are used to determine the coordination number of the silver cation in acetonitrile. The number of coordination for the cation decreases with concentration, due to presence of the contact ion pair. Evidently the nitrate anion gives a lower coordination number for Ag^+ relative to the perchlorate anion, indicating that NO_3^- is more prone to form a contact ion pair with Ag^+. Extrapolation to zero concentration leads to the Ag^+ coordination number of 4 in acetonitirle for both $AgClO_4$ and $AgNO_3$, consistent with the earlier studies. DFT calculations are also done to examine the structures and vibrational characteristics of deuterated acetonitrile coordinated to silver cation. The details will be discussed.

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Comparative Study of Cyclohexanethiol and 4-Hydroxycyclohexanethiol Self-Assembled Monolayers on Au(111)

김유영, 강훈구, 이남석, 노재근

한양대 화학과

Surface structures, adsorption conditions, and electrochemical behaviors of self-assembled monolayers (SAMs) formed by the adsorption of cyclohexanethiol (CHT) and 4-hydroxycyclohexanethiol (HCHT) on Au(111) were characterized by means of scanning tunneling microscopy (STM), X- ray photoelectron spectroscopy (XPS), contact angle (CA), and cyclic voltammetry (CV). High-resolution STM imaging reveals that CHT SAMs have the well-ordered $(5 \times 2\sqrt{10})R48°$ superlattice, whereas HCHT SAMs have a rectangular unit cell containing two molecules, which can be described as a $(\sqrt{3} \times 2\sqrt{5})R46°$ structure. The remarkable differences in the surface structure and packing density between these SAMs on Au(111) can be attributed to the formation of hydrogen bond in HCHT SAMs.

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Novel Smart and Emissive Imide Conjugated Systems Bearing Imine Conjugated Part

정우철, 최수동, *전기석, 이기환, **최창식

*공주대 화학과 *한국화학연구원 나노바이오융합연구센터 **극동대 한약자원학과*

We have been synthesized various imine conjugated systems and imide conjugated ones for the development of the novel emissive photo-materials. In addition, we found the imide systems having considerable emission even if the heavy atom existed in that system. In this presentation, we prepare some more smart designed imide systems connected to imine conjugated part. Furthermore, the photophysical properties of the prepared imide systems will be investigated.

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Theoretical study for Reaction Dynamics of syn-Sesquinobornene disulfones using Variational Transition State Theory including Multidimensional Tunneling.

박기수, *김용호

*경희대 화학 및 신소재과학과 *경희대 화학 및 신소재과학*

syn-Sesquinobornene disulfones 은 두 개의 양성자가 동일한 방향으로 이동하는 특이한 형태의 양성자 이동반응을 일으키고 반응속도론적 동소체효과가 크다고 알려져 있다.본 연구에서는 syn-Sesquinobornene 의 이중 양성자 이동의 반응동력학을 알아보기 위하여 반응물과 생성물, 전이상태 구조, 그리고 포텐셜 에너지 표면을 M06-2X/6-31+G** 방법을 이용하여 계산하였다.그리고 변분법적 전이상태이론과 터널링을 고려한 직접적 반응동력학 계산으로부터 HH, HD, DH, DD 의 반응속도를 구하고 반응속도론적 동소체효과를 얻었다.이중 양성자 이동의 메커니즘은 협동적이지만 계산결과 두 개의 양성자이동이 완전히 동시에 일어나지는 않았다. 터널링 효과가 매우 크며 반응의 활성화 포텐셜 에너지는 34.9 kcal/mol, 반응속도론적 동소체효과는 100ºC 에서 HH/DH = 3.43 과 HH/HD = 3.65 이며, 수소 두 개가 중수소로 모두 치환된 경우, HH/DD = 8.80 였다.

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Theorical study of porphyrin chloride reaction

이효승, *김용호

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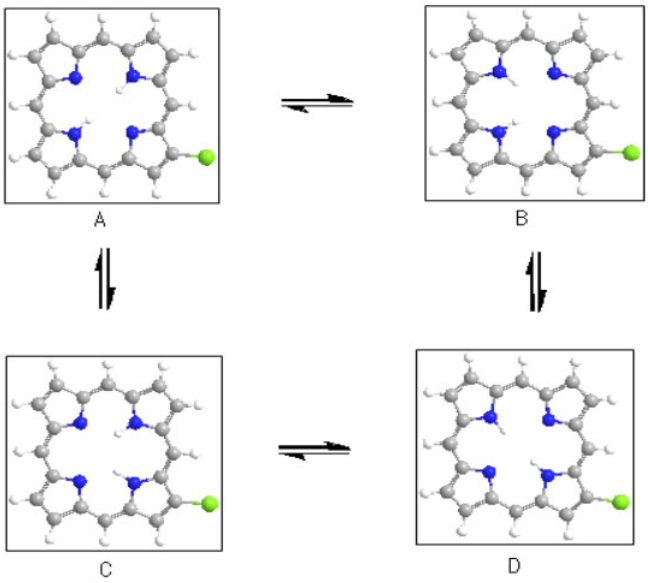
porphyrin 은 혈색소·시토크롬·엽록소 등의 색소성분을 구성하는 화합물로 생체내에서 산화·환원반응에 중요한 작용을 하는 물질이다.본 연구에서는 porphyrin 의 외각 수소원자 하나를 염소원자로 치환시켜 asymmetric 상태의 porphyrin 의 내부 양성자 이동을 알아보았다. 이중 양성자 이동의 메카니즘을 알아보기 위해 반응물과 생성물, 중간체, 전이상태의 구조를 최근에 개발된 계산 방법인 M06-2X/6-31+G** 방법을 이용하여 계산하였다.이중 양성자 이동의 메커니즘은 동시에 일어나지 않고 단계적으로 일어났으며, 여러가지 가능한 토토머 중 A 의 경우가 가장 안정하였으며, 가장 불안정한 토토머는 C 구조였다. A -> B , D -> C 로 가는 과정의 활성화 포텐셜 에너지는 각각 15.9kcal/mol 이였으며, B -> D 의 활성화 포텐셜 에너지는 7.5kcal/mol, C -> A 의 활성화 포텐셜 에너지는 6.1kcal/mol 로 나왔다.



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Photoinduced Disassembly of Gold Nanoparticle Aggregates

박정수, 윤상운

단국대 화학과

We control the assembly behavior of gold nanoparticles (AuNPs) using pulsed laser irradiation. AuNPs with a diameter of 16 nm are synthesized by the Turkevich method. Addition of p-aminothiophenol (p-ATP) to the AuNP solution induces the aggregation of AuNPs. Sixty shots of irradiation at 532 nm at 39 mJ/cm^2 disassemble the AuNP aggregates into well-dispersed individual AuNPs. Once the AuNPs are dispersed, they do not re-aggregate by desorbed p-ATP molecules, remaining stable. Further irradiation induces the fragmentation of the AuNPs. We present the mechanism of the photoinduced disassembly process. Dependence of the disassembly rate on irradiation wavelength and power is also discussed.

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Green-DCF의 열변색 현상에 관한 열역학적 연구

권태필, 김재욱, 지명진, 차병관, 김종규

단국대 화학과

Leuco 염료 중에 Green-DCF 의 열역학적 함수들을 계산하였다. 이전의 연구에서와 같이 염료의 열 변색 현상을 이용하여 평형상수, 엔탈피 엔트로피에 대하여 연구하였다. 본 연구에 사용된 기능성 염료는 양성자성용매와 비 양성자성 용매 모두에서 염료가 무색의 lactone 형으로 존재하나, 산을 첨가하였을 경우 두 가지 용매에서 무색의 lactone 형과 유색의 zwitter-ion 형의 평형 혼합물로 존재함을 확인하였다. 이러한 평형혼합물의 존재는 용매의 수소 결합 주게 능력에 크게 영향을 받는다. 따라서 평형 위치의 결정은 용매의 극성도가 아니라 용매의 양성자 성질임을 확인하였다. 용매에 산을 첨가하였을 경우 무색의 lactone 형과 유색의 cation 형이 평형 혼합물로 존재한다. 따라서 산성 용액 하에서는 평형위치가 유색의 cation 형으로 이동함을 확인하였다. 염료와 용매와의 상호작용을 이해하기 위하여 여러 용매 하에서 흡수 스펙트럼을 측정하였다. 용매의 수소 결합주게 능력이 클수록 최대 파장이 증가한다. 이것은 양성자 용매와 zwitter-ion 형의 COO-의 상호작용이 COO-와 xanthene 고리의 9 번째 탄소와의 결합력을 감소시킨다는 것을 알 수 있다. 염료의 열역학적 함수도 온도 변화에 따른 흡광도의 변화로부터 평형상수를 계산하여 엔탈피 변화량을 측정하였다.

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Leuco 계의 염료인 Blue220의 열 변색 현상에 관한 열역학적 연구

차병관, 김재욱, 권태필, 지명진, 김종규

단국대 화학과

최근 열 변색 기술은 섬유, 광학, 광센서 등의 여러 가지 분야에 응용되고 있으며 상당한 연구가 활발히 진행되고 있다. 또한 열 변색 기술은 앞으로 21 세기를 선도해 나갈 수 있는 과학기술로써 열 변색 현상을 이용한 감열염료에도 이용되어지고 있다. 지금까지 triphenylmethane 염료, Ca 염, Mg 염에 대한 연구는 상당히 진행되어 왔으며 현재는 Leuco 계의 염료에 대한 연구가 활발히 진행되고 있는 상황이다. 이에 따라 본 실험실에서 사용한 시약은 Blue220(7-(4-(diethylamino)-2-methylphenyl)-7-(1-ehtyl-2-methyl-1H-indol-3-yl)furo[3,4-b]pyridin-5(7H)-one)이라는 Leuco 계 시약이며, 이 시약의 열 변색 현상에 대해 UV-Vis, DSC, TGA 와 NMR 을 통한 구조분석, 물리화학적 특성과 열 분석 현상을 조사하고 열 변색 염료로써의 응용성을 타진하였다.

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Blue계열 염료의 열변색 현상에 관한 열역학적 연구

지명진, 김재욱, 김종규

단국대 화학과

다양한 색을 나타내는 기능성 염료인 blue402 (3-(4-(diethylamino)-2-methylphenyl)-3-(1,2-dimethyl-1H-indol-3-yl)isobenzofuran-1(3H)-one) 와 blue502(3-(4-(diethylamino)phenyl)-3-(1-ethyl-2-methyl-1H-indol-3-yl)isobenzofuran-1(3H)-one) 열변색 현상으로부터 열역학적 함수들을 계산하여 비교하였다. 평형상수, 엔탈피, 엔트로피에 대하여 연구하였다. Blue 402 와 Blue 502 의 분자량은 같으나 분자구조의 차이를 이용하여 평형상수, 엔탈피, 엔트로피에 대하여 연구하였다. 양성자성 용매에서는 Lactone 형으로 존재하나 비양성자성 용매에서는 Lactone 형과 Zwitter - ion 형이 같이 존재함을 확인하였다. 이러한 평형혼합물의 존재를 결정하는 요인은 용매의 극성도가 아니라 수소결합 주게의 성질에 큰 영향을 받음을 확인하였다. 용매에 의한 λmax 의 변화는 용매의 수소 결합 주게의 능력이 클수록 장파장으로 이동함을 알수 있었다. 이것은 양성자 용매와 zwitter - ion 형의 COO-의 상호작용이 COO-와 xanthene 고리의 9 번째 탄소와의 결합력을 감소시킨다는 것을 알 수 있었지만, 산성용액에서는 장파장의 경향성을 찾기 힘들었다. 염료의 열역학적 함수도 온도 변화에 따른 흡광도의 변화로부터 평형상수를 계산하여 엔탈피 변화량을 측정하였다.

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Polymorph-tuned Synthesis of α-and β- Bi_2O_3Nanowires and their Polarized Raman Single Nanowire Confocal Microscopy

인준호, 윤일선, *박정희, **주재범, ***이용훈, 김봉수

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We report the selective synthesis of single crystalline α- and β- bismuth oxide (Bi_2O_3) nanowires by using bismuth powder as a precursor in an oxidative atmosphere and their polarized Raman Single Nanowire confocal Microscopy. Factors such as vaporization temperature of bismuth powder, oxygen flow rate, reaction time, and temperature gradient have the influence on the synthesis of two different bismuth oxide nanowires. The growth process of α- and β- bismuth oxide nanowires can be explained by the conventional vapor-solid (VS) mechanism or self-catalyzed vapor-liguid-solid (VLS) mechanism mechanism with the different injection methods of oxygen flow. In the confocal Raman microscopy of bismuth oxide nanowires, we show the single crystalline nature and growth direction of a single nanowire. The thermal stability measurement of bismuth products by shows the phases of α- and β- Bi_2O_3 nanowires are maintained up to 750 ℃ and 300℃, respectively. The blue-shifted emission bands of α- and β-Bi_2O_3 nanowires were observed at 400 nm and 440 nm, respectively, owing to quantum confinement effect.

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Effects of Fe-Mo Catalyst Concentration and Dilution Time on the Growth of Three-Dimensional CNTs Network.

여해구, *이태재, 서정은, 이해원

*한양대 화학과 *한양대 나노과학기술연구소*

Three-dimensional (3D) network of CNTs is useful for applications in electronics, optics, sensors and other fields of materials science. The density and shape of 3D network of CNT are important factors to be utilized for application. In this study, we investigated the effects of concentration of Fe-Mo catalyst and dilution time in ethanol on the density and shape of 3D network of CNTs. CNTs were synthesized on Si pillar substrates by using low pressure thermal chemical vapor deposition (CVD). The Fe-Mo catalyst was deposited on a Si pillar substrate by a dipping method, and then the substrate was rinsed with ethanol. CNTs were grown by CVD by supplying C_2H_2 gas as a carbon source after NH_3 pretreatment at 800℃. The 3D CNTs network was characterized by using both SEM and Raman spectroscopy.

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Construction of a cold quadrupole ion trap at a cryogenic temperature and its application to ultraviolet photodepletion spectroscopy of dibenzo-18-Crown-6 ether complexes with alkali metal cations

최용훈, 김남준

충북대 화학과

We built a quadrupole ion trap that could be cooled down to a cryogenic temperature and employed it to ultraviolet (UV) photodepletion spectroscopy of dibenzo-18-crown-6 ether complexes with alkali metal cations (M+-DB18C6). The M+-DB18C6 ions were produced by electrospray ionization, stored in the quadrupole ion trap, and irradiated by UV laser pulses. The photodepletion spectra were then obtained by monitoring the depletion yields of ions as a function of UV wavelength. The cooling of the ions to a cryogenic temperature was manifested by narrower absorption peaks in the spectra compared to those observed at 150 K.

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Effective Removing and Recovering of Alkanethiolate Self-Assembled Monolayers on Au(111) : Scanning Tunneling Microscopy and X-Ray Photoelectron Spectroscopy Studies

이남석, 박태성, 강훈구, 노재근

한양대 화학과

Molecular-scale desorption processes of fully-covered alkanethiol self-assembled monolayers (SAMs) chemisorbed on Au(111) were monitored by scanning tunneling microscopy (STM) as a function of $NaBH_4$ solution concentration. $NaBH_4$ molecules can be used as an effective reducing agent for reductive desorption of alkanethiolates to free thiols. We found that alkanethiolates can be totally removed from the gold surfaces after the immersion of pre-covered SAMs in a 0.5 M $NaBH_4$ solution for 3 min. STM imaging reveals the phase transitions from the closely packed c(4 x 2) superlattice to the disordered phases via the formation of intermediate striped structure as a function of desorption time. X-ray photoelectron spectroscopy shows a bound peak with a very weak intensity, which implies the desorption of alkanethiolates on Au(111) surfaces. On the other hand, we also clearly demonstrated that the Au(111) substrates formed after removing thiolates can be reused for preparation of organic thiol SAMs.

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Au nanowire-Au nanoparticles conjugated system provides micrometer size molecular sensor

강태준, 윤일선, 김장배, 이효철, 김봉수

KAIST 화학과

We report a new type of molecular sensor using the Au nanowire (NW)-Au nanoparticles (NPs) conjugated system. The Au NW-NPs structure is fabricated by the self-assembly of biotinylated Au NPs on a biotynylated Au NW through the agency of the target avidin, creating hot spots between NW and NPs that strongly enhance the Raman signal. The number of the Au NPs attached to the NW is reproducibly proportional to the concentration of the avidin, and is also proportional to the measured surface-enhanced Raman scattering (SERS) signals. Since this well-defined NW-NPs conjugated sensor is only a few micrometer long, we expect that development of multiplex nanobiosensor of a few tens micrometer size would become feasible by combining individually modified multiple Au NWs together on one substrate.

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Directional growth of single-crystalline FeSi nanowires.

김시인, *서관용, *김봉수

*KAIST 나노과학기술대학원 *KAIST 화학과*

Directionally grown single-crystalline FeSi nanowires (NWs) have been successfully synthesized via halide vapor transport method with no metal catalyst. The FeSi NWs are grown on m-plane and r-plane sapphire substrates placed on mixture of silicon and graphite powders. By controlling the reaction temperature and weight ratio of silicon and graphite powders, we can realize the directionally grown FeSi NWs. Diameters of the as-grown FeSi NWs range from 250 to 300 nm and lengths are up to tens of micrometers. Synthesis of aligned silicide NWs on a substrate with a specific orientation is highly valuable for fabrication of three-dimensional (3D) integrated platform.

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Theoretical Study on the Aggregation Mechanism of Aβ(1-42) peptides Using Targeted Molecular Dynamics Simulation.

이제욱, 함시현

숙명여대 화학과

Aβ42 peptide, the main cause of Alzheimer disease (AD), converts under some conditions from their non-toxic soluble structures into highly ordered toxic fibrillar aggregates. Because such transitions can provoke pathological conditions ranging from neurodegenerative disorder to systematic amyloidoses, much effort has been invested in the development of various experimental and theoretical model systems to study the details of the aggregation processes and the effects of endogenous molecules that have been implicated in AD. In this study, all-atom TMD (targeted molecular dynamics) simulations in explicit water solvent were used to investigate the aggregation mechanism and dynamic properties of full-length aggregation-prone structures (APS) that found from our previous conventional MD simulations. We mainly focus on the conformational changes of APS structure, formation (or deformation) of some important electrostatic interactions, and variations of hydrophobic properties. This study will contribute to improve understanding of progress and control the amyloid diseases.

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Fabrication of Mn-doped Porous ZnO Nanostructures of Hexagonal Shape by Ultrasound Assisted Hydrolysis

Umapada Pal, 김창우, **Nitin Appa Jadhav**, 강영수

서강대 화학과

Mesoporous ZnO nanoparticles doped with Mn at different concentrations are fabricated by hydrolyzing zinc (II) acetate dihydrate in N,N-dimethylformamide - water (9:1) mixture under ultrasonication. The nanostructures are characterized by X-ray diffraction, transmission electron microscopy, nitrogen adsorption-desorption isotherms, and photoluminescence techniques. It has been observed that those hexagonal shaped nanostructures of about 200 nm average size are well crystalline, have uniform dopant distribution and of mesoporous in nature. The emission behavior of the porous nanostructures modifies drastically on Mn doping. These porous nanostructures should have high catalytic activities for the degradation of organic wastes and could be used in cosmetics.

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A Vibrational Transition Moment Angle Study of Several Cytosine Tautomers Using ab Initio and DFT Calculatons

민아름, 최명룡

경상대 화학과

Cytosine, one of the four main nucleic acid bases found in DNA and RNA, is classified as a keto, amino or imino tautomer. Among various tautomers of cytosine, the three lowest energy amino tautomers were chosen for the vibrational transition moment angle (VTMA) studies. We have conducted ab initio and DFT calculations to obtain the angles between permanent and transition dipole moments of several cytosine tautomers. The VTMAs of each tautomer are investigated as function of several dihedral angles associated with the amino (NH2) group. By brute forcing the dihedral angles of the amino group while fully relaxing the other atoms in the molecule, the structural information of the tautomers is well denoted in the corresponding VTMAs. In the near future, we intend to study the nonplanarity of cytosine by comparing the experimental VTMAs obtained from 0.37 K superfluid helium nanodroplets and those from this study.

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Infrared Laser Spectroscopy of Imidazole Dimer and Its Water Complexes in 0.4K superfulid Helium Nanodroplets : Vibrational Transition Moment Angle Study and Free OH stretching Mode Assignments

이승준, 최명룡

경상대 화학과

We present the mid infrared spectra of imidazole(IM) diner and its water complexes in 0.4K superfluid helium nanodroplets. Two different complexes of (IM)2–H2O have been identified in the free OH stretching spectral region of 3710–3755 cm−1. The assignment of the infrared vibrational bands of the clusters is aided by ab initio calculations. Vibrational transition moment angles (VTMAs) provide conclusive assignments for the complexes studied in this work.

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Activity of Au-Pt bimetallic catalysts for CO oxidation

김영독, 김광대, TAIWEISHENG, Luo Yuan

성균관대 화학과

Bimetallic catalysts are commonly used in a variety of catalytic reactions. In this study, CO oxidation activity of nanoparticles prepared by deposition of Pt and Au on Ta2O5/Ta substrates under high vacuum conditions was studied at 190 ℃. In addition, the surface structures and chemical properties of the catalysts were characterized by scanning electron microscope (SEM) and X-ray photoelectron spectroscopy (XPS). When only Au was deposited on the surface, no catalytic activity could be found. Catalytic activity of Pt nanoparticles (

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Interaction between oxygen and Pd films on Ta

김영독, TAIWEISHENG, 김광대, 서현욱

성균관대 화학과

Behaviors of samples with different Pd thicknesses in the reaction with oxygen were studied by in-situ X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM). Depending on the Pd thickness, various behaviors in reaction with oxygen were observed. In the case of the sample with a Pd thickness of 3.0 nm, a new low-binding-energy component appeared in the Pd 3d level upon O2 exposure at 250℃. After CO exposure at 200℃, decrease in the relative intensity of the low-binding-energy component was observed, indicating that the oxygen atoms formed at 250℃ on this Pd film can react with CO to CO2. For the sample with a Pd thickness of 5.0 nm, no change in the Pd 3d spectrum was observed after exposure to O2 at 250℃ while a positive shift of the Pd 3d level due to the oxidation of Pd was observed after exposure to O2 at a higher temperature (300 ℃). A subsequent CO exposure at 200℃ could not reduce Pd-oxide layers, as confirmed by the unchanged Pd 3d spectra after CO treatment, .i.e. Pd-oxide is not reactive for CO oxidation. In the case of P/Ta system, increase in the intensity ratio between oxidic and metallic Ta 4f states could be observed upon O2 treatment at 250℃ while no change in the Ta 4f state could be found for a bare Ta sample without Pd. It indicates that Ta can more easily be oxidized in the presence of Pd.

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One Step Preparation of TiO_2 Nanoparticles by Electron Beam Irradiation

박지현, *이병철

*과학기술연합대학원대 레이저및플라즈마응용공학 *한국원자력연구소 양자광학연구부*

TiO_2 nanoparticles were prepared from titanium tetra-isopropoxide (TTIP) by electron beam irradiation without using surfactant and dispersant at ambient pressure and room temperature. The shape, size and crystal structure of TiO_2 nanoparticles were controlled by concentration of TTIP and electron beam accelerator conditions such as, the electron beam energy, the current density and the absorbed dose. The phase, particle size and structure of prepared TiO_2 nanoparticles were characterized by transmission electron microscope (TEM) and x-ray diffraction (XRD) patterns and the chemical composition was investigated by energy dispersive spectrometer (EDS).

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An NMR Relaxation Study of Borohydrides in Solids

김철, *Jessie Ku, *Son-Jong Hwang, **Robert C. Bowman Jr., **Joseph W. Reiter, **Jason Zan

*한남대 화학과 *Division of Chemistry and Chemical Engineering, California Institute of Technology, USA **Jet Propulsion Laboratory, California Institute of Technology, USA*

The nuclear spin-lattice relaxation of ^{11}B and ^{1}H nuclei in the solid borohydrides was measured by using NMR spectrometers and analyzed with a new relaxation equation and the dynamical model for the reorientational motion of BH_4 unit. A more accurate relaxation equation was derived for the analysis of the nuclear spin-lattice relaxation of a quadrupolar ^{11}B nucleus in the BH_4 unit of solid $LiBH_4$ and $Ca(BH_4)_2$. The relaxation equation obtained with the two-spin approximation was found to be consistent with the previous results for quadrupolar nuclei. Two types of reorientational motion for the BH_4 unit in solid $Ca(BH_4)_2$ were found as $LiBH_4$ and their activation energies and correlation times were obtained. α-to-β phase transition of $Ca(BH_4)_2$ was also observed at around 260 ^{o}C under a high vacuum condition.

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Visible-Light-Driven Degradation of 1,4-Dioxane Using CdS, Cu_2S, and PbS Nanocrystals and Their TiO_2 and Carbon Nanotube Hybrid Nanocrystals

김윤희, 장동명, 명윤, 지경환, 박정희

고려대 소재화학과

The photocatalytic degradation of aqueous 1,4-dioxane under visible light irradiation was first achieved using free CdS, Cu_2S, and PbS nanocrystals (NCs), and their hybrid nanostructures with TiO_2 and carbon nanotubes (CNTs). The free Cu_2S NCs exhibited the higher degradation efficiency than the CdS and PbS NCs. Ethylene glycol diformate (EGDF) and H_2O_2 were detected as intermediates, which eventually decompose into CO_2 and H_2O. We suggest that the degradation of 1,4-dioxane would proceed via the formation of EGDF, through the oxidation reaction of OH radicals. The highest efficiency of the Cu_2S NCs is attributed to their excellent photocatalytic activity toward the redox reaction of H_2O_2. The hybridization with TiO_2 and CNTs enhanced the efficiency, most significantly for CdS NCs. The band gap and valence band/conduction band potentials indicates that the promotion of the interfacial electron-transfer processes takes places most efficiently in the CdS NC hybrid nanostructures.

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Two Gas-Phase Synthesis Routes of Single-Crystalline PbS Nanowires and Their Electrical Transport Properties

장소영

고려대 소재화학과

Single-crystalline PbS nanowires were synthesized using two different routes; chemical vapor transport and gas-phase cation exchange reaction of pre-grown CdS nanowires. They consisted of rock-salt structure PbS nanocrystals uniformly grown in the [100] or [110] direction, controlled by the growth condition. The chemical vapor transport produced the single-crystalline nanowires grown along the [100] direction. Single-crystalline wurtzite structured CdS nanobelts (growth direction = [011(_)0] or [011(_)1]) were converted into rock-salt PbS nanobelts by Pb vapor transport (at 500 C). We first observed the transmission electron microscopy snapshots for the construction of PbS domains by forming the heterojunction with the CdS domains. The conversion takes place through the highest surface energy {110} planes of PbS, producing uniformly [110] axial direction. We fabricated field effect transistors using single PbS nanowire, providing evidence for its intrinsic p-type semiconductor characteristics, for all three routes. The highest value of the carrier mobility was estimated to be 10 cm2V−1s−1 and their concentration was 2 1017 cm-3.

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Water-soluble PbS nanocrystals and their TiO_2, ZnO, carbon nanotubes, and nanodiamond hybrid nanostructures.

박기영, 조용재, 김창현, 김한성, 박정희

고려대 소재화학과

Photocatalysis has attractive potential applications in the conversion of solar energy into chemical energy (e.g., the production of H_2 by water splitting). Recent research demonstrated the improved photocatalytic activity of semiconductor-TiO_2 nanocrystal (NC) hybrid nanostructures toward the degradation of water and organic molecules. The electron transfer from the conduction band of the NC sensitizer to that of TiO_2 can lead to efficient and longer charge separation by minimizing the electron-hole recombination. However, the charge separation abilities of the NC sensitizers have not been compared with other nanocrystals such as ZnO or carbon nanotubes, although this information would provide valuable information on the mechanism of the photocatalytic redox reaction. The present work reports the size-controlled synthesis of water-soluble colloidal semiconductor PbS (Eg (bulk) = 0.4 eV) NCs and their TiO_2, ZnO, carbon nanotubes (CNT), and nanodiamond hybrid nanostructures, which were prepared by the in-situ solvothermal method. Their photocatalytic abilities of hybrid nanostructures toward the production of H_2 from water splitting were compared under visible light irradiation, providing the relative efficiency of charge transfer.

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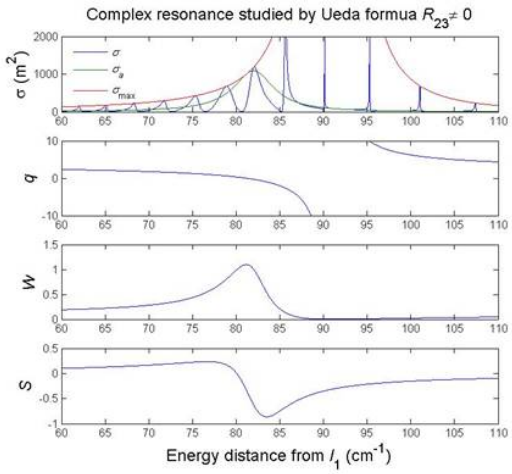
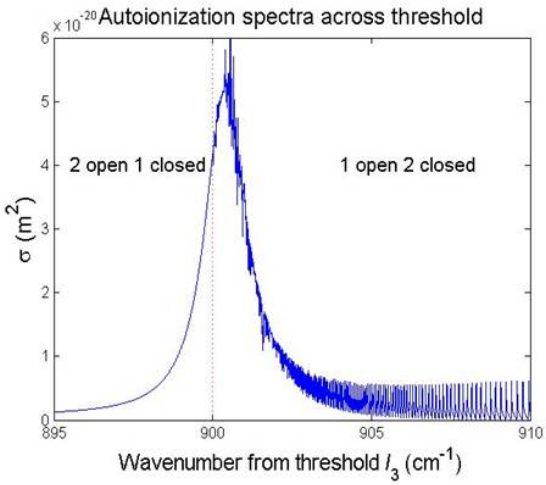
Studies of overlapping resonance phenomena for various 3 channel systems

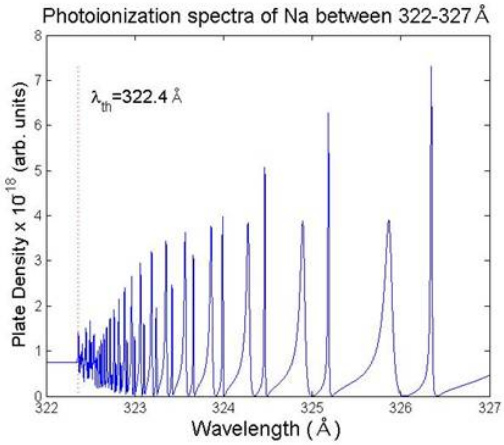
이천우, 조병훈

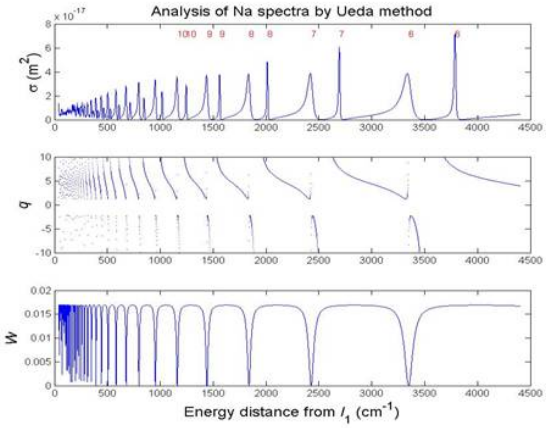
아주대 화학과

여러 형태의 삼채널 계에서의 중첩 공명현상에 대해 다채널 양자 결함 이론에 대한 연구와 이를 실제 계에 대해 적용한 결과를 발표할 것이다. giant resonance 혹은 complex resonance 라 불리는 현상은 Connerade, Lane 등의 R-matrix 기반 방법에 의해 연구되었고, multichannel quantum defect 이론 (MQDT)에 의해서는 2 개의 닫힌 채널과 1 개의 열린 채널계에 대해 Giusti-Suzor 와 Lefebvre-Brion 에 의해 연구되었으나, 후자들의 방법은 수치적 방법에 의존하여 관련 동력학 인자들에 의한 영향을 체계적으로 연구할 수 없었다. 이를 체계적으로 기술할 수 있는 방법이 Ueda 에 의해 오래전 유도되었으나, 이 식은 지금까지 거의 이용이 되지 않았다. 이를 interloper 가 있는 계에 적용하여 얻은 좀 더 체계적인 연구결과를 발표할 것이다. 한편 이들 interloper 가 threshold 에 걸쳐 있을 때는 Ueda 방법을 쓸 수 없고 이천우, 김지현에 의해 연구된 방법을 사용해야한다. 이 둘의 방법은 analytical continuation 에 의해 통합되어야 하는데 이를 통해 얻은 giant resonance 현상에 대해 발표할 것이다. Ueda 방법의 단점으로는 giant resonance 현상에서 isolated resonance 와 overlapping resonance 의 기여를 따로 구할 수 없다는 점이다. 이에 대한 일반 이론은 아직 연구가 되지 못했고, 이천우, 공자현에 의해 연구된 분석법을 두 닫힌 채널이 같은 이온화에너지 threshold 를 가지는 3 채널 단순계에 대해 완벽한 수식유도를 통해 얻은 분석결과를 발표할 것이다.









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A Vibrational Transition Moment Angle Study of 2-Aminopurine using ab Initio and DFT Calculations

김유식, 민아름, 최명룡

경상대 화학과

2-Aminopurine (2AP), an analog of adenine and guanine, can pair with thymine and cytosine as a base-pairing analogue. Therefore, it is of importance in investigating as a mimicking system for mutagenesis. We present ab initio and DFT calculations to obtain the angles between permanent and transition dipole moments of several iso-cytosine tautomers. Among various tautomers of iso-cytosine, the three lowest energy amino tautomers were chosen for the vibrational transition moment angle (VTMA) studies. The VTMAs of each tautomer are investigated as function of several dihedral angles associated with the amino (NH2) group. By brute forcing the dihedral angles of the amino group while fully relaxing the other atoms in the molecule, the structural information of the tautomers is well denoted in the corresponding VTMAs. In the near future, we intend to study the nonplnarity of 2AP by comparing the experimental VTMAs obtained from 0.37K superfluid helium nanodroplets and those from this study.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Theoretical study on the IR spectrum and strain energy of cyclodisiloxane

서현일, *민병진, 김승준

*한남대 화학과 *배재대 화학과*

The two-membered silicon rings (2MRs) is believed to be the most reactive site for the adsorption because of its large strain energy due to having severely deformed angle (about 90) of Si-O-Si, while the idealized silica surface, which has the Si-O-Si angles about 109.5° or 143, 152 and almost no strain, is rather inert to most reagent. Ring opening by chemical reactions with adsorbing molecules, triggered by the large strain energy, is currently being pursued in our groups.Silica surface, in the absence of water, are characterized by three specific infrared (IR) bands: two strong peaks at 888 and 908 cm^{-1}, (and a weaker shoulder at 932 cm^{-1}). The theoretical results for the vibrational frequencies of the parent 1,3-cyclodisiloxane were reported by Kudo and Nagase, Bunker et al., Choi et al.. The calculated IR spectrum of the b-cristobalite slab by the *ab initio* simulation shows the IR doublet (at 791 and 841 cm^{-1}) due to vibrational modes of the 2M ring, strongly supporting the experimental assignment of the IR doublet at 888 and 902.The Si-O bond distances in $(H_2SiO)_n$ decrease in the order 1.717 Å(n=2) > 1.667 Å(n=3) > 1.646 Å (n=4). This may suggest that the strength of the Si-O single bond increase with the increase in 'n'. The locally strained bonds have reduced bond energy, and the ring strain in these structures greatly increases the reactivity of their siloxane bonds, especially in the dimer rings.In this study, the molecular structures and strain energy for the parent 1,3-cyclodisiloxane (R=H), which has not been yet observed experimentally, are investigated using density functional theory and high level *ab initio* quantum mechanical techniques with large basis sets. The highest level of theory employed is cc-pVQZ CCSD(T). The harmonic vibrational frequencies and IR intensities are also determined at the B3LYP and CCSD(T) levels of theory with various basis sets, and compared with each other.

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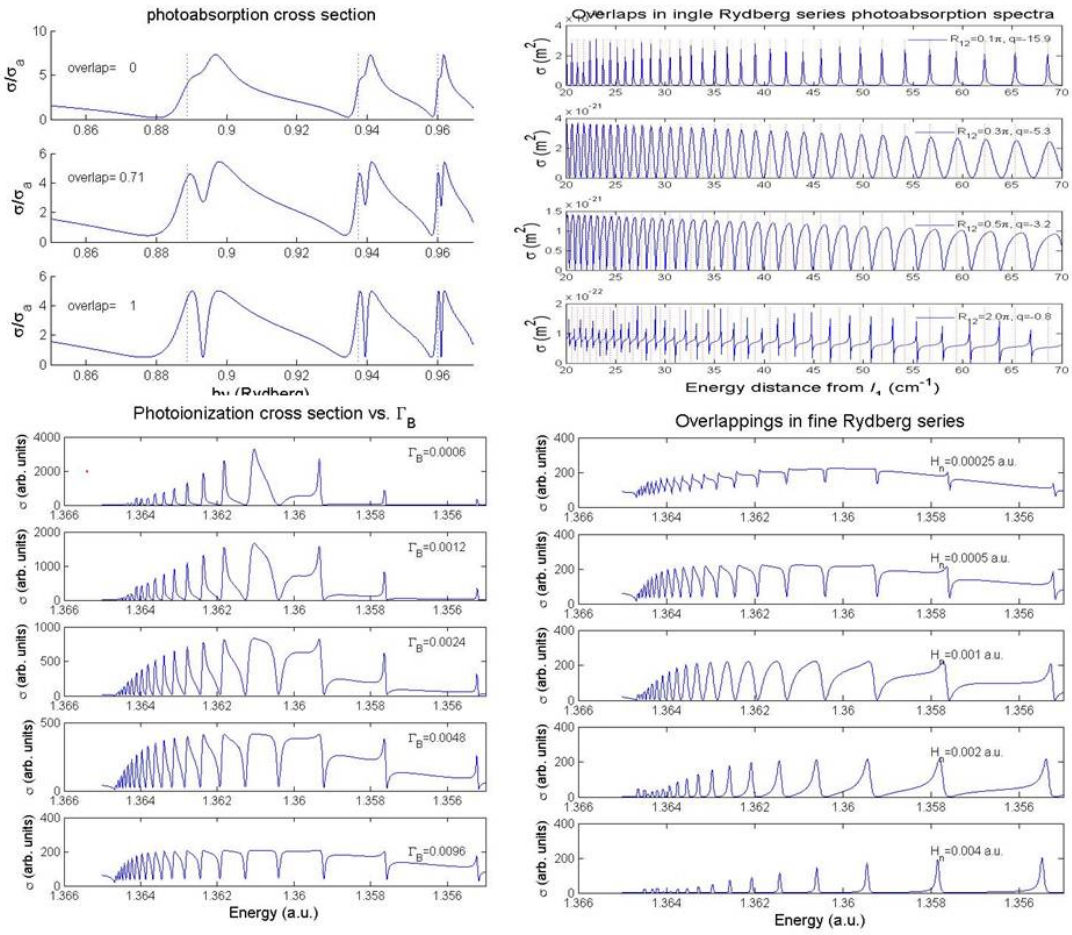
Comparative studies of overlapping resonances of Mies' configuration interaction theory and multichannel quantum defect theory

이천우, 강희원

아주대 화학과

We will present the multichannel quantum defect version of Mies' theory on overlapping resonances. Mies discussed the role of continua in overlapping resonances using the concept of overlap matrix. Although his theory is considered as conclusive work for overlapping resonances, its multichannel quantum defect version has not been exist. Our work fills this gap.



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Catalytic and Photocatalytic Activity of Various Platinum Hybrid Nanocrystals

장동명, 지경환, 김윤희, 명윤, 조용재, 박정희

고려대 소재화학과

We synthesized the Pt hybrid nanostructures with TiO2 (Pt-TiO_2), carbon nanotubes (Pt-CNT), nanodiamonds (Pt-ND), and graphenes (Pt-GR), and compared their catalytic and photocatalytic ability toward the degradation of methylene blue (MB) dye. Under no light irradiation, the Pt-CNT and Pt-GR hybrid nanostuctures exhibit the higher catalytic activity, probably due to the larger adsorption activity. The visible light irradiation enhances dramatically their catalytic ability by more than factor of 2, following the order Pt-ND > -TiO_2 > -GR > -CNT. The hybridization enhances the reductive degradation rate, by the interfacial electron transfer process from the Pt NCs to the attached nanostructures, which retards the recombination of the electrons and holes. The much enhanced photocatalytic ability of Pt-NDs was explained by the oxidative N-demethylation degradation involving the transfer of holes from the NDs to MB, in addition to the reductive pathways.

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Terahertz Emission from Single-Crystalline GaAs and Mn-doped GaAs Nanowires

공강준, 정경복, 조용재, 명윤, 김한성, 박정희

고려대 소재화학과

We observed the terahertz (THz) emission from single-crystalline GaAs and Mn-doped GaAs nanowires (NWs) excited by a 100 fs pulse of 810 nm radiation from a Ti:Sapphire laser system, and compared it with that of a semi-insulating (SI) GaAs film. The frequency spectrum (0-4 THz) of the THz emission from the GaAs NWs and Mn-doped GaAs NWs is red shifted by 0.4 and 0.5 THz, respectively. This red shift is though to originate from the anisotropic nanowire geometry, which causes a decrease of the longitudinal plasmon oscillation frequency. The GaAs NWs consistently show a red shift of the Raman longitudinal optical mode, due to their shape effect. The Mn-doping enhances significantly the intensity of the THz emission, which is correlated with the increase of electron density accompanying the band gap decrease.

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MR relaxivity study of Gd doped Iron oxide nanoparticle

박자영, 최은숙, *백명주, 이강호

*경북대 화학과 *경북대 나노과학기술학과*

We prepared Gd doped Iron oxide nanoparticle for MR contrast agents. So we changed Gd content from 1 to 10%. We characterized them by using HRTEM, XRD, Squid magnetometer, FTIR, and MRI instrument. Increasing Gd content, they had a low r_2/r_1 relaxivity ratio and showed clear dose-dependent T_1 and T_2 map images, indicating that they will be useful as both target-specific T_1 and T_2 MR contrast agents.

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Water soluble GdO@MnO core-shell nanoparticles for T1 MR imaging

최은숙, 박자영, *백명주, 이강호

*경북대 화학과 *경북대 나노과학기술학과*

We synthesized paramagnetic GdO@MnO core-shell nanoparticles for MR contrast agents. We characterized the biocompatible ligands surface modified GdO@MnO core-shell nanoparticles by using XRD, HRTEM, FT-IR, and TGA for studying particle size, crystal structure, coating ligands, and weight percent of pure nanoparticles . We tested the ligands surface modified GdO@MnO core-shell nanoparticles for T1 MR contrast agents by measuring relaxivities and map images by using MRI instrument. We observed high contrast MR images of a rat with tumor.

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Radical-radical reaction dynamics : The OH formation in the reaction of $O(^3P)$ with ethyl radical, C_2H_5

박용팔, 강규원, *정세희, 최종호

*고려대 화학과 *고려대 나노환경과학/화학과*

The radical-radical reaction dynamics of ground-state atomic oxygen[$O(^3P)$] with ethyl radicals(C_2H_5) in the gas phase were investigated using high-resolution laser spectroscopy in a crossed-beam configuration, together with ab initio calculations. The radical reactants, $O(^3P)$ and C_2H_5, were produced by the photodissociation of NO_2 and the supersonic flash pyrolysis of the precursor, azoethane which was synthesized by the Renaud's method, respectively. The nascent internal state distributions of the product OH were probed by the UV laser induced fluorescence spectroscopy. With the aid of the CBS-QB3 level of ab initio theory, it has been found that the barrierless addition of $O(^3P)$ to C_2H_5 forms the energy-rich addition complexes on the lowest doublet potential energy surface, which are predicted to undergo a subsequent isomerization and decomposition steps to generate various exothermic reaction products.

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T1 MR 이미징을 위한 산화가돌리늄 나노입자 합성 및 특성 분석

백명주, *박자영, *최은숙, *이강호

*경북대 나노과학기술학과 *경북대 화학과*

T1 MR 이미징을 위해서 GdCl3 · xH2O 을 전구체로 사용하여 산화가돌리늄 나노입자를 합성하였다. GdCl3 · xH2O, NaOH, 및 각각의 리간드를 1:3:1 의 비율로 N2 flow 하에서 반응을 시켰다. 표면을 코팅한 리간드의 종류를 PEG, D-glucuronic acid, Lactobionic acid 등으로 달리하여 나노입자를 합성했으며, 이 리간드들로 코팅된 산화가돌리늄 나노입자의 특성을 HR-TEM, XRD, FT-IR, TGA 등을 이용하여 분석해보았다.

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A Theoretical Study of the Radical-radical Reactionsof $O(^3P)$ with CH_3 and C_2H_5

정세희, 박용팔, 강규원, 최종호

고려대 화학과

Herein, we present ab initio calculations of the prototypal radical-radical reactions of ground–state atomic oxygen [$O(^3P)$] with methyl (CH_3) and ethyl (C_2H_5) radicals. The reaction mechanisms and dynamics were investigated using the density functional method and complete basis set model. In both radical reactions, two distinctive pathways were predicted to be in competition: addition and abstraction. The barrierless addition of $O(^3P)$ to the hydrocarbon radicals led to the formation of energy-rich intermediates that underwent subsequent isomerization and decomposition to yield various products. The products predicted to be found were H_2CO + H, $^{1,3}HCOH$ + H, and $^{1,3}CH_2$ + OH for $O(^3P)$ + CH_3 and H_2CO + CH_3, CH_3CHO + H, c-CH_2OCH_2 + H, $^{1,3}CH_3COH$ + H, $^{1,3}HCOH$ + CH_3, CH_2CHOH + H, C_2H_3 + H_2O and CH_2CH_2 + OH for $O(^3P)$ + C_2H_5. The minor H-atom abstraction mechanisms producing CH_2 + OH and CH_2CH_2 + OH were calculated to compete with the addition processes in both cases. With the aid of microscopic statistical calculations, the major pathways were predicted to be the formation of H_2CO + H for $O(^3P)$ + CH_3 and that of H_2CO + CH_3 and CH_3CHO + H for $O(^3P)$ + C_2H_5. through the low-barrier, single-step cleavages of the addition intermediates. The characteristics of the major reaction channels were compared with the experimental results reported in the gas-phase kinetics and crossed-beam investigations.

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Light scattering of Ag SNOF(single nanowire on a film)

안지희, 윤일선, 김봉수

KAIST 화학과

Light scattering of Ag SNOF (single nanowire on a film) was studied by using the side-illumination of white light and He-Ne laser light. Ag SNOF was prepared by manipulating Ag nanowires on the Ag thin film. Ag nanowires were synthesized by the chemical vapor transport method. The diameters of Ag nanowires are 100-200 nm and the lengths of the nanowires are 5-10 μm. The Ag film was prepared by the E-beam evaporation on the Si substrate. The thickness of Ag is 300 nm and the surface roughness is about 3 nm. White light and He-Ne laser light were side-illuminated and scattered light SNOF was observed by using the microscope objective (x100). The polarization of the incident light was adjusted by using a linear polarizer. We show that the direction and polarization of the incident lights strongly influence light scattering of SNOF.

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Ionization potential gas sensor using indium oxide(In2O3) coated SWNT

한봉우, 이휘건

한양대 화학과

Gas sensor using ionization breakdown voltage show good sensitivity and selectivity. Each gas has different ionization potential that means breakdown voltage data can be a fingerprint region for gas sensing. Here we report new fabrication methode to lower breakdown voltage. Indium oxide is selectively synthesized to SWNT and bring great field emission enhancement. Thus, indium oxide coaed SWNT is expected to lower ionization potential breakdown voltage efficiently that can be easily applied to gas sensor.

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Simple synthesis and electric properties of TCNQ- and TTF-encapsulated single walled carbon nanotubes

박태희, 이정우, 이휘건

한양대 화학과

Single-Walled Carbon nanotubes(SWNTs) have been found to be have a p-type transfer characteristics in atmosphere. Reaction of single-salled sarbon nanotubes (SWNTs) with molecules having large electron affinity and small ionization energy achieved p-type(TCNQ : Tetracyanoquinodimethane) and n-type(TTF : Tetrathiafulvalene) doping, respectively. Encapsulation of those molecules was carried out inside carbon nanotube under vacuum environment. The simplicity of the synthetic process offers a viable route for the large-scale production of SWNTs with controlled doping states, because of using mat-type SWNT. After encapsulation, TTF- and TCNQ-encapsulated SWNT deposited between electrodes of a bottom gate field effect transistor (FET) fabricated on Si- wafer substrate and investigate their electronic transport properties. FET character depend on changing gate voltages and Near IR were measured to elucidate charge transfer between those molecules and SWNTs.

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The characteristics of pure and N-doped ZnO nanorods on various substrates

박은경, 이정우, 이휘건

한양대 화학과

High-technology applications related on zinc oxide (ZnO) nanomaterials, for instances, photonic crystals, photodetectors, electron emission sources, gas sensors, and solar cells, are attractive research theme in recent. ZnO nanorods with a band gap 3.37eV are promising semiconducting materials. High-quality field emitters are very desirable for applications in a wide range of field-emission-based devices such as flat-panel-displays, X-ray sources, etc.ZnO nanorods were synthesized by the hydrothermal process. ZnO seed layer was deposited on various substrates such as glass, ITO, p-type porous silicon and n-type porous silicon by dipping in ZnO solution and atomic layer deposition (ALD) method. And then, plastic bottles were filled with an mixture of equimolar (0.02M) aqueous solution of zinc nitrate hexahydrate and hexamethylenetetramine (HMT). Consequently, the PL peak of N-doped ZnO nanorods was red-shfted compared to pure ZnO nanorods.

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Enhanced charge transfer and reduced recombination in CdSe/Single-walled carbon nanotubes complexes

안주원

한양대 화학과

Cadmium selenide is an important Ⅱ-Ⅵ group semiconductor and has a band gap of 1.74 eV. It is an n-type semiconductor and being developed for use in laser diodes, nanosensing and high-efficiency solar cells. First, CdSe nanoparticles were synthesized and directly functionalized with amine. And it has been investigated that sidewall functionalisation of purified single-wall carbon nanotubes (SWNT) terminated with carboxylic to acid-chloride. Then, directly attachment of CdSe nanoparticles to SWNTs has been performed. The reaction products were characterized by Scanning Electron Microscope, IR and PL.

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CO_2 제거용 알칸올아민 흡수제의 친핵반응성 및 접근성

전영호

숭실대 화학과

화력발전소 배가스(flue gas) 중의 CO_2 를 제거하는 알칸올아민계 화합물 중, MEA, MAE, 2A1P, 및 AMP 를 선정하여 이들의 친핵반응성과 접근성을 고찰하였다. MP2/aug-cc-pVDZ//B3LYP/6-311++G(d,p)수준의 양자역학 계산과 분자동력학적 계산에 의하면, 친핵반응성은 MAE > AMP > MEA > 2A1P 순서였고 이 경향은 pKa 실험값과 잘 일치하였다. 반응물의 CO_2 접근성은 MEA > 2A1P > AMP > MAE 이었다. 이상의 결과를 토대로 효율적인 CO_2 제거능을 갖는 알칸올아민 흡수제의 요건을 토의하고자 한다

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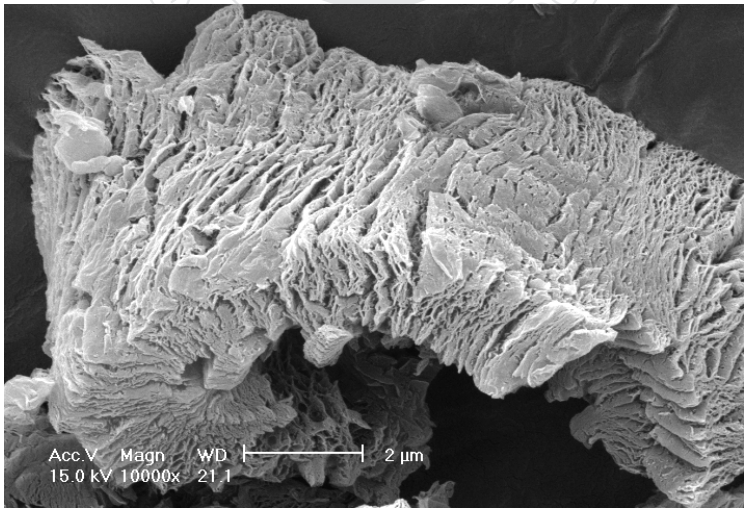
The synthesis of Ag nanoparticles intercalated in graphen with improved the catalytic activity

박경원, *김성규, 정종화

*경상대 화학과 *진주교육대 과학교육학과*

Graphene intercalated with Ag nanoparticles was synthesized in a one-step method. The stable Ag-nanoparticle-intercalated graphene (Ag-NPIGR) composites were fabricated by adding sodium borohydride and an aqueous solution of AgNO3 to the graphene matrix. The prepared graphene were successfully used as a powder phase catalyst for the reduction of 4-nitrophenol (4-NPO) with sodium borohydride.



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Comparative Photocatalytic Ability of Nanocrystal-Carbon Nanotube and -TiO_2 Nanocrystal Hybrid Nanostructures

지경환, 박정희, 장동명, 조용재, 명윤, 김한성, 김윤희

고려대 소재화학과

We synthesized various nanocrystal (e.g., CdS, CdSe, and Cu_2S)-carbon nanotube (NC-CNT) and NC-TiO_2 hybrid nanostructures using the solvothermal method and compared their photocatalytic ability toward the visible-light-driven degradation of methylene blue (MB) dye. The free CdS NCs exhibited higher degradation efficiency than the CdSe and Cu_2S NCs. The photocatalytic abilities of the NCs were found to determine the relative degradation efficiency of their CNT and TiO_2 hybrid nanostructures. These results suggest that the oxidative N-demethylation degradation involves the transfer of holes from the NCs to MB. The hybridization of the NCs with the TiO_2 NCs and CNTs enhances the oxidative degradation rate to the same extent, suggesting that the interfacial electron transfer process from the NCs to the attached CNTs (or TiO_2), which retards the recombination of the electrons and holes, is comparable for both hybrid nanostructures.

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Synthesis of InAs and InGaAs nanowires using vapor transport method, and twinned structure using electron tomography

정찬수, 김한성, 명윤, 김창현, 박정희

고려대 소재화학과

Nanowires of zinc blende crystal structure, grown in the [111] direction, which is the favoured direction of growth, usually have a large number of twin-plane defects. Such defects limit the performance of optoelectronic nanowire-based devices. To investigate this defect formation, we examine InAs and InGaAs nanowires grown by vapor transport method. We show that the nanowire segments between the twin planes are of octahedral shape and are terminated by {111} facets, resulting in a microfaceting of the nanowires. This investigation contributes to the understanding of defect formation in nanowires. We employed electron tomography and high-resolution transmission electron microscopy were used to characterize the unique 3-dimensional structures. One future prospect of such knowledge is to determine strategies on how to control the crystallinity of nanowires.

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Photoinduced Dissociation Spectroscopy of Protonated Naphthalene and Water Cluster in the Gas Phase

김민호, *김상수, *강혁

*아주대 에너지시스템학부 *아주대 화학과*

Protonated polycyclic aromatic hydrocarbons constitute an important class of closed-shell molecules because they occur as short-lived intermediates in a broad range of environments, ranging from astrochemistry, jet engine gas exhaust, and organic chemistry to biochemistry. It is interesting that protonated naphthalene absorbs visible radiation around 500 nm while naphthalene has absorption in the UV. In this study, we obtained the absorption spectra of protonated naphthalene-water clusters using photoinduced dissociation spectroscopy and calculated their geometries using Gaussian03. The 1:1 cluster of protonated naphthalend-water showed similar visible absorption as in the protonated naphthalene monomer, while 1:2 cluster had no visible absorption but only absorbed in the UV. The result of ab initio calculation showed that the 1:1 cluster has the form of protonated naphthalene solvated by one water molecule. On the other hand, the proton in the 1:2 cluster resides on the water moiety, which results in the UV absorption similar to that of neutral naphthalene.

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Vibrations and structures of *m*-aminophenol·NH_3 H-bonded cluster studied by IR-UV double resonance spectroscopy in supersonic jet

김상수, *김민호, 강혁

*아주대 화학과 *아주대 에너지시스템학부*

We have investigated OH and NH stretching vibrations of *m*-aminophenol (*m*-AP) clustered with one ammonia (*m*-AP·NH_3) in the electronic ground state by IR-UV double resonance spectroscopy in supersonic jet. Meta-substituted phenol has two rotational isomers according to the orientation of OH group. Our previous REMPI spectroscopy has shown that only the trans-form of the cluster exists but not the cis-form. For further investigation of *m*-AP·NH_3, we observed the IR spectrum of this cluster by fixing the UV laser at 34 411 cm^{-1}, wavelength of its 0-0 transition, and scanning the IR from 2.84 to 3.07 μm (from 3257 to 3521 cm^{-1}). The vibronic structure of this cluster was assigned based on ab initio calculation on the ground state at MP2 level with 6-311++G** basis set. The calculated frequencies of OH and NH stretching vibrations of *m*-AP·NH_3 agree very well with those of the IR-UV double resonance spectrum. The broad red-shifted OH frequency confirms that the geometry of the cluster is the one in which the ammonia is hydrogen-bonded to the OH group of the *m*-AP.

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Study on the hybrid plasma-polymer thin films of different ratio between toluene and TEOS

조상진, 부진효

성균관대 화학과

Organic-inorganic hybrid co-polymer thin films were deposited on silicon(100) substrates under the sevral ratio of TEOS (tetraethoxysilane) against toluene by plasma enhanced chemical vapour deposition (PECVD) method. Toluene and TEOS were also utilized as organic and inorganic precursors each, and hydrogen and argon were used as a bubbler and carrier gases, respectively. In order to compare the difference of the electrical and the mechanical properties of the plasma polymerized thin films, we grew the hybrid co-polymer thin films under the conditions of various ratio between toluene and TEOS with fixed RF (radio frequency using 13.56 MHz) powers at 30 W. The as-grown polymerized thin films were in first analyzed by FT-IR and XPS. The result of FT-IR showed that the co-polymer thin films were totally polymerized with fragment each precursor. Also, X-ray photoelectron spectroscopy (XPS) results showed the chemical species and binding energies of each species. Si 2p core-level spectra from the hybrid polymer thin film showed the status of Si oxidation number. Impedance analyzer was utilized for the measurements of I-V curves and capacitance values. Also, the thin films were analyzed for hardness and Young's modulus by nano-indenter.

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The effect of the shape and distance Si pillar structure on the three-dimensional carbon nanotubes network

서정은, 주해나, *이태재, 이해원

*한양대 화학과 *한양대 나노과학기술연구소*

The single walled carbon nanotubes(SWNTs) are expected to provide a great advantage in their various applications such as electronic devices, biosensors, energy storage, and solar cells. For application using unique properties of SWNTs, various methods of synthesis of SWNTs were developed only two-dimensional substrates. We demonstrate a growth of three-dimensional(3D) SWNTs network on suspended between silicon pillars with different shape and distance. The growth direction and shape of SWNTs were decided by Si pillar structures. As-grown 3D networks SWNTs were characterized using SEM, Raman, and HR-TEM analysis.

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Physical properties of zinc oxide thin films for photovoltaic divices

김명화, 부진효

성균관대 화학과

Zinc oxide (ZnO) films have been investigated in recent years as transparent conducting oxide layers, because of their good electrical and optical properties in combination with large band gap, abundance in nature, and absence of toxicity. Zinc oxide thin films were prepared at deposition thickness in the range of 50 nm to 150 nm by RF magnetron sputtering on glass substrates with pure zinc oxide target. The crystallinity nanostructure and surface morphology of zinc oxide thin films were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM). As the thickness of the films increased, the grain size and surface roughness increased. Also, we studied the optical-electrical properties of the zinc oxide thin films such as carrier concentration, mobility, and resistivity by hall measurement. As changed by thickness of zinc oxide thin films, concentration become increasing. But mobility and resistivity become decreasing.

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Theoretical study on the Cu complexes

chenjunxian, 이해황, 김찬경

인하대 화학과

Theoretical computation has been performed to study the stable structures of various Cu(I) and Cu(II) complexes with hetero-aromatic compounds. All the structures were optimized using Gaussian 03 or DMol 3 packages. Two possible conformers were identified depending on the types of the ligands – penta- and hexa-coordinated. These compounds might be involved in the oxidation reduction reactions occurring in the active site of the fuel cell.

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Synthesis and Application of Porous Silica Nanospheres Encapsulating a Hollow Gold Nanoparticle

김인현, 조영관, *박민호, 신권수, **김관

*숭실대 화학과 *숭실대 자연대 / 화학과 **서울대 화학부*

Porous spherical silica nanoparticles are a class of nanomaterials with potential applications in catalysis, separation, and drug delivery. In this study, we report the synthesis of porous silica nanospheres encapsulating a hollow gold nanoparticle (Porous-SiO2@Hollow-Au) through a two-step procedure. First, hollow Au nanoparticles were synthesized by sacrificial galvanic replacement of cobalt nanoparticles. It was possible to tune the peak of surface plasmon band absorption by controlling particle size and wall thickness. And then surface-protected etching strategy was used for constructing core-shell systems where a hollow Au nanoparticle was embedded in porous silica shell for enhanced stability against aggregation. We will also demonstrate that Porous-SiO2@Hollow-Au nanospheres can be applied not only as catalysts for the reduction of 4-nitrophenol to 4-aminophenol by NaBH4 but also as stable surface-enhanced Raman scattering substrates.

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Plasmonic Coupling between Gold Nanoparticles and a Gold Surface

김동길, 김진욱, 김지환

고려대 화학과

We experimentally studied the coupling between the surface plasmons (SPs) of Au nanoparticles and a thin Au film. The strength of coupling is determined by the degree of red-shift of scattering resonance with respect to the resonance of isolated nanoparticles. We examined the influences of particle size, particle-plane separation, change in dielectric constant, and the thickness of plane on the plasmonic coupling strength. The numerical electrodynamic simulation results agree with the experimental trends, which supports our interpretation of the plasmonic coupling mechanism.

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Prediction of the Melting Points of Organic and High Energetic Compounds

Li Jun, 김창곤, 이해황, 김찬경

인하대 화학과

The melting point of a solid organic compound is one of basic and important properties, and many studies have been performed so far. One of the well-known methods is to calculate the melting point from the enthalpy and entropy changes at the melting point of a compound. Another interesting method is using the topology model based on the molecular connectivity. In this work, QSPR method based on various descriptors including three-dimensional descriptors will be developed for organic molecules. We will examine if this method also can be applied to high energetic materials.

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3D-Suspended single wall carbon nanotube with storngly improved response time for IR detector

이동환

한양대 화학과

The properties of a Single wall carbon nanotube (SWCNT) wire about photonics and electorics have been known for infra red (IR) detector for last two decades. many researchers made an effort to use CNT for the detector. Thus, some of them have achieved the result about the detector. However, it has not been applied to the detector completely despite of its great intrinsic characters. Because of Its too much slow response time that has been the most difficult problem for application for the IR detector. Many studies has tried to reach fast response time so they found the way to improve the time. Suspended SWCNTs film or wire was the most prospective solution. Unfortunately, this way, which suspended the CNTs as two-dimensional, has just grown current intensities. Those experiment included fatal shortage that 2d suspended CNTs could not utterly separately each tubes. A lot of tubes of entire tubes in those experiments might be able to contact to themselves that probably brought about inter-tube interaction causing thermal effect. Now I suggest a brilliant method to improve response time that is 3-dimensional suspended SWCNT wire. I could obtain what i want exactly. This is an easy and convenient way.

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Effects of Amide-to-Ester Backbone Mutation on the Structural Properties in the Model Polypeptides

조예진, 함시현

숙명여대 화학과

Amide-to-ester backbone mutation is an excellent method to investigate the backbone-backbone hydrogen bond ability of hydrogen bond between protein backbones. In this study, peptide backbone mutation effects of model polypeptides, from monomer to pentane, were investigated by using density functional theory. All calculations were performed with B3LYP/6-31+G* level of theory. Upon amide-to-ester mutation in model polypeptides, changes in the structural properties will be discussed in view of the changes in the backbone hydrogen-bond ability. Also, the effects of vibrational properties with respect to the position of backbone amide-to-ester substitution will be discussed.

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Structural and dynamic properties of the modified OSS2 water

이송희

경성대 화학과

Classical molecular dynamics (MD) simulations using the modified OSS2 model potential derived from ab initio calculations can be used to understand the structural and dynamic properties of the model water at several different states. We found that reducing the total potential energy of the original OSS2 water model as well as decreasing the density or increasing the temperature of the system invokes the vivid mobility of the OSS2 water molecules. By choosing the proper scaling factor λ of the total potential energy from the obtained MD results for the self-diffusion coefficients of the modified OSS2 water, the radial distribution functions of O-O, O-H, and H-H, and the self-diffusion coefficients are compared with the SPC/E water and the experimental results.

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Computational Study on the Mechanism of Thermal Decomposition of Diazetine N,N'-Dioxide

Wu Yong, *이해황, *김찬경

*인하대 유기-나노하이브리드분자설계연구사 *인하대 화학과*

The NO release mechanism from diazetine N,N'-dioxide was studied using the MP2 method. We considered three possible pathways: Path 1 was a concerted mechanism; Path 2 was a stepwise mechanism involving a dinitroso intermediate; Path 3 was a stepwise mechanism to release two NO molecules one by one. The mechanism strongly depended on the type of solvent. Path 1 was favorable in CH_2Cl_2, while Path 2 was favorable in DMSO. The origin of mechanism was further analyzed by NBO and AIM.

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Real-Space Mapping of the Strongly Coupled Plasmons of Nanoparticle Dimers

김덕수, 안성현, *한상우, **윤완수, 김지환

*고려대 화학과 *KAIST 화학과 **한국표준과학연구원 나노소자연구단*

We carried out the near-field optical imaging of isolated and dimerized gold nanocubes to directly investigate the strong coupling between two adjacent nanoparticles. The high-resolution (～10 nm) local field maps (intensities and phases) of self-assembled nanocube dimers reveal antisymmetric plasmon modes that are starkly different from a simple superposition of two monomeric dipole plasmons, which is fully reproduced by the electrodynamics simulations. The result decisively proves that, for the closely spaced pair of nanoparticles (interparticle distance/particle size ～0.04), the strong Coulombic attraction between the charges at the interparticle gap dominates over the intraparticle charge cillations, resulting in a hybridized dimer plasmon mode that is qualitatively different from those expected from a simple dipole-dipole coupling model.

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Structure and Dynamics of Subtilisin Carlsberg in Nonaqueous Media

어유진, 함시현

숙명여대 화학과

Enzyme structure and flexibility are important determinants of catalytic activity. Therefore, Subtilisin Carlsberg which has 65 crystallographic waters was investigated by using molecular dynamics simulations to understand its structure and dynamics which are changed by solvent polarity. The simulations of Subtilisin Carlsberg were carried out in organic solvent (chloroform, methanol) and in pure water. Trajectories from the simulations are analyzed with a focus on enzyme structure, flexibility, and hydration of active site. In this study, we will discuss about overall structures of enzyme in aqueous and organic media. Also, it will be discussed that the hydration of active site and behavior of crystallographic water molecules bound with active site because those are important components of enzyme activity.

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Investigations for Selectivity of Chlorinated Thiophene Derivatives

최호준, *아루마렌, *정광주, *윤용진, **구인선, **김봉곤, **박종근

*경상대 화학교육전공 *경상대 화학과 **경상대 화학교육과*

The geometrical structures, relative energies, and atomic charges (NBO) of thiophene derivatives substituted with 1-6 chlorine cations were fully optimized at the MP2/6-311+G** level. The regioselective chlorination reaction on thiophene derivatives is mainly depended by the relative stability. The relative stability of the transition π-complexes is related to the atomic charges of the carbon atom on the thiophene ring and the π-conjugation of p-orbital on the ring. The transition π-complexes are classified as three groups such as 3,3'-substituted, 4,4'-substituted, and 5,5'-substituted π-complexes. The atomic charges of 5,5'-positions are largest than the others. The 5,5'-substituted π-complexes are most stable than the others. The relative stability of the neutral derivatives is mainly related to the Cl-substituted positions and the HOMO-LUMO energy gaps.

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Ab initio molecular dynamics study of the reductive decomposition of battery electrolyte in Li-ion battery

한영규, 김혜미

(주)LG화학기술연구원 CRD연구소

지금까지 배터리 전해질 분자 (용매, 첨가제 혹은 염)에 대한 이론적 연구는 양자 계산 혹은 고전적 분자 동역학 계산 방법을 통해 주로 이루어져 왔다. 양자 계산은 많은 반응 가능성에 대해 일일이 계산해야 하며, 특히 전이상태 계산에 시간이 오래 걸리는 단점을 가지고 있다. 고전적 분자 동역학 계산은 결합이 생기거나 끊어지는 현상을 관측할 수 없고, 배터리 모델링에 적합한 force field 가 부족한 계산상의 단점이 있다. 위 두 가지 계산법의 장점을 모두 가지는 양자 분자 동역학 계산은 산업체에서 원하는 수준의 정성적 결과를 얻는데 가장 경제적이고 믿을만한 방법이라고 할 수 있다. 우리는 음극에서 일어나는 carbonate 계 전해질 분자의 환원 반응에 대한 양자 분자 동역학 결과를 발표하고자 한다.

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Ab initio study of the reaction of SiH_4 with O

김상현, 장성우, 곽현태, 박찬량

국민대 화학과

The reaction mechanism of $O(^3P)$ with SiH_4 for the production of OH has not been well documented compared with that with the saturated hydrocarbons which is well known to proceed via direct abstraction. To elucidate the reaction mechanism, abstraction vs. insertion, ab initio calculations have been conducted using GAUSSIAN 03W package at the MP2/6-31G(d,p) and MP2/6-311G(2d,2p) levels. Optimized stationary points and transition states relevant to the reaction products were calculated. On the triplet PES, a transition state correspon ding to direct abstraction channel was found while that corresponding to insertion-elimination was not found. A possibility of the intersystem crossing (ISC) from the triplet PES to singlet PES was discussed to explain the experimentally observed bimodal rotational distribution of OH product.

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Molecular rotor dynamics influenced by the elastic modulus of polyethylene nanocomposites

이민영, *지아영, *배은혜

*이화여대 화학나노과학부 *이화여대 나노과학부*

We have observed that the excited-state twisting motion of 3,3'-diethyloxacarbocyanine in polymer nanocomposites (PNCs) depends strongly on the elastic modulus of medium. PNCs consist of low density polyethylene dispersed with surface-functionalized nanodiamonds with various alkyl groups. The mechanical properties of the PNCs were measured by a nanoindentation method, and the photoisomerization processes of the cyanine dye doped in the composites were investigated by time-resolved fluorescence spectroscopy. It was found that the molecular rotor dynamics in rigid media should be quantitatively describable by the elastic modulus of polymer.

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Atomic force microscopy of amyloid oligomers interacting with polyamines

이민영, *권하늘

*이화여대 화학나노과학부 *이화여대 화학/나노과학과*

Aggregation of -amyloid (A) monomers has been known for a main cause of the pathogenesis of Alzheimer's disease. Among A aggregates, oligomers having the size of a few nanometers are highly toxic to neuron, and thus their formation and characterization have been subjected to intensive studies. In this work, we have investigated the formation of A oligomers in the presence of various polyamines by atomic force microscopy (AFM). We observed that the aggregation process of A oligomers interacting with polyamines are strongly affected by their molecular structures, which may provide a clue to understand A aggregation mechanism at the molecular level. Our results also show that AFM-based assay can be used as an effective means for drug screening in Alzheimer's disease therapeutics.

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Theoretical Study on the Thermodynamic properties of Chiral Dipeptides

이정은, *함시현

*숙명여대 자연과학부/화학과 *숙명여대 화학과*

Molecular chirality is one of the key factors to control and to manipulate molecular functions in biological systems. Although L-amino acid is the predominant enantiomer in nature, D-amino acid has been found as neurotransmitter or building block for bacterial cell-membrane synthesis. Herein, we chose 19 model dipeptides containing chiral center and employed ab initio density functional theory (DFT) method. We present thermodynamic properties including the effects of side-chain substitution for optical isomer of each model dipeptide.

THE KOREAN CHEMICAL SOCIETY

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Crystallographic Studies of Fully Dehydrated Fully Sr^{2+}-exchanged Zeolite Y (FAU) and its Benzene Sorption Complex, $|Sr_{37.5}|[Si_{117}Al_{75}O_{384}]$-FAU and $|Sr_{37.5}(C_6H_6)_{33}|[Si_{117}Al_{75}O_{384}]$-FAU

이재명, *이석희, **박종삼, 임우택

*안동대 응용화학과 *부산교육대 과학교육과 **대구보건대학 방사선과*

The single-crystal structure of fully dehydrated $|Sr_{37.5}|[Si_{117}Al_{75}O_{384}]$-FAU ($a$ = 25.075(3) Å, crystal 1) and of its benzene sorption complex $|Sr_{37.5}(C_6H_6)_{33}|[Si_{117}Al_{75}O_{384}]$-FAU (($a$ = 24.984(3) Å, crystal 2) have been determined by single-crystal X-ray diffraction technique in the cubic space group $Fd3$-m at 294 K. The single crystal was prepared by ion exchange in a flowing stream of 0.05 M aqueous $Sr(ClO_4)_2 \cdot 6H_2O$ for 3 days, followed by dehydraton at 673 K and 1×10^{-6} Torr for 2 days, followed by exposure to about 92 Torr of benzene vapor at 294 K. The single-crystal structures were refined using all intensities to the final error indices (using only the 1109 and 590 reflections for crystals 1 and 2, respectively, for which $F_o > 4\sigma(F_o)$) R_1/R_2= 0.044/0.169 and 0.058/0.141 for crystals 1 and 2, respectively. About 37.5 Sr^{2+} ions per unit cell are found at an unusually large number of crystallographically distinct positions, six, in crystal 1. In crystal 2, 37.5 Sr^{2+} ions are found at four crystallographic sites and 29 benzene molecules are found at two distinct sites within supercages.

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Synthesis of PVP – CTAB Stabilized Copper Nanoparticles for Conducting Ink Paste

Pham Quoc Long, 강영수

서강대 화학과

Copper nanoparticles of about 56 nm average size are prepared in aqueous solution by reducing copper chloride solution (0.02M) by hydrazine hydrate in the presence of CTAB (Cetyl trimethylammonium bromic) and PVP (Poly vinylpyrrolydone) stabilizers. While using only CTAB as stabilizer, copper nanoparticles are aggregated and partially oxidized to Cu_2O. On the other hand, while using both PVP and CTAB, copper particles of uniform shape and size were formed and they are protected from oxidation. Copper nanoparticles dispersed in ethanol revealed an absorption band at about 614 nm. Use of the nanoparticles for application as conducting ink paste has been studied by dispersing them in PEDOT/PSS.

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Fluorescence lifetime studies from encapsulation of FITC inside single-walled carbon nanotubes

이종택, 이정우

한양대 화학과

FITC (Fluorescein isothiocyanate) is fluorescent material that has high fluorescence quantum yield. But generally, when fluorescent materials are in a solution, they can lose their excitation by nonradiative means : through collisions with other atoms or molecules. It is called dynamic quenching. Thus if FITC is encapsulated into SWNTs (single-walled carbon nanotubes), losing their excitation by nonradiative means may decrease.In this way, we expect to increase fluorescence lifetime of FITC.We inserted FITC into the inside SWNTs. And to confirm that FITC was encapsulated into SWNTs, We used simultaneously AFM(Atomic Force Microscope) and PL (Photoluminescence). Afterward we measured lifetime of FITC using TRS (Time-resolved fluorescence spectroscopy).

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Single Point Mutation Effects of FAS1 Protein in Relation to Corneal Dystrophy using Molecular Dynamics Simulation

박미래, 이제욱, 함시현

숙명여대 화학과

The transforming growth factor beta induced protein (TGFBIp, also known as big-h3) is an extracellular matrix protein and it contains four FAS1 domains. It has been reported that mutations on the big-h3 gene cause amyloid deposits and induce a corneal dystrophy disease in eyes. In this study, we have investigated the effect of point mutation on the wild-type FAS1 domain composed of six a-helices and six beta-sheets by using molecular dynamics simulation. We mainly discussed about conformational changes and thermodynamic stabilities of wild-type FAS1 domain 4 and its two single point mutants (R555W and R555Q). Also, other important properties related with protein aggregation are analyzed.

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Single-crystal Structure of Fully Ba^{2+}-exchanged Zeolite Y (FAU), $|Ba_{35.5}|[Si_{121}Al_{71}O_{384}]$-FAU

김후식, *김경화, **김영훈, ***박종삼, 임우택

*안동대 응용화학과 *포항가속기연구소 빔라인부 엑스선운영2팀*
***안동대 환경공학과 ***대구보건대학 방사선과*

The single-crystal structure of $|Ba_{35.5}|[Si_{192}Al_{71}O_{384}]$-FAU per unit cell, a = 25.096(1) Å dehydrated at 723 K and 1 × 10^{-6} Torr for 2 days, has been determined by single-crystal X-ray diffraction techniques in the cubic space group *Fd*3-*m* at 294 K. The crystal was prepared by ion exchange in flowing stream of 0.05M aqueous $Ba(OH)_2$ solution for 2 days. The structure was refined using all intensities to the final error indices (using only the 906 reflections for which $F_o > 4\sigma(F_o)$) R_1 = 0.0721 (based on F) and R_2= 0.2019 (based on F^2). In this structure, about 35.5 Ba^{2+} ions per unit cell are found at six equipoints crystallographic sites. Two different site-I positions in the center of the double 6-rings(D6Rs) are occupied by 7 and 6 Ba^{2+} ions per unit cell;(site I; Ba(I)-O(3)=2.804(8) Å and Ba(Ia)-O(3)=2.627(14) Å, O(3)-Ba(I)-O(3) = 87.4(2) and O(3)-Ba(Ia)-O(3)=86.5(2) and 92.6(2)^o). The 1.5 Ba^{2+} ions are located at site-I' positions in the sodalite cavity; the Ba^{2+} ions were recessed 1.32 Å in to the sodalite cavity from their three oxygen plane(Ba(I')-O(3) = 2.687(14) Å and O(3)-Ba(I')-O(3) = 97.9(6)^o). The 21 Ba^{2+} ions are found at three nonequivalent site II (in the supercage) with occupancies of 1, 13, and 7 ions, respectively; Ba(IIa)-O(2) = 2.475(15) Å, Ba(IIb)-O(2) = 2.692(9) and Ba(IIc)-O(2) = 2.859(14) Å and O(2)-Ba(IIa)-O(2) = 116.1(10)^o, O(2)-Ba(IIb)-O(2) = 102.6(3)^o, and O(2)-Ba(IIc)-O(2) = 94.6(5)^o)

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Atomic Force Microscopy Lithography for Nanostructure Fabrication using CNT Tip

SONGYIBIN, 유재범, 주해나, *권광민, 이해원

*한양대 화학과 *한양대 나노공학과*

AbstractMany technologies have been developed as new generation lithography, such as extreme UV lithography, electron beam lithography, atomic force microscopy (AFM) lithography and so on. As the technique which can be used in ambient condition, AFM lithography is widely used for nanopattern fabrication. Especially, carbon nanotube(CNT) tips, with their high aspect ration and small diameter, are very important for high resolution pattern fabrication. Polymer copolymerized by methylmethacrylate and 4-biphenyl sulfonium triflic benzyl methacrylate was applied to CNT tip lithography. Cross-linked resist pattern with high resolution and aspect ratio was fabricated by controlling the voltage, lithography speed and oscillation amplitude.

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Synthesis and Photophysical Properties of Voltage Sensitive Dyes with Ionic Naphthalene Derivatives

백남섭, 김용희, 정상돈

한국전자통신연구원 신경계인터페이스연구팀

The aminonaphthlethenylpyridium (ANEP) dyes are commonly used for detection of membrane potential change. These dyes undergo changes in fluorescence intensity (10~20%/100 mV) in response to applied electric field. However, the drawbacks of these dyes are rather low quantum yield in aqueous media and their low photostability due to the nonradiative pathway. One of the key enabling materials for imaging electrical activity of cell membrane is a rigid block naphthalene-pyridinium chromophore consisting of donor-acceptor units. In this presentation, the origin of the solvatochromic phenomena of voltage-sensitive dyes will be discussed.

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Size controlling of Cu nanoparticles fabricated by electron beam irradiation

박옥경, 이병철, *박지현

*한국원자력연구소 양자광학연구부 *과학기술연합대학원대 레이저및플라즈마응용공학*

Recently, the electron beam(EB) irradiation technique has been developed for the synthesis of nanostructures and nanomaterials. Hydrated electrons(e^-_{aq}) and hydrogen atoms produced from solution irradiated by EB act as reducing agent and reduce high valence metal ion to low valence metal ion or metal. In this study, copper nanoparticles were synthesized by irradiating solutions, prepared by mixing $CuSO_4 \cdot 5H_2O$, Polyvinylpyrrolidone(PVP) and Isopropanol(IPA), with 1MeV electrons under room temperature and pressure. Copper nanoparticles size was controlled by EB irradiation condition (Energy, absorbed dose, current), type and content ofsurfactant,and solvent sort. fabricated particles size range was from 5nm to several hundred nm. The morphology, size and chemical composition of the irradiated samples were characterized by transmission electron microscopy(TEM), scanning electron microscopy(SEM) and energy-dispersive X-ray spectroscopy(EDX). Crystal structures of copper nanoparticles were studied by X-ray diffraction(XRD).

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Hydrogen adsorption on alkali metal-doped silicon nanotubes calculated using the density functional theory

박민희, 이윤섭

KAIST 화학과

The adsorption capacity of hydrogen in silicon nanotubes (SiNT) doped with alkali metal atoms (M=Li, Na, K) is studied via first-principles theory based on DFT and Quantum Mechanics/Molecular Mechanics (QM/MM) approach. It is shown that H_2 is physisorbed on pure silicon nanotube, which agrees with earlier studies. The binding energy increases when H_2 binds to alkali metal-doped on silicon nanotube. The origin of the increase in binding energy is the charge transfer from the alkali metal atom to the nanotube. The possibility of SiNT as a hydrogen storage material is discussed.

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Theoretical Study of Pentadehydrobenzene Radical and Ion

정규성, 이동춘, *이덕환

*건양대 화학과 *서강대 화학과*

The electronic structures and molecular properties of pentadehydrobenzene radical and ion (C_6H and C_6H^-) found in the interstellar medium are investigated with multiconfiguration-SCF method and the density functional theory. The CASSCF calculations show that the doublet radical has several local minimum structures with various electronic configuration, whereas negative ion has only one local minimum with singlet state. It turns out from CASSCF as well as DFT calculations that all possible triplet states of negative ion are transition state with one negative hessian. In addition, the ionization energy and the proton affinities of C6H radical are examined by CASSCF+MCQDPT2 method. The results show that sigma nonbonding characters are crucial for understanding the mechanism of electron and proton addition to radical.

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DNA Mediated Energy Transfer from DAPI to Porphyrins

정진아, 전선희, *이길준, **한성욱, 김석규

*영남대 화학과 *경운대 한방자원학부 **경운대 환경공학과*

Horizontal energy transfer through the DNA stem between simultaneously bound [4',6-diamidino-2-phenylindole (DAPI) and porphyrins has been investigated. From earlier study, we reported that the excited energy of DNA bound DAPI was effectively transferred to porphyrin molecule namely, meso-tetrakis(N-methylpyridinium-4-yl) porphyrin (TMPyP) or *cis-bis*(N-methylpyridinium-4-yl) porphyrin (*cis*-BMPyP). Here, we studied the effect of DAPI concentration to the DNA mediated energy transfer efficiency. As results, the fluorescence of the DNA bound DAPI was effectively quenched by TMPyP and *cis*-BMPyP. DAPI-DNA and DAPI-poly[d(A-T)$_2$] quenching by porphyrin appeared to be upward bending curve in the Stern-Volmer plot. While quenching of the DAPI's fluorescence showed downward bending curve in the Stern-Volmer plot in the poly[d(G-C)$_2$]. The quenching efficiency of DAPI-DNA complex by TMPyP was significantly decreased at high DAPI concentration relative to DNA, while no remarkable change of quenching efficiency was observed in *cis*-BMPyP case.

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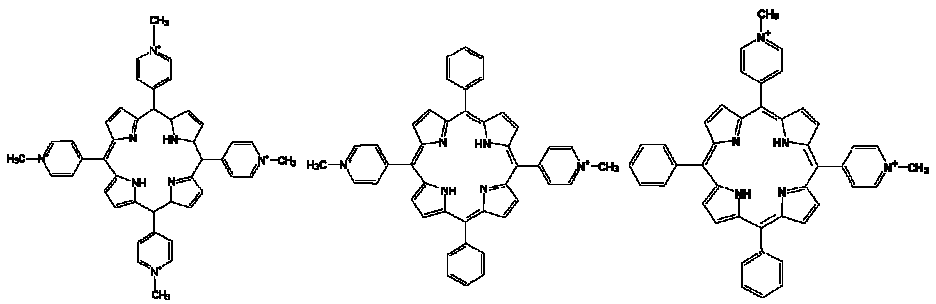
Number and position dependent change in the binding mode of cationic porphyrins on the poly[d(A-T)$_2$] template

이상화, 권용준, *이동진, **이재철, 김석규

*영남대 화학과 *경일대 공업화학과 **삼척대 식품영양학과*

Binding modes of cationic porphyrins to DNA are affected by various factors including the salt concentration and temperature of medium, position and number of positive charges on the periphery group, coordination number of the central metal, and the DNA sequence. The binding modes change also with time. Change in binding mode of various cationic porphyrins (Figure) on poly[d(A-T)$_2$] was investigated by absorption, circular and linear dichroism (CD and LD), and fluorescence techniques in this study. For all porphyrins, rapid decrease in absorbance in the Soret absorption band followed by a very slow decrease was observed: the latter change likely due to the aggregation of the DNA-porphyrin complex. The extent of change was the largest for TMPyP. In the CD spectrum, magnitude of the bisignate CD spectrum decreases in TMPyP case while the negative band in the short wavelength region becomes positive in both *trans*- and *cis*-BMPyP case as the time pass by suggesting the appearance of monomerically bound porphryin in *trans*- and *cis*-BMPyP case.



TMPyP **Trans-BMPyP** **Cis-BMPyP**

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Structual and Electronic Analysis of Lanthanide Complexes : A DFT Study

서영선, 이기학, *이지현, **이왕로

*원광대 화학과 *원광대 생명나노화학과 **전북대 고분자나노공학과*

The chemistry of lanthanides has attracted a great deal of interest, due to their high potential in molecular catalysis. It is commonly assumed that the f electrons of lanthanides are not involved in the chemistry of their complexes, because the f orbitals are significantly more contracted than the valence d d or s orbitals in rare earths. This is widely understand because of the dependence of the orbital radii with the pricipal quantum number, which makes of 4f orbitals closer to the nuclei than the 5d and further than th 6s orbitals. Moreover, the relativistic effects will contract s and p orbitals with respect to nonrelativistic ones, and because the nuclei are accordingly more shielded, the f and d orbitals are on the contrary slightly relaxed, leading to destabilized energy levels. Because most of the electronic density originating from the f orbitals exhibits a rather small overlap with the density of neighbor atoms, taking account the f orbitals into geometry optimization calculations usually leads to geometries quite close to that obtained in calculations where the f orbitals are frozen into the so-called pseudopotential s or frozen core approximations Computations are performed using Gaussian 03. The hybrid density functional method denoted as B3LYP consisting of Becke's three-parameter exchange functional combined with the correlation functional of Lee, Yang and Parr was utilized. 6-311+g* basis set was utilized for C, H, N atoms and Lanthanide atoms were using stuttgart RSC segmented ECP.

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Silica Mesoporous Shell Grown on Core Material via Metal Oxide Core/Meso Shell Strategy

김창우, **Umapada Pal, Nitin Appa Jadhav,** 강영수

서강대 화학과

Here, we report a general approach to a one-pot and one-step synthesis of metal oxide core/mesoporous silica shell (MO@mSiO_2). Micelles are formed on the surface of negatively charged core nanoparticle with cation surfactant under basic conditions. After hydrolysis and condensation of silicate precursors, silica-surfactant nanocomposite can be fabricated with micelle. This designed MO@m$SiO_2$2 materials can be formed by the electrostatic interaction between the partial negative charge of metal oxide core and the positively charged surfactant after the calcination. Various sized silica core materials was prepared and various mesoshell thickness can be fabricated on the surfactant of silica core materials.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Investigation of Magnetic Behavior of One-Dimensional Copper Oxide Nanostructures

차현길, 김창우, 강동인, 강영수

서강대 화학과

Among copper oxide compounds, cupric oxide (CuO) has unusal magnetic properties. Some of them are shared by the supercondutiong one dimensional (ID) copper oxides nanostructure. The effect of the particle size and defects on the magnetic properties of cupric oxide has been assessed by magnetic and optical measurements. Up to room temperature, instead of the increasing susceptibility found in bulk samples, a Curie- Weiss-like behavior is observed above the ordering temperature (Neel temperature) of 230 K.

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Synthesis and Characterization of Volatile Liquid Cobalt Amidinates asALD Molecular Sources

강동인, 차현길, 강영수

서강대 화학과

Cobalt metal are promising in many areas of technology including magnetic information storage, computer chips and catalysis. Volatile cobalt amidinate compound cobalt bis(N,N'-Diisopropylacetamidinate was synthesized. It was characterized by several analytical methods in order to elucidate its structure with single-crystal X-ray diffraction, ^{1}H NMR and FT-IR, optical properties with UV-vis absorption spectroscopy and thermal behavior with thermogravimetric analysis. They are highly reactive compounds that have been found to be suitable precursors for vapor deposition of cobalt metal, cobalt nitride and cobalt oxide. Preliminary atomic layer deposition (ALD) experiments highlight its very promising features as a atomic layer deposition molecular source for cobalt oxide nanosystems.

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Effects of dynamic heterogeneity on adsorption-isotherms

박보정, 양성은, 정원, 성재영

중앙대 화학과

We study the effects of dynamic heterogeneity on adsorption-isotherms. We obtain an analytic expression for binding fraction θ and compare that with the simple Langmuir isotherm. The plot of $(1-\theta)/(1-\theta_0)$ versus θ_0^2 has positive initial curvature when adsorbates have dynamic disorders.Also we find that the new isotherm reduces to the simple Langmuir isotherm in fast fluctuation limit. In between fast and slow fluctuation limits, the isotherm is controlled by the rate fluctuating constant λ. We monitor the equilibrium binding fraction θ by varying λ values .

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Behavior of carbon nanotubes in a shear flow : Simulation studies

권계민, *신관우, 성봉준

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

The influence of the shear on the percolation network of carbon nanotubes (CNT) in CNT/polymer composites is studied using Monte Carlo (MC) simulations and a percolation theory. The percolation behavior of CNTs is crucial to electrical conductivity of CNT/polymer composites, which has been considered a promising material in various applications. It has been well known that the shear has deteriorated the percolation behavior of CNTs significantly. In this work, the shear, which is mimicked in simulations by implementing the biased potential, is exerted on the composite of CNTs and polymers confined between two hard walls. Upon the imposition of shear, CNTs lie parallel to the shear direction and their distribution within the composite is also altered significantly. After a certain amount of time, however, the shear leads the CNTs to get entangled forming clusters of CNTs, which breaks down the percolating network of CNTs, if any, and decreases the electric conductivity of the composite. We carry out MC simulations extensively changing the shear rate, the CNT aspect ratio, and the CNT concentration and obtain a pseudo-phase diagram for the cluster formation.

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Computational Study on the Inversion of Possible Secondary Structures of the β-Peptides

이주희, 함시현

숙명여대 화학과

Interest in β-peptides has recently turned towards the residue-based control of secondary structure formation, and it was proved that the stereochemistry effects on the β-peptides folding. β-peptides composed of trans-2-aminocyclohexanecarboxylic acid (trans-ACHC) and trans-2-cyclopentanecarboxylic acid (trans-ACPC) had been reported to exhibit a high propensity to form helical structures. Unlike that, β-peptides composed of cis-2-cyclopentanecarboxylic acid (cis-ACPC) were assigned to be strand structures by using the NMR spectroscopy. In this study, the homo-oligomers composed of (1R,2R)-trans-ACPC and (1R,2S)-cis-ACPC as model systems were employed to examine the effects of the stereochemistry for the stability of β-peptides. Here, we performed the conformational annealing method by using molecular dynamics simulation and selected model ACPC conformers were optimized by the density functional theory to evaluate briefly the conformational preference and the thermodynamic properties such as relative stability, dipole moment, free energy, enthalpy, and entropy of the model systems. The results of these theoretical approaches would give the structural propensities and thermodynamic stabilities of the secondary structures in the β-peptides.

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The infrared photodissociation spectroscopy of hydrated Aniline cationMd. Alauddin, Sang Hwan Nam, Nuri Cheong, Jae Kyu Song and Seung Min Park

MD.ALAUDDIN, *김준일, 남상환, 정누리, 송재규, 박승민

*경희대 화학과 *연세대 화학과*

Infrared photodissociation spectra of hydrated Aniline cation (n=1-6) are measured in the 2800-3800 cm-1 region. The spectra are interpreted with the aid of density functional theory calculations. It was found that several isomers coexisted. A linear type cluster is the main component for small clusters. A ring type cluster in which the NH2 group of aniline and water molecules form a ring appears in the spectrum of the clusters of n=3, and it becomes the main component in the clusters of n ≥ 4.For n=1 ion, there exist four strong bands at 3099, 3436, 3626 and 3711 cm-1, which has been assigned to the bonded NH vibration of aniline ion, free NH stretching vibration of aniline ion, the symmetric and anti-symmetric stretching vibrations of H2O, respectively. The analysis of the spectrum suggests that there is a hydrogen bond between one of the NH bonds of the Aniline cation and the lone pair of the oxygen atom of H2O.

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Infrared Spectroscopic Studies of Free OH Vibrational Stretching Modes of Imidazole Trimer-Water Complexes in 0.4K Superfluid Helium Nanodroplets.

안아름, 이승준, 최명룡

경상대 화학과

We present infrared spectra of imidazole trimer-water (IMTW) complexes formed in 0.4K superfluid helium nanodroplets. Specific free OH band assignments of IMTWs were employed by varying the oven temperatures of imidazole and the pick-up pressures of water. Ab initio and DFT frequency calculations are also conducted to help the band assignments. Two different complexes of IMTW have been identified in this study.

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The Effect of Quenching Concentration of Fe^{3+} in $LiAl_5O_8$:Fe^{3+} Prepared by Sol-gel Method

Abhijit Pandurang Jadhav, Amor Uttaam Pawar, Umapada Pal, 강영수

서강대 화학과

The nanoparticles of $LiAl_5O_8$:Fe^{3+} were synthesized by sol-gel method. The concentration of dopant Fe^{3+} was varied between 0.00025 mol to 0.006 mol to study the effect on optical properties as well as particle size. The optical properties of $LiAl_5O_8$:Fe^{3+} at various concentration of activator was studied at room temperature. The decrease in luminescence intensity was observed with increase in dopant concentration which corresponds to quenching concentration phenomenon. The quenching process between Fe^{3+} ions is determined and the critical quenching concentration of Fe^{3+} in$LiAl_5O_8$:Fe^{3+} was found to be 0.0005 mol. The luminescence peak at 709.8 nm corresponds to $^4T_1(^4G)$-$^6A_1(^6S)$ transition shows that the synthesized material is red phosphor with highly crystalline nature. The nanoparticles formed were highly crystalline with uniform size distribution.

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Theoretical Studies of Solvent Effect on the Nucleophilic Substitution of Halides and Amine at Sulfonyl and Carboxylic Esters

김태준, 성대동, *이익춘, **류준하

*동아대 화학과 *인하대 화학과 **동의대 화학과*

The solvent effect is inverstigated on the nucleophilic substitution reaction of halides and amine at sulfonyl and carboxylic easters. We compared the theoretical results with our previously reported experimental results. The $E_T(30)$ parameter of many of solvent mixtures are shown as a good measure to show the solvent effects on the nucleophilic substitution reactions and the parameter is accord with well the theoretical calculation results. Other solvent parameters are also well applied to understand the reaction mechanism and orientation of water moleculer around the substrates and solvents.

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A New Photochemical Probe in Detection of Biological Moleculer.

이화진, 성대동, *류준하, **이익춘

*동아대 화학과 *동의대 화학과 **인하대 화학과*

A new photoaffinity probe was developed by using chlorophenyldiazirine. The probe is useful to apply identification of a kind of special protein fibrils as Aβ-Amyloid. The developed method is very effective on the protein fibrils selectively compared to the trifluoromethyldiazirine. In this study, we examined the effectiveness of chlorophenyldiazirine on 15-crown ether in DMF schematically. The substituent effect shows that the electron donating groups are moved to red shift, on the contrary the electron withdrawing groups are constant during the carbene reactions occur. The carbene intermediates are inserted into the substrate effectively selectively without any other side-reactions and this reaction mechanism is useful to detect the protein fibrils.

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Photoaffinity Labeling of Aβ-Amyloid with Aromaticdiazirine

류선아, 성대동, *류준하, 이종팔, **이익춘

*동아대 화학과 *동의대 화학과 **인하대 화학과*

The Photochemical reaction of Aβ-Amyloid with 3-trifluoromethyl-3-phenyldiazirine gives a kind of photoaffinity labeled Aβ-Amyloid derivatives. The Amyloid fibrils were detected for the cross-links which reacted with a single trifluoromethylphenyl carbene. This probe is useful to identify the Aβ-Amyloid fibrils which could not separate in protein using effective MALDI-MS. The method of photoaffinity labeling is more developed to detect the Aβ-Amyloid fibrils effectively compared to the reported method of the photo-induced cross-lingking probe. This photoaffinity labeling method is based on the mechanism of self-insertion reaction into the Aβ-Amyloid selectively by the electron-withdrawing carbene intermediate.

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Characterization of a double-stage membrane interface for sample introduction into a miniature TOFMS

장유미, 정광우, 이명기

원광대 화학과

The benefits of on-site analysis of environmental pollutants are well known, with such techniques increasing sample throughput and reducing the overall cost of pollution level monitoring. Characterization of double-stage membrane inlet have been performed using a time-of-flight mass spectrometer (TOFMS). Temporal evolution of volatile organic compounds (VOCs) through the two 127 ㎛ thick polydimethylsiloxane (PDMS) membranes were measured by monitoring the ion signal after a step change in the sample concentration. The detection limits for VOCs were found to be in the range of ppb by volume. Initial results indicate that the TOFMS will be capable of use in a wide range of applications, particularly for real-time environmental monitoring.

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Energy Transfer and Photophysical Properties of NIR Emitting [Ln(III)(2-ATFB)$_3$(phen)] Complexes

신정식, 강준길

충남대 화학과

The NIR emitting Ln(III) (Ln = Pr, Nd, Ho, Gd, Er, Tm and Yb) complexes with beta-diketonate containing anthracene moiety (2-ATFB, 1-(2-anthrancenyl)-4,4,4-trifluoro- 1,3-butanedione) and phen (1,10-phenanthroline) were synthesized and investigated their photophysical properties using various spectroscopic techniques. The synthesized Ln(III) complexes were confirmed with the EA, ICP and TGA. Their photophysical properties were comprehensively investigated, including absorption, emission and excitation spectra, quatum yield, and luminescence lifetimes.

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Synthesis and luminescence properties of Eu(III) complexes with beta-diketone and phen (phen = 1,10-phenanthroline)

김현준, 강준길

충남대 화학과

Europium(III) complexes of [Eu(beta-diketone)$_4$]$^-$ and [Eu(beta-diketone)$_3$(phen)] were synthesized and their photophysical properties were investigated. The beta-diketones used in this work were 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione, 4,4,4-Trifluoro-1-(2-naphthyl)-1,3-butanedione, 1-(2-Thenoyl)-3,3,3-trifluoroacetone, 4,4,4-Trifluoro-1-phenyl-1,3-butanedione and dibenzoylmethane. The synthesized Eu(III) complexes were confirmed with EA, ICP and TGA. The Eu(III) complexes excited at UV produced sensitized red-luminescence. The excitation spectra measured by monitoring the emission proved that the energy transfer took place effectively via the beta-diketone ligand, no matter whether phen was included or not in the complex. In this presentation, the energy transfer between the beta-diketone ligands and the europium(III) ion will be precisely discussed.

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Effective Electron Transfer species of Ruthenium and Osmium Derivatives

윤혜진

동아대 화학과

A new effective electron transfer compounds Ru[H_2O(2,2'-bipyridyl-4,4'-dicarboxylic acid)]H_2O and Os[H_2O(2,2'-bipyridyl-4,4'-dicarboxylic acid)]H_2O were synthesized and applied to photosensitizing materials. The synthesized molecular are excellent candidate to the molecular photoconversion. The molecules are shown short-lived life time as shown as 0.484ns detected by a pico seconds Nd : YAG laser operating at a wavelength of 467nm at 20MHz.The Ru and Os bipyridyl sensitizer are useful to show a relatively high quantum yields for the sensitization of nanocrystalline TiO_2.

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The photochemical reaction mechanism of Ru and Os containing photoelectron systems.

윤지원, 윤혜진, 성대동, *이익춘

*동아대 화학과 *인하대 화학과*

The photochemical reaction mechanism is studied on the photochemical reactions of [Ru(H_2O)(2,2'-bipyridyl-4,4'-dicarboxylic acid)].H_2O and [Os(H_2O)(2,2'-bipyridyl-4,4'-dicarboxylic acid)].H_2O in the colloidal TiO_2 systems. The dependence of the fluorescence quantum yield of the [Ru(H_2O)(2,2'-bipyridyl-4,4'-dicarboxylic acid)].H_2O and [Os(H_2O)(2,2'-bipyridyl-4,4'-dicarboxylic acid)].H_2O onto TiO_2 colloid on the solution composition gives the 'infinite' concentration of TiO_2 and enables to estimate which part of the label is bound to the surface of colloid particles. The photochemical evidence that the quantum yield of the fluorescence of the label on the surface is smaller than in the bulk solution. The logaritm of the quenching rate constant k_1 against the surface potential for the two compounds with different chemical environments shows that the process in the layer are accord with for the observed results.

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New try for correlation energy on a ground state.

박성준

중앙대 화학과

I suggest two ways for correlation energy. They have very simple principles. In the first method, We start the fact that the interaction of two molecular orbitals is thought to associate the overlap integral of the two molecular orbitals. If this is right, We will evaluate correlation energy using only occupied orbitals. Otherwise, In the second method, We use variation method that is added correlation energy term. This method is similar to get Fock operator. We indicate only methods on this document, not results.

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Macroporous Zirconium Oxide Thin Films Prepared by Simple Spin – Coating Using Polystyrene Grafted Carboxyl Latex as Template[발표 취소 10-7]

Mai Xuan Dung, 정현담

전남대 화학과

Porous materials are of scientific and technological interests because of their potential applications such as: separation, catalysts, air – like layer electro - optics. Ordered porous materials are usually fabricated with help of various templates. High band gap, high refractive index materials possessing macro pores are designed to improve the pe[illegible]OLED device.In current research, macroporous zirconium oxide [illegible] – coating sol containing zirconium precursor, catalyst, and polysty[illegible]PS – AA) on silicon wafer followed by thermal remove of organic template. PS-AA latex whose particle size is controllable in macro range confirmed by Zeta – PSA was pre - prepared by miniemulsion polymerization from polystyrene and acrylic acid monomers. The morphology, electrical, and optical properties of final macroporous zirconium oxide were thoroughly characterized by several techniques as a function of sol compositions.

발 표 취 소

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Synthesis of Mesoporous TiO_2 using F-68 Triblock Co-polymer as Template

Nitin Appa Jadhav, 김창우, **Umapada Pal**, 강영수

서강대 화학과

Porous metal oxides are of high demand for catalytic and photocatalytic applications. Recently several research groups have reported on the synthesis of $TiO_2$and ZnO_2 porous structures using ultrasonic hydrolysis of the precursors,[1] tri-block copolymers,[2] or using porous silica as hard template.[3] However, reports on the synthesis of porous TiO2 structures with ordered and size controlled pores are rare.Here we report on the synthesis of mesoporous TiO_2structures with ordered pores using Pluronic F-68 triblock co-polymer as soft template. The porous TiO_2 powders were prepared by simple EISA method using titanium (IV) butoxide as precursor. The pore size and their order have could be varied by varying the polymer concentration. The porous materials were analyzed by transmission electron microscopy (TEM), X-ray diffraction and nitrogen adsorption-desorption isotherms.

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Synthesis of Blue Phosphor $CaMgSi_2O_6:Eu^{2+}$ with Different Volume Ratios of Water/Ethanol Solvent Mixture.

Amor Uttaam Pawar, Abhijit Pandurang Jadhav, 강영수

서강대 화학과

In this work, $CaMgSi_2O_6:Eu^{2+}$nanoparticles were synthesized by co-precipitation method with different volume ratio of water and ethanol as a solvent mixture. These synthesized nanoparticles were calcinied at different temperatures. We observed $CaMgSi_2O_6:Eu^{2+}$ particles obtained from volume ratio of W: E as 0:1 and calcinied at 1000 OC for 2 hrs gave uniform particle size and high photoluminescence intensity. The dielectric constant of solvent depends upon volume ratio of solvent mixture which is responsible for electrostatic interaction and nucleation rate of particles. The synthesized blue phosphor shows absorption band in UV range with emission at 478 nm.

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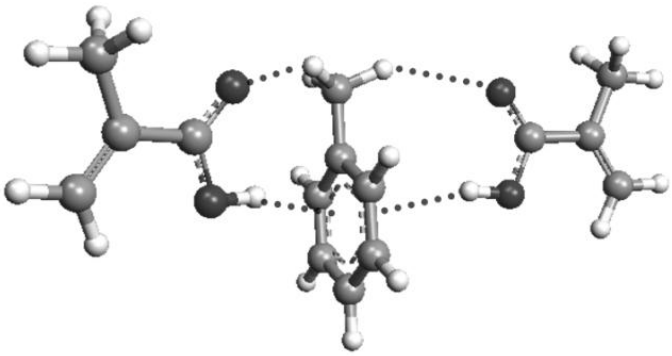
Compuational study of the weak interactions between toluene(or xylene) and functional monomers used in molecular imprinting

장성우, *임상규, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We studied the weak interactions between template molecules(toluene or xylene) and functional monomers(acrylic acid, methylacrylate, methacrylic acid, allylamine and etc) in order to improve the efficiency of molecularly imprinting technique using density functional theory and ab initio methods. The possible complex conformations of toluene and xylene with functional monomers were calculated by Density Functional Theory(B3LYP, BHandH and BHandHLYP) method using 6-311++G(d,p) basis set and ab initio(HF and MP2) method using 6-31G(d,p) and cc-pVDZ basis sets. The binding energy(ΔEbind) of the complex between template and functional monomers were calculated applying the basis set superposition error(BSSE) and the zero-point vibrational energies(ΔZPVE) corrections. The binding affinity and the geometry of the conformations between template molecule and functional monomers revealed the mechanism of molecular recognition process in molecular imprinting technique.



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Conformation-Selective Photoionization of Diaryl Compounds: Excimer-mediate R2PI of Ultracold 1,3-Diphenylpropane

부봉현, *이재광, **Richard H. Judge, *E. C. Lim

*충남대 화학과 *Department of Chemistry, University of Akron*
***Department of Chemistry, University of Wisconsin*

Hole-burning spectroscopy and ionization threshold measurement were combined with fluorescence excitation (FE) and resonant two-photon ionization (R2PI) spectroscopies to probe conformation dependence of photoionization for jet-cooled 1,3-diphenylpropane (DPP). The S_1<-- S_0 excitation energy dependence of excimer fluorescence and that of one-color R2PI indicate formation of an intramolecular excimer and an efficient photoionization of the excimer that occur at higher energies. The energy threshold for the enhanced photoionization, which concurs with that for the excimer formation, is considerably lower for the trans-gauche (tg) conformer than for the trans-trans (tt) or the gauche-gauche (gg) conformer.

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Ab Initio and Density-functional Theory Studies of Molecular Structures and Energies of Ga_xN_x (x=1-3) Clusters

부봉현

충남대 화학과

An ab initio and DFTcalculations on Ga_xN_x (x=1-3) clusters were performed to predict stable clusters which are responsible for the formation of thin films of GaN. We have optimized various conformers of Ga_xN_x (x=1-3) by using the DFT B3LYP/6-31G(d) method and then performed single point calculations by using B3LYP/6-31G(d)//B3LYP/6-31G(d) and MP2/6-31G(d)//B3LYP/6-31G(d) methods in order to estimate the relative energies of conformers. Also we have simulated Raman spectra by calculating the Raman frequencies and the intensities with the DFT B3LYP/6-31G(d) and HF/6-31G(d)//DFT B3LYP/6-31G(d) methods, respectively. A simulated Raman spectrum of the zigzag conformer is relatively well consistent with the experimental Raman spectra of powder and thin film reported elsewhere. Therefore we presume that the zigzag clusters are converted at the surfaces on the substrate to the wurtzite type crystals due to the high deposition temperature.

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Ab Initio and DFT Studies of the Thermal Rearrangementof Trimethylsilyl(methyl)silylene. Remarkable Rearrangements of Silicon Intermediates

부봉현, *이성렬

*충남대 화학과 *경희대 화학과*

A reaction scheme for the rearrangement of trimethylsilyl(methyl)silylene (Me_3Si-Si-Me) discovered in a pioneering work of organosilicon chemistry (J. Am. Chem. Soc. 100, 6236) was studied by the MP2 and DFT methods. We report a thermal reaction scheme for the rearrangement of Me_3Si-Si-Me with the structures and energies of various silicon species along the isomerization paths, that can account for the experimentally found product ratio. The experimental product ratio is in good agreement with the theoretical one derived from the Gibbs free energy changes calculated in the present study.

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Fe-Mn 합금으로 이루어진 Grain boundary에서의 Boron 영향에 대한 연구

양혁, 이억균, *이영주, *김상원

*KAIST 화학과 *포항산업과학연구원 부품신소재연구본부*

철강은 소량으로 첨가되는 원소들의 함량과 이후 처리과정에 따라 가공성 및 기계적 특성에 큰 차이를 가져오며 이것은 첨가된 원소들의 분포 및 화학결합의 차이에서 기인한다고 알려져있다. 철강에 큰 영향을 주는 미량원소 중 Boron 은 고망간강에 약 3~40ppm 정도 첨가됨으로서 기계적 특성과 강도를 향상시키는 것으로 알려져 있다. 적은 양의 Boron 이 고망간강에 첨가되면 오스테나이트로 이루어진 grain 의 boundary 에 들어가 구조내에서 페라이트의 핵 생성을 억제하지만 필요 이상으로 들어가면 Fe_2B 결정으로 석출되기 때문에 오히려 강도를 약화시킨다. 산업적으로 Boron 이 첨가된 고망간강은 시료의 열처리 조건에 따라 다양한 종류의 기계적인 특성을 보이고 이것은 Boron 원자의 분포 및 이웃한 철원자와의 결합 조건에 영향받는다고 추정되지만 이를 실험적으로 확인하기 어렵다. 일반적으로 사용되는 재료분석 방법으로는 수십 ppm 정도의 Boron 의 화학결합 및 분포를 규명할 수 없는 상태이다. 이번 발표에서는 원자단위에서 Boron 의 농도를 계산하고 제일원리 전산모사를 이용하여 고망간강의 다양한 환경 내에서 Boron 의 분포 및 구조를 해석하고 특히 입계에너지에 미치는 Boron 의 영향에 대해서 논의한다. 이번 연구에서 사용된 제일원리 계산은 전자밀도함수이론을 이용하였고 전이금속 원자들을 효과적으로 표현할 수 있는 generalized gradient approximation 과 norm-conserving pseudopotential 을 이용하였다.

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FCC Fe로 이루어진 Grain boundary 생성에너지의 Boron 효과 연구

양혁, 이억균, *이영주, *김상원

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Grain boundary 는 산업적으로 철강을 이용할 때 매우 중요한 변수가 되는데 이들 주변은 상대적으로 에너지가 높기 때문에 핵의 생성이나 결함의 제거가 이루어지는 자리가 된다. FeMn 합금에 소량의 Boron 을 첨가하면 철강의 전체적인 인장강도도 증가하고 핵생성을 억제하는 효과를 나타낸다고 알려져있다. 이는 Boron 이 grain boundary(GB)에 들어가 서로 다른 두 grain 의 중간부를 채워서 grain 사이의 결합을 강하게 해주며 grain boundary 생성엔탈피를 낮추어주어 GB 를 안정하게 만드는 역할을 한다고 생각된다. 하지만 이러한 역할에 관한 실험적, 이론적 근거는 전무한 상태이다. 이에 대해 명확히 검증하기 위해서는 GB 의 정확한 원자구조를 생성한 뒤 GB 에너지/생성엔탈피 및 GB 에서의 화합결합 상태를 조사해야 한다. 이번 연구에서는 순수철에서 스핀상태에 따라 GB 의 정확한 원자구조를 얻고 GB 에너지 및 화학결합 상태가 어떻게 다른지는 원자단위 제일원리 계산으로 밝혀내고자 한다. 이를 위해 fcc 순수철에 들어가는 Boron 의 원자단위 농도 계산법 및 제일원리 전산모사를 사용하고 철원자를 효과적으로 표현할 수 있는 generalized gradient approximation 과 norm-conserving pseudopotential 을 이용하였으며 모든 계산은 스핀상태별로 구분하여 진행하였다.

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Single-crystal Structure of Fully Dehydrated Partially Cs^+-exchanged Zeolite Y (FAU, Si/Al = 1.56), $|Cs_{45}Na_{30}|[Si_{117}Al_{75}O_{384}]$-FAU

서성만, *김경화, **이석희, 임우택

*안동대 응용화학과 *포항가속기연구소 빔라인부 엑스선운영2팀 **부산교육대 과학교육과*

Large single crystals of zeolite, $|Na_{75}|[Si_{117}Al_{75}O_{384}]$-FAU (Na-Y, Si/Al = 1.56), were synthesized from gels with composition of $3.58SiO_2$: $2.08NaAlO_2$: 7.59NaOH : $455H_2O$: 5.06TEA : 2.23TCl. One of these, a colorless single-crystal was ion exchanged by allowing aqueous 0.02 M CsOH to flow past the crystal at 293 K for 3 days, followed by dehydration at 673 K and 1×10^{-6} Torr for 2 days. The crystal structure of fully dehydrated partially Cs^+-exchanged zeolite Y, $|Cs_{45}Na_{30}|[Si_{117}Al_{75}O_{384}]$-FAU per unit cell ($a$ = 24.9080(10) Å) was determined by single-crystal X-ray diffraction technique in the cubic space group $Fd3$-m at 294 K. The structure was refined using all intensities to the final error indices (using only the 877 reflections for which $F_o > 4\sigma(F_o)$) R_1 = 0.0966 (based on F) and R_2 = 0.2641 (based on F^2). About forty-five Cs^+ ions per unit cell are found at six different crystallographic sites. The 2 Cs^+ ions occupied at site I, at the centers of double 6-ring (D6Rs, Cs-O = 2.774(10) Å and O-Cs-O = 88.9(3) and 91.1(3)^o). Two Cs^+ ions are found at site I' in the sodalite cavity; the Cs^+ ions were recessed 2.05 Å into the sodalite cavity from their 3-oxygen plane (Cs-O = 3.05(3) Å and O-Cs-O = 77.4(13)^o). Site-II' positions (opposite single 6-rings in the sodalite cage) are occupied by 7 Cs^+ ions, each of which extends 2.04 Å into the sodalite cage from its 3-oxygen plane (Cs-O = 3.067(11) Å and O-Cs-O = 80.1(3)^o). The 26 Cs^+ ions are nearly three-quarters filled at site II in the supercage, being recessed 2.34 Å into the supercage (Cs-O = 3.273(8) Å and O-Cs-O = 74.3(3)^o). The 4 Cs^+ ions are found at site III deep in the supercage (Cs-O = 3.321(19) and 3.08(3) Å), and 4 Cs^+ ions at another site III' (Cs-O = 2.87(4) and 3.38(4) Å). About 30 Na^+ ions per unit cell are found at one crystallographic site; the Na^+ ions are located at site I' in the sodalite cavity opposite double 6-rings (Na-O = 2.578(11) Å and O-Na-O = 97.8(4)^o).

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Synthesis and Characterization of Fully Dehydrated Fully Ca^{2+}-exchanged Zeolite Y (FAU), $|Ca_{35.5}|[Si_{121}Al_{71}O_{384}]$-FAU

서성만, *김경화, 최식영, **김영훈, 임우택

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The single-crystal structure of $|Ca_{35.5}|[Si_{121}Al_{71}O_{384}]$-FAU, $Ca_{35.5}Si_{121}Al_{71}O_{384}$ per unit cell, a = 24.9020(10) Å, dehydrated at 673 K and 2×10^{-6} Torr, has been determined by single-crystal X-ray diffraction techniques in the cubic space group $Fd3\text{-}m$ at 294 K. The large single crystals of zeolite Y (Si/Al = 1.70) were synthesized up to diameters of 200 μm and Ca^{2+}-exchanged zeolite Y were prepared by ion exchange in a batch method of 0.05 M aqueous $Ca(NO_3)_2$ for 4 hrs at 294 K. The structure was refined using all intensities to the final error indices (using only the 971 reflections for which $F_o > 4\sigma(F_o)$) R_1 = 0.038 (based on F) and R_2 = 0.172 (based on F^2). About 35.5 Ca^{2+} ions per unit cell are found at an unusually large number of crystallographically distinct positions, four. Nearly filling site I (at the centers of the double 6-rings), 14.5 octahedrally coordinated Ca^{2+} ions (Ca-O = 2.4194(24) Å and O-Ca-O = 87.00(8)^o) are found per unit cell. One Ca^{2+} ion per unit cell is located at site II' in the sodalite cavity and extends 0.50 Å into the sodalite cavity from its 3-oxygen plane (Ca-O = 2.324(13) Å and O-Ca-O = 115.5(10)^o). The remaining twenty Ca^{2+} ions are found at two nonequivalent sites II (in the supercages) with occupancies of 10 and 10 ions, respectively. Each of these Ca^{2+} ions coordinates to three framework oxygens, either at 2.283(3) or 2.333(5) Å, respectively, and extends either 0.24 or 0.54 Å, respectively, into the supercage from the three oxygens to which it is bound. In this crystal, site I is the most populated; sites II' and II are only sparsely occupied. Ca^{2+} appears to fit the octahedral site I best. No cations are found at sites III or III', which are clearly less favorable for Ca^{2+} ions in dehydrated zeolite Y.

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Tuning of Refractive Indices and Optical Band Gaps in Oxidized Silicon Quantum Dot Solids

최진규, *장승현, *손홍래, 정현담

*전남대 화학과 *조선대 화학과*

Quantum dots (QDs) or nanocrystalline semiconductors whose radii are less than tens nanometers have discrete energy levels resulted from the confinement of carriers in all three spatial dimensions, known as quantum confinement effect. Different from well-investigated Ⅱ-Ⅵ QDs containing cadmium, silicon QDs (Si QDs) are nontoxic, cheap, and relatively easy to integrate into industrially well-established silicon process. We have initiated compelling research into silicon quantum dots (Si QD) solids in order to utilize their synergetic benefits with quantum dot solids through fabrication of Si QD thin films. The oxidation problems of the Si QD thin films were confirmed using Fourier transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS). The refractive index value of the Si QD thin film at a 30 oC curing temperature was 1.61, while 1.45 for 800 oC, due to complete oxidation of the Si phases. The optical band gap values of 5.49 - 5.90 eV corresponded to Si phases of diameters between 0.82 - 0.74 nm dispersed in the oxidized Si QD thin films, modeled by Si molecular clusters of approximately fourteen silicon atoms. The photoluminescence (PL) energy (2.64 – 2.61 eV) in the proposed Si QD thin films likely originated from the Si=O bond terminating the Si molecular clusters.

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Time-Average Approximation for Calculation of Line Shape of Coupled Chromophores

양민오, *J.L. SKinner

*충북대 화학과 *Department of Chemistry, University of Wisconsin-Madison*

Semiclassical calculation of vibrational absorption and Raman spectra of a large number of coupled chromophores is a demanding task because of the dimensionality of Hamiltonian matrix. Therefore it is desirable to develop an approximate and efficient theoretical method. Recently, as a candidate, a time-average approximation was developed by Skinner group. In this work, we extend the method so that more accurate prediction is available with much less computing cost than exact numerical calculation. The present approximate method is applied to the IR and Raman line shapes of water and shows an excellent agreement with exact numerical calculations.

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Semiclassical calculation of IR pump-probe anisotropy and two-dimensional IR spectra of water

양민오, *J.L. Skinner

*충북대 화학과 *Department of Chemistry, University of Wisconsin-Madison*

We developed a mixed quantum/classical method to calculate the IR pump-probe and two-dimensional (2D) IR spectra of coupled chromophores. The theoretical calculations for water are compared in good agreement with experimental results. With the calculated frequency-integrated pump-probe signal, we constructed the anisotropy decay of water. The comparison of the theoretical and experimental anisotropy shows that the OH vibrational energy is transferred to other OH bonds in an extremely short time scale via inter-molecular dipole-dipole interaction as well as intra-molecular couplings.

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Anomalous Electron Binding Energy for the Dimers of 2-, 3-, 4-Bromochlorobenzene

김남두, 손태일, 이상학, *김성근

*서울대 화학부 *서울대 화학부, 서울대 생물물리 및 화학생물학과*

The extraordinary behaviors of 2-, 3-, 4-bromochlorobenzene (BCB) cluster anions upon electron attachment were investigated by using TOF-MS, photoelectron spectroscopy (532 nm 2.329 eV and 355 nm, 3.496 eV) and ab initio calculations. In the mass spectrum, Br^- shows a distinctly more intense peak than any other moieties, indicating dissociative attachment of electron to bromine. In photoelectron spectrum, the vertical detachment energies (VDEs) of all three isomers of monomer were determined to be ~2.5 eV, which agrees well with the calculated values. Dissociated bromine atom was found to form a van der Waals complex with its parent molecule. In contrast to the monomeric cases, the VDE of 4-BCB dimer is extremely small at ~0.3 eV, while that of 2-BCB and 3-BCB are 1.1 eV and 2.69 eV. We calculated several possible structures and found that a parallel-staggered structure and a T-shaped one are the most likely structures for 4-BCB dimer anion, with a VDE value of 0.36 and 0.30 eV, respectively.

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Relatively short silver nanorods for surface-enhanced Raman scattering

구근회, *서정쌍

*서울대 화학과 *서울대 화학부*

Silver nanorods were fabricated by electrodepositing them evenly near the mouth of the pores of anodic aluminum oxide templates with a very shallow depth. The SERS intensity increased almost linearly with increasing the concentration of the mother solution in the range of sub-monolayer level. From the data of the enhancement and the number of molecules irradiated by the laser beam at the detection limit, the minimum SERS enhancement factor for non-resonant single molecule detections was assumed to be approximately 10^{11}.

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Silver nanorods in ultrathin porous anodic alumina as a quantitative analytical tool by SERS

구근회, *서정쌍

*서울대 화학과 *서울대 화학부*

Fabrication of silver nanorod electrodeposited in porous anodic aluminum oxide templates was done. The SERS intensity of Malachite green isothiocyanate increased linearly with the concentration of the mother solutions in the range of sub-nanomolar concentration. These results showed that silver nanorods fabricated on AAO templates could be used as a SERS substrate for quantitative analyses.

THE KOREAN CHEMICAL SOCIETY

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Abstraction of Oxygen Chemisorbed on a Silicon Surface by Atomic Hydrogen

김은영, 이종백, 김성희, *김유항, **H. K. Shin

*전남대 화학교육과 *인하대 물리화학부 **University of Nevada,Reno, USA*

We have calculated the probability of the OH formation and energy deposit of the reaction exothermicity in the newly formed OH, particularly in its vibrational motion, in the gas-surface reaction H(g)＋O(ad)/Si→OH(g)＋Si on the basis of the collision-induced Eley-Rideal mechanism. The translational and vibrational motions share most of the energy when the adatom-surface vibration is initially in the ground state. When the initial excitation increases, the vibrational energy of OH rises accordingly, while the energies shared by other motions vary only slightly. The product vibrational excitation is significant in OH and the population distribution is strongly inverted. Flow of energy between the reaction zone and the solid has been incorporated in trajectory calculations. The amount of energy propagated into the solid is only a few percent of the available energy in the OH formation.

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Dynamics of OH dissociation and CH_3O formation in the CH_3 + OH collision

김성희, 이종백, *김유항, **H. K. Shin

*전남대 화학교육과 *인하대 물리화학부 **University of Nevada, Reno, USA*

The collision-induced OH dissociation and CH_3O formation in the CH_3 + OH collision have been studied over the temperature range of 1000 – 2500 K using classical dynamics procedures for an analytical form of the interaction potential composed of numerous short-range and long-range terms. The OH dissociation occurs with the rate constant k(T), which decreases slightly from 3.35 $X10^{14}$ cm^3 mol^{-1} s^{-1} at 1000 K to 3.00 $X10^{14}$ cm^{-1} mol^{-1} s^{-1} at 2500 K. k(T) for CH_3O formation varies from 4.86 $X10^{13}$ to 3.99 $X10^{13}$$cm^3$ mol^{-1} s^{-1} over the same temperature range, exhibiting a weak negative temperature dependence which is typical of free radical reactions. As the temperature increases, an increase in the translational and rotational motions tends to disrupt the preferred alignment of the free radicals for the reaction, which is strongly affected by attractive forces. Majority of reactive events occur in a direct-mode collision between the radicals. CH_3O is found to be highly vibrationally excited and acts as a precursor state for other reaction pathways. Also studied is the reaction of the dissociation product H with CH_3 to form CH_4, which is found to be extremely inefficient with k(T) smaller than the CH_3O values by two orders of magnitude.

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Rapid Synthesis of Aligned Zinc Oxide Nanowires

허창순, 이상국

부산대 화학과

A rapid growth approach for zinc oxide (ZnO) nanowires is highly appealing because of the low growth temperature and possibility for large area synthesis. Reported reaction times for ZnO nanowire synthesis, however, are long, spanning from several hours to days. In this work, we report on the rapid synthesis of ZnO nanowires on various substrates (such as ITO, silicon and sapphire) using a microwave plasma enhanced chemical vapor deposition(MPECVD) method.The crystal structures and morphology of the products were characterized by high resolution field emission scanning electron microscope (FE-SEM) and transmission electron microscope (TEM). Energy dispersive X-ray spectrum (EDS) demonstrated that the various microstucture consist of element.

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Identification of 3,5-Difluorobenzyl Radical in a Corona Excited Supersonic Expansion

이승운, 정승환, 이상국

부산대 화학과

Over the last ten years, we have developed a technique of corona excited supersonic expansion (CESE) to observe the vibronic emission spectra of transient molecules such as benzyl-type radicals, from which many benzyl-type molecular radicals have been identified from the analysis of vibronic spectra. The precursor, 3,5-difluorotoluene was corona discharged with high voltage DC current with a large amount of inert carrier gas helium. The relatively strong emission emitted from the molecular radicals generated in a corona excited supersonic expansion was collected to observe the vibronic structure of 3,5-difluorobenzyl radical, in which many bands were identified to belong to other isomers, possibly through rearrangement of fluorine atom or methylene group.

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Identification of Benzyl-type Radicals Generated from 1,2,3,5-Tetramethylbenzene in a Corona Excited Supersonic Expansion

정승환, 이기우, 이상국

부산대 화학과

Methyl-substituted benzyl-type radicals are excellent candidates for analysis of internal rotation of methyl group, from which the interaction between methyl groups and torsional barrier can be identified. The precursor, 1,2,3,5-tetramethylbenzene seeded in a large amount of inert carrier gas helium has been discharged by employing a technique of corona excited supersonic expansion, from which the fluorescence of benzyl-type radicals were observed with a long-path monochromator to see the vibronic structure of molecules in the ground electronic state. From the analysis of band structure and intensity observed, we can easily identify the electronic transition and vibrational mode frequencies of each isomer produced.

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DFT study of small boron cluster as a building block for larger nanodevice design

장효원

순천대 화학과

As an alternate to the carbon nanostructure, boron clusters have been considered to be applied for high temperature semiconductors, for example.Various forms have been studied experimentally and theoretically including rings, cages, tubes, and sheets to name a few.In this work, a novel boron cluster is introduced to be used as a building block for larger and/or longer nanostructures.The energetics and MO structures of the present cluster and its oligomers are compared with the known stable isomers where appropriate.Interesting properties incurred by doping with other elements are also discussed.

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A Kinetic Studies of the Solvolyses of Phenyl 4-methylphenoxy Thiophosphinyl Chloride

고한중

전주교육대 과학교육과

The sensitivity values (l = 1.08 and m = 0.53) of Phenyl 4-methylphenoxy Thiophosphinyl Chloride ((Ph,4-CH_3PhO)PSCl, 1) were similar to those obtained for diphenyl thiophosphorochloridate ($(PhO)_2PSCl$, 2), diphenyl phosphorochloridate ($(PhO)_2POCl$, 3), diphenylphosphinylchloride (Ph_2POCl, 4) and diphenylthiophosphinylchloride (Ph_2PSCl, 5). [The extended Grunwald-Winstein equation : log (k/ko) = l N_T + mY_X + c]. As with the previously studied of 2~5 solvolyses, a S_N2 pathway is proposed for the solvolyses of 1. The activation parameters, $\Delta H^{\neq}$(= 12.8~13.9 kcal/mol) and $\Delta S^{\neq}$(= -32.3~34.6 cal/molK), were in line with values expected for a S_N2 reaction. The large kinetic solvent isotope effect (= 1.99) is also well explained by the proposed S_N2 mechanism.

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Second-harmonic generation and multiphoton induced photoluminescence in ZnO

한노수, 박승민, 송재규

경희대 화학과

Among II-VI semiconductors, zinc oxide (ZnO) possesses attractive properties such as a wide band gap (3.37 eV) and a large exciton binding energy (60 meV). Thus, nonlinear optical responses of ZnO have been investigated to understand the optical nonlinear properties. We present the nonlinear optical properties of ZnO, which were investigated by nonresonant optical excitation of femtosecond laser pulses in the range of 710 nm-850 nm. In order to figure out the mechanisms of UV emission and SHG, emission spectra were obtained as a function of the excitation intensity. The power dependence suggested that SHG was the two-photon process and UV emission was affected by both 2PA and 3PA.

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In Situ Surface-Enhanced Raman Scattering (SERS) of Current-Carrying Molecules at Metal Nanoparticle-Molecule-Plane Junctions

박원화, 김지환

고려대 화학과

We present the important aspect of molecular conformational rearrangement in developing molecular-based electronic device using well-established SERS-active metal nanoparticle-molecule-plane junction system. Electrical contact between Au(Ag) nanoparticle and Au plane via conducting atomic force microscopy (C-AFM) is employed and simultaneous SERS measurement with I-V curve can help interpreting the molecular dynamic behavior under certain electrical potential bias voltage. Relative SERS intensity changes including broadband continuum background are dominantly observed with varying bias voltage. We address this phenomenon in association with molecular conformational rearrangement under the specific potential bias voltage with certain amount of electron flow between metal nanoparticle and plane. Exploring the detailed and more quantitative relationship between electrical property and the corresponding molecular conformation of the interconnected-SAM via SERS will be unprecedentedly emerged in terms of understanding charge transport in organic system as well as developing molecular-based electronic device.

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Excited-state reversible geminate recombination in two dimensions

박기현, *김효준, 신국조

*서울대 화학부 *동아대 화학과*

Excited-state reversible geminate recombination with two different lifetimes and quenching is investigated in two dimensions. From the exact Green function in the Laplace domain, analytic expressions of two-dimensional survival and binding probabilities are obtained at short and long times. We find that a new pattern of kinetic transition occurs in two dimensions. The long-time survival probabilities show a pattern of $(\ln t)^{-1} \rightarrow$ constant $\rightarrow e^{t}$ depending on the rate constants while the binding probabilities show $t^{-1}(\ln t)^{-2} \rightarrow t^{-1} \rightarrow e^{t}$.

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Whole-process Monitoring of 10-23 Deoxyribozyme and DNA Substrate with Dual RNA

박윤희, 고혜란, *김성근

*서울대 화학부 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

Deoxyribozyme is a synthetic enzyme composed of DNA, which efficiently catalyzes reactions related to RNA/DNA cleaving, DNA ligation and modification thought to belong only to the realm of protein and RNA enzymes. In our study, we studied 10-23 deoxyribozyme which can cleave almost any RNA substrate under ion-, temperature-, and pH-dependent conditions. A particularly interesting point of this study was to demonstrate the capability for whole-process monitoring by single-molecule detection method in the form of total internal reflection fluorescence. We observed a series of processes where the target ribonucleotide located within a substrate domain was attached to the potential catalytic domain of 10-23 deoxyribozyme, followed by the separation of the catalytic and substrate domains, allowing the DNA to carry out a fully enzymatic function. Also, we were able to directly measure the RNA cleavage rate while varying temperature and Mg^{2+} ion concentration through real-time monitoring of binding between 10-23 deoxyribozyme and DNA substrate with dual RNA.

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Photoelectron Spectroscopy and *ab initio* Study of Bromochlorobenzenes

손태일, 김남두, 이상학, *김성근

*서울대 화학부 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

The properties of all three bromochlorobenzenes (BCBs) have been investigated by using photoelectron spectroscopy and ab initio calculations. Full molecular orbital calculations of neutrals and the corresponding anions have been performed by the DFT and MP2 methods. Photoelectron spectra were obtained at 355nm to identify and characterize the electron structure of anionic BCB. The electron binding energies (EBEs) of all BCB isomers were rather similar. The negative charge was found to be localized in the bromine atom and the aromatic ring for all isomeric BCB anions, indicating that the position of chlorine atom little affects the EBE of BCB isomers. Mass spectrum shows the formation of various negative ions, including Br^-, BCB^-, $[(BCB)_11(H2O)_1]^-$, $(BCB)_2^-$, and $(BCB)_3^-$. The predominance of the Br-containing clusters has been explained by simple molecular orbital theory.

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Imaging of Soft Materials with Molecular-level Spatial Resolutionby Frequency-modulation Atomic Force Microscopy

김지아, *이상학, **김성근

*서울대 화학과 *서울대 화학부 **서울대 화학부& 서울대 생물물리 및 화학생물학과*

AFM (atomic force microscopy) is widely used to obtain topographic images of molecular-level spatial resolution. However, the contact mode of AFM is difficult to apply to soft materials such as organics, polymers, and biological samples because they tend to be easily damaged or perturbed by direct contact with the AFM tip. New methods such as non-contact mode and force-modulation AFM have been developed to overcome such an obstacle. Here we introduce the frequency-modulation AFM technique based on the detection of high harmonic frequency oscillations of the AFM tip, which enhances the spatial resolution. Imaging of several soft materials was readily carried out at a molecular-level spatial resolution.

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Two Low-lying Excited States of Riboflavin Studied by Multi-photon Spectroscopy

허현, *김성근

*서울대 화학부 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

Riboflavin, known as vitamin B2, is the key structure of the redox cofactors, FAD and FMN, which play important roles in metabolic reactions. We used infrared multi-photon spectroscopy to investigate the excited state dynamics of riboflavin. In the liquid phase, the multi-photon spectra show that two low-lying excited states of riboflavin reached by photoexcitation at 368 nm and 460 nm have different relaxation processes. With the characterization of the excited states, we carried out time-resolved spectroscopy under various conditions of concentration and solvent environment.

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Interaction of Proline with Cu^{+} and Cu^{2+} Ions in the Gas Phase

이갑용, *권혁재, **송영대

*대구가톨릭대 생명화학과 *대구가톨릭대 화학과 **경운대 한방자원학부*

The structures and metal affinities of the binding configurations of Cu^{+} and Cu^{2+} to proline have been investigated using the hybrid three-parameter Density Functional Theory(DFT/B3LYP). We found that the metal-proline bonding and the energy ordering of several conformers were very different in Cu^{+}-proline and Cu^{2+}-proline. For Cu^{+}-proline, the ground state structure was found to have a bidentated coordination in which Cu^{+} was coordinated to the carbonyl oxygen and imino group nitrogen of neutral proline. On the contrary, the ground state structure of Cu^{2+}-proline involves chelation between the two oxygens of the carboxylate group in a zwitterionic proline. The metal ion affinity of proline of the most stable Cu^{+}-proline complex was calculated as 76.0kcal/mol at 6-311++G(d,p) level, whereas the Cu^{2+} ion affinity of proline was calculated as 258.5kcal/mol.

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Secondary Solvent Effect on the Excited-State Triple Proton Transfer of 7-Hydroxyquinoline along a Hydrogen-Bonded Water Chain in Ethers

박선영, 장두전

서울대 화학부

A large secondary solvent effect on the reaction rate has been experimentally observed in the excited-state tautomerization of a 7-hydroxyquinoline (7HQ) molecule complexed cyclically with two water molecules in ethers. The proton acceptance of a water molecule from the acidic enolic group of 7HQ to form a cation having the Eigen configuration is proposed to be the rate-determining step while the proton donation of the Eigen cation to the basic imino group of 7HQ is followed rapidly to complete the triple proton transfer of the 7HQ-$(water)_2$ complex in both diethyl ether and dipropyl ether without accumulating the reaction intermediate. The rate constant of the proton transfer is larger in diethyl ether than in dipropyl ether due to the more polar environment around the complex in diethyl ether. Although the activation energies of the proton transfer are similar each other in both ethers, the kinetic isotope effect of the rate constant is larger in dipropyl ether than in diethyl ether. We attribute these kinetic differences to dissimilarity in the polarities of the two secondary solvents.

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Facile Controlled Synthesis and Spectroscopy of $CdS_{1-x}Se_x$ and $(CdS)_{1-x}@(CdSe)_x$ Nanotetrapods

김미란, 장두전

서울대 화학부

High-dimensional nanostructures having great optical and electronic properties and chemical reactivities possess high possibilities in applications such as photovoltaics, single-nanoparticle transistors, electromechanical devices, and scanning probe microscopes. In particular, tetrapod-shaped semiconductor nanocrystals have attracted considerable interest in photovoltaic devices, which ideally would require a uniform film of tetrapods. We report that nanotetrapods of alloy $CdS_{1-x}Se_x$ and core-shell $(CdS)_{1-x}@(CdSe)_x$ have been fabricated facilely in aqueous solutions using ethylenediamine as a solvent-coordinating molecular template, and then their optical properties have been investigated using diverse static and time-resolved spectroscopic methods. Compared with pure CdS nanotetrapods, the photoluminescence of $CdS_{0.9}Se_{0.1}$ shifts to the red by 40 nm whereas that of the $(CdS)_{0.9}@(CdSe)_{0.1}$ does only by 5 nm. Although the mean luminescence lifetime of alloy $CdS_{1-x}Se_x$ is shorter than that of pure CdS, it is still much longer than that of core-shell $(CdS)_{1-x}@(CdSe)_x$.

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An Approach to Molecular Electronic Transport Using Bacteriorhodopsin

김종엽, 장두전

서울대 화학부

A functional protein of bacteriorhodopsin has been employed for a new approach to develop molecular single-electron transistors. A purple-membrane nanofragment loaded on gold electrodes with gap spacing of 50 nm has shown a characteristic, cyclic, and reproducible *I–V* curve having negative differential resistance and an extremely large on-off peak-to-valley ratio of 660. The abrupt changes of the electric current have been attributed to the voltage-induced oxidation-reduction and structural changes of bacteriorhodopsin. The conductance increases exponentially with temperature increase with an activation energy of 47 meV, comparable to the charging energy of a bacteriorhodopsin molecule. The Coulomb staircase is apparent at low temperature below 47 K and the interval of its onset voltages increases enormously with temperature decrease. In particular, the current at 4 K is essentially zero up to the V_T value of 13 V. The ζ value of $I \approx (V/V_T - 1)^{\zeta}$ has been found to be as large as 3.0. These indicate that the Coulomb blockade is the primary conductance-limiting feature and that charges are carried by well-defined and arrayed Coulomb islands of bacteriorhodopsin in the lipid of the purple-membrane nanofragment.

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Development of thermal lens detector using image analyzing technique

박은미, 김지웅, 최중길

연세대 화학과

A simple and rapid method has been developed to detect the thermal lens (TL) effect by utilizing the image analysis of the probe beam using a camera. The excitation beam and probe beam were coaxially irradiated into a sample solution. The generated TL effect due to the absorption of the excitation beam was obtained from the variation of image area of the probe beam. The image size was determined by counting pixels of the digitalized image at the probe beam. The frequency character of the image variation were analyzed through Fourier transformation in real time and the height of the signal peak at chopping frequency was also recorded at the same time. Sunset yellow solution was used in order to determine sensitivity of this method. The detection limit of this method was determined to be 5 x 10-9 M(S/N=3) for sunset yellow diluted in water. It strongly suggests that this particular method of the thermal lens effect is believed as a unique detector and can be applied to the remote sensing detection.

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Structural study of Ice ; As conbinations of H_2O configurations.

배태열, 최철호

경북대 화학과

In hexagonal or other ice surfaces we can easily find their conformations. Many kinds of these conformations of water dimer on the surface, as model grow up its size, its H-bond could change we think, but in these situations our purpose is to find less changable ice cluster models. It is basis on the H-bond, it is important component of the ice surfaces for compare with oter conformations.In this study we will see the some kinds of conformations and compare their H-bond.

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Isomerization and dissociation of the thiophenol molecular ion: A theoretical study

김선영, 최중철

동국대 화학과

We have explored the potential energy surface (PES) for the isomerization and dissociation of thiophenol molecular ion by quantum chemical calculations at the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) level. We obtained the minium energy pathways to form the $C_6H_6S^+$, $C_5H_6^{+\cdot}$, and $C_4H_4S^{+\cdot}$ ions by loss of H, CS, and C_2H_2, respectively. The five-, six-, and seven-membered ring structures were the intermediates in the dissociation processes. Based on the PES obtained, the dissociation kinetics will be discussed.

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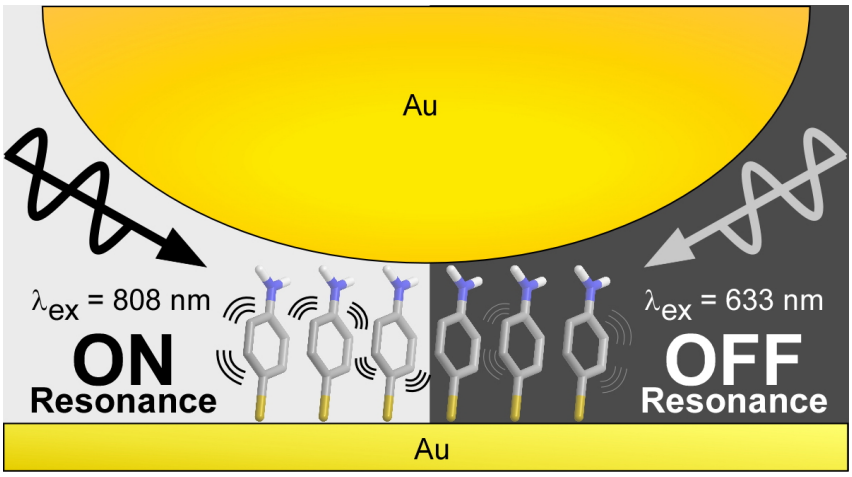
Quantitative SERS measurements for Au particle – Au film junction in on/off plasmonic resonant conditions

안성현, 김지환

고려대 화학과

A metal particle on a metallic thin film separated by a few nanometers is strongly coupled to the metallic film. This capacitive coupling is dependent on the excitation wavelength as well as their separations. The Raman active molecules adsorbed between the Au particle and Au film exhibit strong Raman enhancement. However, by varying the incident excitation wavelength, resonance condition can be turned on and off for fixed particle-film separation. The molecules in the particle-film junction exhibit different SERS intensity by turning on or off the junction resonant condition. In this work, we measure plasmonic resonance spectrum of particle-film junctions separated by ~ 1 nm. For optimized on- and off-resonance spectral region, 808 nm and 633 nm respectively, we investigate quantitative SERS intensities by changing excitation wavelength. SERS of 4-aminothiophenol between Au 100 nm particles in diameter and a thin Au film with 20 nm thickness is stronger for junction resonant condition and relatively weak for off-resonant condition.



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Development of the Femtosecond-Resolved Nano Tip Electron Microscope

정다희, *연기영, *김상규

*KAIST 화학과 *KAIST 화학과*

The novel femtosecond-resolved nano tip electron microscope system can be used to identify the reaction dynamics on surfaces, and nano-, bio-structural change on the surfaces. Also we can measure reaction mechanism on surfaces in real space of nanometer scale and real time of femtosecond scale by using pump and probe method. We produced tungsten nano tip using the electrochemical etching method. After then, this nano tip is attached on the tuning fork. We can control the distance between the nano tip and the sample using the shear force. When the oscillating tip at a resonance frequency close to its resonance frequency approaches the surface of sample, the amplitude of the oscillation is decreased. At that time the resonance frequency shifts slightly. We achieved images with nickel mesh and micro channel plate. And also, we generated electron pulses using the tungsten nano tip and femtosecond laser system.

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Size-dependent extinction characteristics of dielectric colloidal particles of high refractive indices

채원식, 최은진

한국기초과학지원연구원 강릉센터

Manipulation of dielectric colloids of high refractive indices with a broad size ranging from a few tens to a few hundred nanometers are a key to develop a variety of applications, such as assembled photonic materials, lasing media, and optical waveguides. Recently, there are several good approaches for the synthesis of dielectric colloids from solution-based systems. Among dielectric colloids of high refractive indices, in this study, we synthesized semiconductors (ZnS and PbS) and metal (Au) colloidal particles, which have a size ranging from 10nm to 1000nm, and measured optical extinction spectra for them. The resulting experimental data (products and extinction spectra) were well correlated with calculated spectra by Mie theory in a broad size range. We expect that the monodispersed and high refractive indexed dielectric colloidal materials should be quite useful for the development of novel photonic micro- and nanomaterials.

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Synthesis and characterization of $Sr_2SiO_4:Eu^{2+}$ phosphors prepared using different fluxes

Nguyen Hoang Duy, 모선일, *여인형

*아주대 에너지시스템학부 *동국대 화학과*

Light-emitting diodes (LED) with phosphor materials to generate white light have been investigated extensively because of their advantages over the existing incandescence and halogen lamps in terms of power efficiency, reliability, and long lifetime. The phosphors for LED should have strong absorption and excitation in the region from ultraviolet to blue light from LED emission. Divalent europium (Eu^{2+})-activated silicate phosphors are suitable for this purpose. In this work, $Sr_2SiO_4:Eu^{2+}$ phosphors were prepared by a solid state reaction method using different fluxes such as Li_2CO_3, LiCl, NH_4Cl in reducing environment. Morphology, crystal structure, and optical properties of the phosphors were examined by a scanning electron microscopy (SEM), a powder X-ray diffraction meter (XRD) and a spectrofluorometer. The effect of variety in flux, flux concentration and annealing temperature on the emission characteristics of the phosphors were examined and discussed. The emission spectra of $Sr_2SiO_4:Eu^{2+}$ under 330 nm excitation are shown two emission bands peaking at 490 nm and 560 nm. The origin of the two emission bands are studied.

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Theoretical Studies on the Effects of Meta-Substituents in the Aromatic Nucleophilic Substitution Reactions of Halopyridine, Halopyrimidine and Halotrizine with halide anions.

한인숙, 김창곤, 김찬경, *이본수, 이해황

*인하대 화학과 *인하대 총장실*

The effects of meta-substituents in the aromatic nucleophilic substitutions (S_NAr) for C_6H_5X, C_5H_4NX, $C_4H_3N_2X$ and $C_3H_2N_3X$ (X = F, Cl and Br) with halide anions have been studied theoretically at MP2 and B3LYP level of theory in the gas phase. For reactions with F^-, the S_NAr reactions proceed via a multistep mechanism with the formation of a σ-complex intermediate. On the contrary, for reactions of with Cl^- and Br^-, the S_NAr reactions proceed via a concerted mechanism without a formation of any stable σ-complex. The effects of meta-substituents are predicted to be considerably higher in energy as compared to those of ortho- and para-substitutents. All the stationary point species have been fully optimized and characterized by frequency calculations at MP2(FC) level with 6-31+G(d) and at B3LYP level with 6-311+G*, 6-311+G(2d,p) basis sets. In order to obtain more accurate energetics, the sophisticated calculations at G3(X=F, Cl) and G2(X=Br) levels on the geometries at the MP2 level have been carried out. All the calculations have been performed by using the Gaussian-03 program.

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Molecular Modeling Studies: Enantioselectivity of Candida Antarctica Lipase B for Lactate Isomers

이주민, 장락우

광운대 화학과

Polylactic acid or polylactide (PLA) is a biodegradable, thermoplastic, aliphatic polyester. Many studies for its synthesis and application have recently been carried out as a candidate for green chemistry. The mechanical and thermodynamic properties of PLA such as melting temperature mainly depend on its tacticity. Since syntactic PLA such as PLLA and PDLA are difficult to obtain by conventional chemical catalysts with harsh reaction conditions, there have been some attempts to accomplish their synthesis by using modified enzymes. In this study, we are trying to guide this enzyme engineering by molecular modeling such as molecular dynamics simulations and docking simulations.A lipase is a water-soluble enzyme that catalyzes the hydrolysis of ester bonds. One of the lipases, Candida Antarctica lipase B (CALB), which catalyzes the trans-esterification reaction in organic solvent, is found to have enantioselectivity toward the dimerization reaction (lactide formation) of lactates in organic solvents: CALB only catalyzes the dimerization of D-lactate.It has been generally believed that the enantioselectivity of CALB results from the free energy difference between enantiomers in the transition state of enzyme-substrate complex formation. However, we experimentally found that the hydrolysis reaction of methyl lactate enantiomers catalyzed by CALB shows no difference between enantiomers, which implies that the activation free energy difference is not a key factor for the enantioselectivity of CALB. Furthermore, molecular dynamics simulations and docking simulations of atomistic models of enzyme-lactate complexes have confirmed that the enzyme-L-lactate complex hides the reaction center for the dimerization reaction from the open pocket so that the nucleophilic attack of the second L-lactate is blocked. It implies that L-lactate can act as an irreversible competitive inhibitor for the dimerization reaction of D-lactate.

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TiO_2/CdS and ZnO/CdS Core/Shell Nanocable Arrays for Efficient Solar Energy Conversion

명윤, 성태광, 조용재, 김한성, 손용재, 박정희

고려대 소재화학과

High-density TiO_2/CdS and ZnO/CdS core/shell nanocable array were synthesized on large-area Ti substrates. The CdS outerlayers were uniformly deposited on the pre-grown vertically-aligned TiO_2 (rutile) and ZnO nanowire array, using vapor transport method. The thickness of the CdS shell was controlled in the range of 10-50 nm using the deposition time. The CdS outerlayers consisted of a number of single-crystalline domains whose wurtzite [001] direction aligned along the wire axis, irrespective to TiO_2 or ZnO core. The structural and optical properties were analyzed by XRD, XPS, XANES, UV-visible absorption, PL, and Raman spectroscopy, showing that the defects at the interface would influence less the exciton generation for the thicker CdS outerlayers. The thicker CdS outerlayer results in a higher value of photocurrent and photoelectrochemical cell efficiency. As the thickness of CdS shell in the CdS/TiO_2 and ZnO core/shell nancables increases to 50 nm, the conversion efficiency reaches to 2.7 and 4.3%, respectively.

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Synthesis of Visible Light-Sensitive ZnO Nanoplates: Optical Properties and Photocatalytic Activities

이주란, 박진형, 윤민중

충남대 화학과

Single crystalline ZnO nanoplates were synthesized by hydrothermal reaction with liposome-ZnO nanocomposites, and they were characterized to be hexagonal wurtzite structure by measurements of XRD patterns, SEM and TEM images. The UV-Visible absorption spectrum of the nanoplates was observed to exhibit a very high absorption of visible light at longer wavelengths than 400nm. Enhancement in optical absorption of ZnO nanoplates indicates that it can be used as an efficient photocatalyst under visible light irradiation. Therefore these results suggest that the present ZnO nanoplates will be a promising nanomaterial for future photoelectronic devices and solar cell.

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Immunoassay Using Surface-Enhanced Raman Scattering

윤경진, 서형균, 정영미

강원대 화학과

Surface-enhanced Raman scattering (SERS) has proved to be a very effective analytical tool due to its high sensitivity, high selectivity, and fluorescence-quenching properties. SERS has been widely used for ultrasensitive chemical analysis down to single molecule detection, and it expands its realm of applications from chemical-biochemical analysis to nanostructure characterization and biomedical applications. In this study, colloidal silver and gold nanoparticles were prepared by reducing silver nitrate with hydroxylamine hydrochloride and by reducing gold chloride hydrate with trisodium salt dehydrate, respectively. These particles have excellent optical properties for a sensitive detection of Prostate-Specific Antigen (PSA) as a biomarker. Highly sensitive immuno-analysis of those complexes was performed using SERS. In this presentation, immunoassay techniques based on the SERS will be discussed.

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Characterization of Formation for Surface Film on the Cathode of Li-Ion Battery

박연주, 김남훈, *최현철, 정영미

*강원대 화학과 *전남대 화학과*

Li-ion batteries are widely used as competitive in many portable devices. However, Li-ion batteries have safety problems, such as explosion. Especially overcharged cathode or anode has been studied most extensively, but the overcharge mechanism is still not clear.To study the formation of surface film (SEI) on the overcharged cathode, we have applied 2D correlation spectroscopy to the IR and XPS (X-ray photoelectron spectroscopy) spectra of Li-ion battery. In this presentation, the overcharge mechanism of cathode of Li-ion battery will be discussed in more detail.

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Characterization of Raman Optical Activity Spectra of pH-dependent Bovine α-lactalbumin

유수련, *Boguslawa Czarnik-Matusewicz, 정영미

*강원대 화학과 *Faculty of Chemistry, University of Wroclaw*

Raman optical activity (ROA) measures vibrational optical activity by means of a small difference in the intensity of Raman scattering from chiral molecules in right and left circularly polarized incident laser light. Proteins in aqueous solution are now accessible to ROA measurements, which provide an incisive new probe of secondary and tertiary structure. Two-dimensional (2D) correlation spectroscopy has attracted a high level of interest of analytical science community, as it provides considerable utility and benefit in many fields of spectroscopic studies. In this study, we have applied 2D correlation spectroscopy to Raman and ROA spectra of the pH-dependent bovine α-lactalbumin to investigate the molten globule state. The details of molten globule state of bovine α-lactalbumin will be discussed.

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Combined theoretical modeling of photoexcitation spectrum of an isolated protonated tyrosine

권장숙, 최창민, 김남준, *장준경, 양민오

*충북대 화학과 *부산대 나노정보소재공학과*

A photodepletion spectrum of gaseous protonated tyrosine molecules was obtained at 150 K by a UV laser spectroscopic technique in conjunction with mass spectrometry and interpreted by theoretical methods. The spectrum exhibits three distinct bands separated each other by about 800 cm-1. Stable conformers of the molecular ion were determined by quantum mechanical density functional theory, and their electronic transition energies were obtained by a semiempirical quantum chemistry calculation. The whole pattern of the spectrum was reasonably reproduced by a combination of theoretical methods, the second-order cumulant expansion, a semiempirical quantum chemistry method, molecular dynamics simulation, and a semiclassical timecorrelation function approach. The three spectral bands turned out to arise from the vibronic transition of two vibrational modes constituted by the “benzene breathing” mode and a torsional mode of the amino acid backbone. It is suggested that the major factor in spectral broadening is not conformational disorder or lifetime broadening but thermal fluctuation of the stable conformers. The good agreement between experimental and theoretical spectra exemplifies the validity of the theoretical methods applied for the present molecular system.

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Gas-phase Sequencing of DNA Aptamer by Infrared Multiphoton Dissociation: Interactions of Thrombin-Binding Aptamer with Dicationic Organic Ligands

홍은선, 윤혜주, 신승구

포항공과대 화학과

We investigated interactions of dicationic organic ligands, such as methyl viologen (MV), DAPI, and berenil, with thrombin-binding aptamer [TBA, d(GGTTGGTGTGGTTGG)] in the gas phase using Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. TBA–ligand complexes were generated by electrospray ionization (ESI) and the 4– charge states were selected for gas phase sequencing by infrared multiphoton dissociation (IRMPD). The 1:1 TBA–MV complex, both 1:1 and 1:2 TBA–DAPI complexe, and both 1:1 and 1:2 TBA–berenil complex were detected. The binding constants of the TBA–ligand complexes were determined using ESI-MS. The binding sites of ligand to TBA were determined from the IRMPD fragmentation pattern, while the binding motif was identified by circular dichroism (CD) in solution. All dicationic organic ligands bind to the central TGT loop of TBA. All dicationic organic ligands suppress the CD amplitude of isopropanol-induced G-qaudruplex (G4) of TBA. It appears that dicationic organic ligands disturb the G4 structure of TBA by binding to the central TGT loop of G4 as shown by the IRMPD sequencing.

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Relative Stabilities of Tetracationic Porphyrin–Fullerene Complexes in the Gas Phase

정성한, 신승구

포항공과대 화학과

Relative stabilities of cationic porphyrin–fullerene complexes were studied in the gas phase by collision-induced dissociation (CID) with Xe. Tetracationic porphyrin ions with charged substituents in the *meso*-positions and their complexes with C_{60} and C_{70} were produced by electrospray ionization. The total charge states of porphyrin ions were determined by the number of counter anions (*p*-toluenesulfonate) attached. Doubly-, triply-, and quadruply-charged porphyrin ions yielded 1:1 complexes with fullerenes. Collisional activation of 1:1 porphyrin–fullerene complexes led exclusively to loss of fullerene. The dissociation yield measured as a function of collision energy was used to determine the center-of-mass collision energy at 50 % dissociation ($E_{50\%}$). $E_{50\%}$ Values were used to compare the relative stabilities of cationic porphyrin–fullerene complexes. Porphyrin ions bound C_{70} more strongly than C_{60}. For the same porphyrin, more stable complexes were formed with higher charge states due to the ion–induced dipole interaction. In addition, the location of charge and steric hindrance also influence the interaction between porphyrin and fullerene. As the charges are closer to the center of porphyrin, fullerene binds to porphyrin more strongly. However, steric hindrance caused by substituent exerts repulsive interaction between porphyrin and fullerene.

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The effect of surface treatment on ethylene bridged silsesquioxane thin films for gate insulator

이덕희, 정현담

전남대 화학과

Ethylene bridged silsesquioxane copolymers were prepared by using sol-gel process. 1,2bis(trimethoxy-silyl)ethane and methyltrimethoxysilane monomers were hydrolyzed by a diluted HCl solutions in anhydrous THF solvent. The diluted HCl solutions were prepared in each other ratio of [HCl]/[-OR] and [H_2O]/[-OR]. Ethylene bridged silsesquioxane copolymer resins obtained by using above procedure have the difference in mole ratio of [Si-OH], [Si-CH_2CH_2-Si], and [Si-OCH_3]. Molecular structures of resins were investigated by using nuclear magnetic resonance (NMR) and Fourier transform infrared (FT-IR) spectroscopy.Thin films were fabricated by spin – coating the above resins on Si-wafer followed by curing at 150°C for 30 minutes on hot plate. The result films were divided in to two portions. Ones were further treated with HMDS. MIS (metal – insulator – semiconductor), MIM (metal – insulator – metal), OTFT (organic – thin film transistor) devices in which silsesquioxane copolymer resins used as insulator layer and P3HT (poly – 3- hexylthiophene) as organic semiconductor were prepared employing thermal evaporator equipment in order to investigate the effects of resin compositions and HMDS layer on electrical properties and mobility of ethylene bridged silsesquioxane.

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Synthesis and dispersion of Dendrimer-Encapsulated Pt nanoparticles on gamma Al_2O_3 and MgO-Al_2O_3

Pullur Anil Kumar, 배현숙, *유창용, **이경주, 하헌필

*KIST 기능금속연구센터 *부경대 재료공학과 **고려대 화공생명공학과*

Dendrimer encapsulated Pt nanoparticles were prepared by using hydroxyl terminated generation four (G4OH) PAMAM dendrimers as the templating agents. The resulting Pt nanoparticles were dispersed on gamma Al_2O_3 and MgO-Al_2O_3 at room temperature by impregnation. Pt/Al_2O_3 and Pt/MgO-Al_2O_3 catalysts were subjected to thermal treatments in oxidizing and reducing atmospheres from room temperature to 500 ℃. These prepared and dispersed Pt nanoparticles were characterized by Transmission Electron microscopy (TEM), XRD, TPR and in-situ FTIR. The resulting Pt nanoparticles size was analyzed from TEM analysis which shows in 2 to 4 nm range. It is obvious to observe an increase in Pt particles size upon thermal decomposition of the dendrimer. The in-situ FTIR results suggest that the presence of oxygen in the gas phase and the Pt particles in the Pt-dendrimer nanocomposite accelerate the dendrimer decomposition from low temperatures.

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Surface-enhanced Raman Spectroscopy of benzimidazolic fungicides: benzimidazole and thiabendazole

김막순, 김민경, 김희진, *이철재, **정영미, 이무상

*경북대 화학교육과 *영남이공대학 화장품화공계열 **강원대 화학과*

Surface-enhanced Raman Scattering (SERS) spectroscopy is applied to the study of the adsorption of benzoimidazolic fungicides benzimidazole(BIZ) and thiabendazole(TBZ) on silver mirrors. The influence of pH on the adsorption mechanism was investigated. In case of BIZ, two different adsorption mechanisms are deduced depending on the experimental conditions: via the π electrons of the ring in neutral conditions and through an ionic pairing of protonated nitrogen atom with the chloride adsorbed on the metal surface. The SERS spectra of TBZ revealed that most molecules were adsorbed on silver surface by the π electrons in neutral and acidic conditions but in acid conditions, some molecules were adsorbed via the sulfur and nitrogen atoms tilted slightly to the surface.

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Measurement of Nanoscale gap by Förster Resonance Energy Transfer

김원정, 김용욱, 서민수, 임성준, 윤혜주, 신승구

포항공과대 화학과

Förster resonance energy transfer (FRET) between Cy5 and TAMRA was measured using near-field scanning optical microscopy (NSOM). Cy5 was immobilized on an NSOM tip and TAMRA was immobilized on a glass substrate. FRET was monitored while drawing the Cy5 tip closer to the TAMRA substrate in nanometer steps. Both the fluorescence spectra and fluorescence decay were recorded simultaneously. FRET between TAMRA and Cy5 allows the measurement of nanoscale gap between the tip and substrate as well as the effective FRET radius of TAMRA-Cy5 pair. The present methodology enables the absolute distance measurement of a sub-10 nm scale gap without physical contact.

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Preparation and Luminescence Properties of HPPC derivatives

이효성, 강준길

충남대 화학과

Some derivatives of HPPC (4-Hydroxy-5-phenylpyrido[3,2,1-*jk*]carbazol-6-one) were prepared by the esterification of OH with carbonyl compounds and their optical properties were investigated in solution and solid states. Carbonyl compounds used in this study were acetyl chloride, benzoyl chloride, naphthoyl chloride, furoyl chloride, and thiophenecarbonyl chloride. The derivatives excited at UV produced markedly enhanced blue-luminescence, compared with that of HPPC. In this presentation, the luminescence properties of the derivatives will be precisely discussed.

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Local Field Calculation on Layer-by-layer Close-packed Gold Nanoparticles

김성규, 오민경, 박성호

성균관대 화학과

The close-packed gold nanoparticle film is unique in that the surface enhanced Raman scattering (SERS) signal is dependent not only on the packed nanoparticles and but also on the 3-dimensional layer structure. To understand the observed phenomena, computation approaches, the finite difference time domain (FDTD) method and the discrete dipole approximation (DDA), were taken to investigate the local field distribution in the film. High local electric fields were found at small interstices among neighboring nanoparticles. In general, the sum of the local field intensities of the so-called 'hot spots' in a layer was greater in the nanorod assemblies than in the nanosphere assemblies. High local electric fields, polarized along the light propagation direction, were found at interlayers of the nanorod assemblies, while they were small in the nanosphere assemblies. These results are in accord with the SERS results and can be explained mostly by larger contact area in the NR assemblies than in the NS assemblies. However, the calculated layer-by-layer local field distribution was not good enough to explain the SERS intensity variation with the number of layers. We will discuss implications of the mismatch and possible limitations of the computation.

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Structures and electronic spectra of CdSe – Adenine complexes:DFT study of a model DNA-coated nanocluster

김호성

경희대 화학과

We present DFT and TD-DFT study of the structures and electronic spectra of small CdSenanocluster-adenine complexes CdnSen – Ade (n = 3, 6, 10, 13). We examine the changes inthe geometries and excitation spectra of the nanoclusters induced by DNA base-binding. Bycomparing the results calculated for the bare (CdnSen), hydrogen-passivated (CdnSenH2n), aswell as the corresponding Ade-bound clusters (CdnSen – Ade, CdnSenH2n – Ade, CdnSenH2n-2– Ade), we find that binding with Ade slightly blue-shifts (up to 0.18 eV) the electronicexcitations of bare nanoclusters, but strongly red-shifts (< 1.2 eV) those of hydrogenpassivatednanoclusters. Natural bond orbital analysis shows that the LUMO of CdnSenH2n – Ade is a π^* orbital located on the purine ring. The large red-shift in the excitation energiesof CdnSenH2n – Ade is therefore caused by the introduction of particle traps by the nucleicacid.

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Expression, Purification, and NMR Structural Studies of Transmembrane Peptide, Syndecan-4

이민혜, 박태준, 김용애

한국외국어대 화학과

Syndecan-4 is a transmembrane heparan sulfate proteoglycan belonging to the syndecan family and they are present on most cell types. Syndecan-4 is known to bind to various molecules, such as basic fibroblast growth factor, midkine, and tissue factor pathway, via its heparan sulfate chain, and is thought to play many biological roles through its binding bio-mediators. To get better understand the mechanism and function of Syndecan-4, it is critical to elucidate the three-dimensional structure of it. Unfortunately, Syndecan-4 is membrane-bound protein that transverse the lipid bilayer of the cell membrane, so large-scale production of such integral membrane proteins has been limited by experimental adversities due to insufficient yields and low solubility of protein. And also it is hard to characterize the membrane-bound three-dimensional structure using conventional solution NMR and X-ray crystallography. In this study, we demonstrate the successful high level expression and purification of Syndecan-4 transmembrane domain to facilitate structural studies in complex with membrane environments by solid-state NMR spectroscopy. And we also present the solution NMR structural studies of Syndecan-4 in lipid micelle.

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The Detailed Kinetic Studies of Competing Multiple-Barrier Unimolecular Dissociations of Chlorotoluene Radical Cations

서종철, *서현일, *김승준, 신승구

*포항공과대 화학과 *한남대 화학과*

Most unimolecular reactions involve a number of intermediates interconnected through multiple barriers. These multiple-barrier reactions cannot be described by a simple kinetic model assuming the steady-state approximation. To better understand the kinetics of multiple-barrier reactions, we need to evaluate the temporal variations of intermediates in terms of population and internal energy distribution using the time-dependent master equation. In the present work, we apply the time-dependent master equation to study unimolecular dissociations of *o*-, *m*-, and *p*-chlorotoluene radical cations. The overall dissociation rates are evaluated based on molecular parameters and potential energy surface provided by density functional theory (DFT) calculation. By time-dependent kinetic simulation, the predominant long-live intermediates are identified and the internal energy distributions of products (benzyl cation or tropylium ion) are derived.

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Synthesis of Visible Light-Responsive Titanate Nanorods: Optical and Photophysical Properties

배은주, 윤민중

충남대 화학과

Titanate nanorods were synthesized by the hydrothermal processing in NaOH solutions. The structure of as-synthesized titanate nanorods were characterized by measuring x-ray diffraction (XRD) patterns, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images. These results proved that it has monoclinic single crystal structures and shapes of nanorods. The UV-visible reflectance absorption spectra of the titanate nanorods were observed to have low band gap energy (3.04eV), exhibiting surface absorption band in the visible range from 400 to 700nm. Visible light-induced photophysical properties of the titanate nanorods were investigated by measuring photoluminescence (PL) spectra properties.

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Synthesis of Visible Light-Responsive TiO_2 Nanopearls: Optical and Photocatalytic Activities

박진형, 배은주, 윤민중

충남대 화학과

TiO_2 nanopearls were synthesized by the hydrothermal processing in HCl solutions. The structure of as-synthesized TiO_2 nanopearls were characterized by measuring x-ray diffraction (XRD) patterns, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images. These results proved that it has anatase structures and shapes of nanopearls. The UV-visible reflectance absorption spectra of the TiO_2 nanopearls were observed to have low band gap energy (3.04eV), exhibiting surface absorption band in the visible range from 400 to 600nm. The visible light-induced photocatalytic activities of the TiO_2 nanopearls were investigated by measuring photodecomposition of methyl orange, which were found to be very efficient as compared with any other conventional visible-light responsive TiO_2 nanomaterials.

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Preparation and photocatalytic properties of TiO2@ HCC nanoparticles

정용광, 강준길

충남대 화학과

Hollow carbon capsule (HCC) nanoparticles were prepared from non-mesoporous silica template through polymerization and carbonization. The surface of the prepared HCC nanoparticles were coated by TiO2 via the hydrolysis and condensation of TiCl4 in aqueous or mixed-solvent solution. The morphology, crystal structure and optical properties of TiO2@HCC were characterized by XRD, SEM, UV-absorption, reflectance and photoluminescence techniques. It was found that the morphology and crystal structure of TiO2 were dependent on surface area of HCC nanoparticle, pH of the precursor solution and temperature of calcination. Under visible light illumination, the photocatalytic activity of TiO2@HCC was investigated by observing the photocatalytic degradation rates of methyl orange and xanthenes

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Wavepacket Dynamics of NH_3Cl

박영춘, 최희철, *백경구, 이윤섭

*KAIST 화학과 *강릉대 화학과*

Ammonium chloride(NH_3Cl) is one of famous examples which have charge transfer state. In electron photodetachment of NH_3Cl, anion is excited to two netral states. Lower neutral state is 4.0 eV above from the anion, and upper neutral state is charge transfer state which is 6.45 eV above. In this poster, dissociation of neutral NH_3Cl is disscussed. Initial nuclear wavepacket of ground anion is vertically excited to charge transfer state. For the nonadiabatic dynamics of wavepacket, two adiabatic potential energy surfaces(PES) are diabatized from the unitary transformation. Quantum dynamic simulation shows most of upper state are transfered to lower dissociation state. However, some portion of upper state still remain in tens of femtoseconds. In lower state PES, two different dissociation occur (NH_3+Cl and NH_2+HCl) from the wavepacket motion. Product ratios are analyzed in each time step. For the influences of different initial wavepacket, several vibrational wavepackets were prepared by Fourier grid hamiltionian (FGH) method. Different vibrational states affect dissociation procedures as well as final branching ratios.

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Novel Fabrication of Au/Ag Bimetallic Thin Films on Glass for Efficient SERS Substrates

심세운, 이상아, 김지훈, 신권수, *김관

*숭실대 화학과 *서울대 화학부*

Noble metallic nanostructures exhibit a phenomenon known as surface-enhanced Raman scattering (SERS) in which the Raman scattering cross-sections are dramatically enhanced for the molecules adsorbed on thereon. In this investigation, Au/Ag bimetallic thin films on glass were successfully produced via galvanic reaction between the surface Ag atoms and AuCl4– ions. A two-step procedure was used to produce Au/Ag films on glass. Firstly, Ag film was formed on glass by soaking a glass substrate in ethanolic solution of AgNO3 and butylamine, and then as-prepared Ag-coated glass substrates were subsequently subjected to the galvanic reaction with HAuCl4. The Au/Ag bimetallic films thus prepared were characterized in terms of the optical property and SERS activity depending on the conditions of galvanic reaction.

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Superhydrophobic Single-walled Carbon Nanotube Networks grown on Texturing Si Surfaces

이재승, 이동환, 이종택, 이휘건

한양대 화학과

Single-walled Carbon Nanotube Networks grown on Texturing Si surfaces are Superhydrophobic as the hierarchical structures created by nanostructures on microstructures. Their liquid–solid wetting behaviors with both a large contact angle and small sliding angle are contributed on the cooperation of micro- and nanostructures as the lotus effect and also interestingly on the induction Electric field. The electric field changes the wetting property from the immobile water droplet to the mobile water droplet on the surfaces. In conclusion, the combined effects of the geometrical roughness and electrical potential create the increase of the contact angle and the decrease of sliding angle as superhydrophobic surface.

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A quantum chemical perspective on the CO_2 removal using metal-organic frameworks

박지영, *정유성, 이윤섭

*KAIST 화학과 *KAIST EEWS 대학원*

Direct removal of CO_2 from the flue exhaust of cars and power plants before its reaching the atmosphere can be an effective way of addressing the global climate changes that can be applied immediately. One of the methods to achieve the latter goal is to chemisorb/physisorb CO_2 reversibly onto the highly porous materials by tuning the chemical interactions between CO_2 and the building blocks of the materials. Here, we explore various possibilities and aspects of using Metal organic framework (MOF), a highly porous, thermally and chemically stable material, to capture CO_2 at room temperatures using quantum chemical calculations.

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Conformational analysis of trimannoside and bisected trimannoside using aqueous molecular dynamics simulations

김현명, 정갑주, *정선호

*건국대 신기술융합과 *건국대 특성화학부 생명공학과*

The conformational properties of oligosaccharides are important to understand carbohydrate-protein interactions. A trimannoside, methyl 3,6-di-O-(α-D-Man)-α-D-Man (TRIMAN) is a basic unit of N-linked oligosaccharides. This TRIMAN moiety was further modified by GlcNAc (BISECT), which is important to biological activity of N-glycan. To characterize the trimannoside and its bisecting one we performed a molecular dynamics (MD) simulation in water. The resulting models show the conformational transition with two major and minor conformations. The major conformational transition results from the ω angle transition; another minor transition is due to the ψ angle transition of α(1→6) linkage. The introduction of bisecting GlcNAc on TRIMAN made the different population of the major and minor conformations of the TRIMAN moiety. Omega (ω) angle distribution is largely changed and the population of *gt* conformation is increased in BISECT oligosaccharide. The inter-residue hydrogen bonds and water bridges via bisecting GlcNAc residue make alterations on the local and overall conformation of TRIMAN moiety. These changes of conformational distribution for TRIMAN moiety can affect the overall conformation of N-glycan and the biological activity of glycoprotein.

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Structures and electronic spectra of CdSe-Cys complexes : Canonical vs. zwitterionic Cys

김주영, *이성렬

*경희대 일반대학원 화학과 *경희대 화학과*

DFT 와 TD-DFT 를 사용하여 CdSe nanocluster, Cys, 물 복합체 Cd_nSe_n-Cys-$(H_2O)_m$ 및 $Cd_nSe_nH_{2n}$-Cys-$(H_2O)_m$ (n=10,13, m=0,1)의 구조와 전자흡수 스펙트럼을 계산하였다. $Cd_{10}Se_{10}H_{20}$ 에서는 Cys 의 Zwitterionic(Z) 형태가 Canonical(C) 보다 에너지적으로 조금 더(1~4kcal/mol) 높았다. $Cd_{13}Se_{13}H_{26}$ 에서는 이 경향이 역전되어 Z 형태가 C conformer 보다 약 3kcal/mol 정도 낮아졌다. 또한 물 분자가 Cys 주변에 있을 경우 Z 형태가 더 안정화 되어 C 형태와의 에너지 차이가 약 3.4 kcal/mol 정도로 증가한다. 이러한 결과로 보아, CdSe nanocluster 및 용매가 Cys 의 Zwitterion 을 안정화하며, 수백 개의 Cd 및 Se 를 가진, 실험적으로 합성되는 용매 중의 CdSe - Cys 에서 Cys 는 Zwitterion 일 것으로 예측된다. 한편, $Cd_nSe_nH_{2n}$-Cys-$(H_2O)_m$, $Cd_nSe_nH_{2n-1}$-Cys-$(H_2O)_m$ (n=10,13, m=0,1) 등, 수소로 리간드화 된 CdSe 의 전자흡수스펙트럼에서, Z cys 가 CdSe 에 결합될 경우, 흡수파장의 red-shift 정도가 C cys 에 비하여 약 < 0.11 eV 정도 더 작은 것으로 나타났다. Z cys 가 수소로 리간드화 되어 있지 않은 CdSe cluster 와 결합할 경우 C 형태보다 blue shift 의 크기가 더 작게 (< 0.34ev) 나타났다.

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Surface enhanced Raman scattering of graphene on gold film substrates

김나영, 오민경, 이충선, 김성규, 홍병희, 박성호

성균관대 화학과

Nayoung Kim, Minkyung Oh, Chung Sun Lee, Seong Kyu Kim*, Sungho Park and Byung Hee Hong*Department of Chemistry, Sungkyunkwan University, Suwon 440-746, Korea*E-mail : byunghee@skku.edu, skkim@skku.eduWe applied surface enhanced Raman scattering (SERS) to a single layer graphene placed on or between various gold film substrates. The SERS substrate is a single or a double layer of either a flat gold film produced by a thermal evaporation or a close-packed gold nanoparticle film. In general, the Raman scattering signal was enhanced on most of the SERS substrates. However, the details of the Raman spectra varied with the layer composition or the excitation laser wavelength; in a few SERS substrates, a broad background emission showed up, the D and G bands were distorted or split, and new vibrational peaks appeared. We will discuss the implications of the observations.

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The Effect of Substrate Dynamics Near Active Site on the Reaction Rate of Acetylcholinesterase

이상윤, *김지현, *이상엽

*서울대 자연과학대학 화학부 *서울대 화학부*

Acetylcholinesterase catalyzes acetylcholine hydrolysis reaction which extinguishes a neuronal signal after the signal transmission at the synapse. This enzyme reaction is so fast that its kinetic belongs to the diffusion controlled regime, which means the rate-determining step is at the stage that the substrate gets close to the active site of the enzyme. (overall reaction rate (kcat/kM) ~ $7X10^7$ /M·sec) The size of substrate is not small enough to pass the narrow enterance(gorge) of active site smoothly and it makes the high energy barrier. It can be inferred that not only substrate's diffusional encounter from bulk to the gorge, but also its dynamics in the gorge influence the overall reaction rate of the enzyme. It was not evaluated correctly in the previous studies, and it can clarify the reason that the predicted rates in the previous studies were commonly overestimated by one or two orders of magnitude. The potential of mean force of enzyme substrate complexm, and the substrate's diffusion coefficient along the reaction coordinate were measured by molecular dynamics simulation using the program CHARMM.

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Characterization of Hydrophobic and Hydrophilic membrane using Portable membrane introduction mass spectrometer

박민정, 김태규

부산대 화학과

We have developed a sheet-membrane interfaced portable time-of-flight mass spectrometer with an electron impact ionization source. It has several advantages that include high sensitivity, simplicity, low cost, rapid analysis, in-situ monitoring, and ease of operation. Selective transport of volatile organic compounds in air into a time-of-flight mass spectrometer through a hydrophobic polydimethylsiloxane(PDMS) membrane was measured and monitored. The detection limits for the volatile organic compounds(VOCs) studied were determined to be 0.2~10 ppm, which have a dynamic range of over three order of magnitude. The total analysis of sample takes less than 1 minute. Unlike the PDMS membrane, a hydrophilic Nafion membrane allows to transport the hydrophilic compounds. We have monitored the behavior of the Nafion membrane for the analysis of low molecular weight alcohols. The permeability of hydrophilic compounds was converted to diffusion coefficients. The transport process of analyte through the membrane can be described by using non-steady state permeation equation. These results indicate that not only hydrophobic compounds but also hydrophilic compounds can be detected by portable membrane inlet mass spectrometer. The sheet-membrane interfaced time-of-flight mass spectrometer can be applicable to various fields, such as monitoring of environmental, biological and chemical processes.

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Relativistic effect and electron correlation in Kramers restricted, and spin-orbit configuration interaction methods: Ground state calculations

김인구, 박영춘, 이윤섭

KAIST 화학과

A comparison of Kramers restricted and spin-orbit configuration interaction (KRCI and SOCI) with regard to spin-orbit coupling and electron correlation for both closed- and open-shell systems is presented. Two-component calculation incorporating relativistic effective core potential is employed. We give the ground state energy and equilibrium bond distance for each CI wavefunction with different exctations and discuss a convergence to *full*-CI analogues. The studied systems include TlH as a closed-shell system, and PbH radical as a open-shell system. Each system is further investigated with differing spin-orbit coupling strength by a manipulation of the potential parameters.

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Photoionization dynamics of the photofragment atomic chromium from bis(eta-6-benzene)chromium

이정묵, 안두식, 김상규

KAIST 화학과

Bis(eta-6-benzene)chromium, one of the commonest sandwich organometallic molecule, is dissociated to cold excited atomic chromiums by UV photons. We studied the photoionization of fragment chromium with photoelectron imaging technique in the range of 366~383nm. The kinetic energy and angular distributions of photoelectron from photofragmented atomic chromium are obtained and analyzed from measured photoelectron images. The remarkable changes are found in terms of photoelectron kinetic energy and angular distribution which depend on both ionization channels of the excited atomic chromium and photodissociation dynamics of bis(eta-6-benzene)chromium.

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Experimental and Theoretical Investigations of the photodissociation dynamics of Substituted Thioanisoles

윤준호, *김상규

*KAIST 화학 *KAIST 화학과*

We compare recoil energy distributions and anisotropy parameters(β) of thioanisole(TA) and substituted analogs[4-XTA, X=F (1) and CH3 (2)] at the para position using ion velocity map imaging. Energy gap between the Ã and X state of XC6H4S radical which is essential for so-called intramolecular orbital alignment is determined theoretically and experimentally. The X/Ã branching ratio is also estimated from the total translational energy distribution to find the energetic location of the S1/S2 conical intersection (CI). It shows chemical substitution at the para position of TA significantly changes the dynamics in the vicinity of the CI. We will describe potential energy surface (PES) of reduced dimensionality using the complete active space self-consistent field (CASSCF(12,11)/6-31G**) method to explain the photodissociation dynamics of substituted thioanisoles. We plan the adaptation of the complete active space second-order perturbation theory (CASPT2) in order to reveal a coupling mode at the CI.

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Direct Observation of Transient Ligand-Field Changes in Transition Metal Complexes via Time-Resolved Soft X-ray Spectroscopy

조하나, 홍기룡, 김태규

부산대 화학과

Here we report the first time-resolved soft x-ray spectroscopy of electron and spin dynamics in solvated molecules. We observe changes in ligand-field splitting, spin-state and orbital populations, and electron delocalization in the studied Fe^{2+} spin-crossover complex by probing photo-initiated transient absorption changes of the iron $L_{2,3}$-edges. The large shift of the $L_{2,3}$-edges to lower energies upon spin crossover is not only caused by a reduction in ligand-field splitting and changes Fe-3d orbital occupancy but necessitates a strong reduction in Fe-3d electron interaction with the π-electron system of the ligands. Upon spin crossover, the ligand-field splitting reduces by more than 1 eV while the iron 3d metal character increases through changes in metal-ligand orbital covalency with indications for spin-orbit quenching in the high-spin state. Our time-resolved measurements directly capture the transients valence-orbital structure in a solvated system, offering future opportunities to investigate important classes of transition metal compounds such as protein co-factors (e.g. metalloporphyrins in Myoglobin and Hemoglobin) or mixed-valence compounds, and more generally the solvent influence on ultrafast dynamics of electronic and spin states.

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Ion-Molecule Reaction Dynamics of $Fe^+(C_2H_5OC_2H_5)_n$ Heteroclusters

폴다바브라타, 홍기룡, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

The ion-molecule reaction dynamics that occur inside $Fe^+(C_2H_5OC_2H_5)_n$ heterocluster ions were investigated using a laser ablation-molecular beam/reflectron time-of-flight mass spectrometer. The mass spectra show major sequences of cluster ions with the formula $Fe^+(C_2H_5OH)(C_2H_5OC_2H_5)_n$ and $Fe^+(C_2H_5O)(C_2H_5OC_2H_5)_n$ which are mainly attributed to bond insertions of Fe^+ into the C-O bond of diethylether molecule within the heteroclusters. The observation of $Fe^+(CH_3CHO)(C_2H_5OC_2H_5)_n$ ions is attributed to the insertions of Fe^+ ions into the C-O bond in the diethylether molecules, leading to a β-H atom transfer and C_2H_6 elimination. The product ions such as $Fe^+(C_4H_8O)(C_2H_5OC_2H_5)_n$ and $Fe^+H(C_2H_5OC_2H_5)_n$ are also observed and interpreted as arising from insertion of Fe^+ into the C-H bond. The formation mechanisms and reaction energetics for the observed heterocluster ions are discussed both experimentally and theoretically.

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Intramolecular ion-molecule reactions within $Ti^+(CH_3COCH_3)_n$ heteroclusters: Oxidation pathway via C=O bond activation

홍기룡, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

The intracluster ion–molecule reactions of $Ti^+(CH_3COCH_3)_n$ complex produced by the mixing of a laser vaporized plasma and a pulsed supersonic beam were investigated using a reflectron time-of-flight mass spectrometer (RTOFMS). The reactions of Ti^+ with acetone clusters were found to be dominated by the oxidation reaction, which produces $TiO^+(CH_3COCH_3)_n$ clusters. This sequence is attributed to the insertion of Ti^+ ions into the C=O bond of the acetone molecules within the heteroclusters, followed by hydrogen migration and neutral propene elimination. The reaction energetic and formation mechanisms of the observed heterocluster ions are supported by the density function calculations.

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Formation of nano sized ferric oxide particles on glass

김희진, 소수정, 한종수

전남대 화학과

A thin ferric oxide film on ceramic can be used in photocatalytic decomposition of water under visible right and the practical formation methods are interesting topics. In this study, ferrous ion was attached to the surface of glass through hydroxyl group and the ferrous ion wad oxidized with $NaNO_3$ solution to obtain nano sized ferric oxide particles. The nano sized particle or ferric oxide film was characterized with Scanning Electron Microscope, Electron Spectroscopy for Chemical Analysis, and Scanning Probe Microscope. It was observed that the reputation of the immersion of glass to ferrous ion and followed $NaNO_3$ solution increases Fe content and roughness of the glass while the size of the ferric particle retains about ~20 nm.

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Excited electronic states of KRb near 480 nm

이용훈, *김봉수

*광주과학기술원 고등광기술연구소 *KAIST 화학과*

We have investigated the excited electronic states of KRb near 480 nm by resonance-enhanced two-photon ionization in a pulsed molecular beam. The 1 $^3\Delta$, 4 $^1\Sigma^+$, and 5 $^1\Sigma^+$ states have been assigned for the first time. From the vibrational analysis and rotational contour fits, the molecular constants of the 1 $^3\Delta$ and 4 $^1\Sigma^+$ states have been determined. Also, the empirical potential energy curves have been constructed by the Rydberg-Klein-Rees method. The experimental results are compared with those from ab initio calculations.

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DNA Minor Groove Binders interaction

김우성

고려대 화학과

Diatamycin A(DST) and Netropsin(NET) are a well known polyamide antibiotic that can bind in the minor groove of duplex DNA primarily at AT-rich sequences. An FTIR and CD study of the DNA binding modes of DST and NET were investigated binding studies with oligomeric duplexes of the form d(CGCGAAAAACGCG)·(CGCGTTTTTCGCG). Distamycin A can bind both as a monomer or as a side-by-side antiparallel dimer. In case of oligomer duplexes with AAAAA binding sites,1:1 complexes are formed at low distamycin:DNA ratios and 2:1 complexes are formed at the ratios >1. It was found that 1:1 and 2:1 drug-duplex complexes exhibit distinctly different circular dichroic(CD) spectral characteristics and can, thus, serve as diagnostic tools for binding mode differentiation. It the infrared spectra of antiparallel-stranded(aps) DNA have been studied. Significant differences have been found in the region of the thymine C=O stretchingvibrations. Interaction with three drugs known to bind in the minor groove of aps-DNA - netropsin and distamycin A - induces shifts of the C = O stretching vibrations of ps-DNA even at low ratio of drug per DNA base pair.

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Polarization angle scan (PAS) 2D IR spectroscopy of RDC

이경구, 조민행

고려대 화학과

The Two-dimensional Infrared spectroscopy (2D-IR) is to be an essential tool which reveals a molecular structure and a chemical exchange of a molecule having extremely fast motions. 2D-IR is based on heterodyned photon-echo detection. It uses four infrared laser pulses of femto-second.I developed the PAS (Polarization Angle Scan) two-dimensional infrared spectrometer which improves the conventional 2D-IR spectrometer. It uses the way of revolving the polarization angle of four infrared laser pulses. It could be possible to get new information to reveal the 3D structure of molecule in the atomic resolution. There is crucial information in cross peaks. However, because of the bigger a diagonal signal, it is not easy to measure the cross peaks separately in the many cases. Once the PAS two-dimensional infrared spectrometer is use, the signal in diagonal areas will be reduced and the resolution of spectrum could be improved by enhancing the cross peaks selectively.RDC (dicarbonylacetylacetonato rhodium) was used for verifying the PAS 2D-IR. I showed the conventional 2D-IR spectrum and the diagonal-peak-diminishing 2D-IR spectrum of RDC.

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Preparation and characterization of polyaniline nanostructure-palladium nanoparticles composites through seed mediated polymerization

Shanmuga sundaram Komathi, *S. Palaniappan, *P. Manisankar, **이세희, ***A.Gopalan, ***이광필

*경북대 화학과 *Department of Industrial Chemistry, Alagappa University*
***경북대 나노과학기술과 ***경북대 화학교육과*

Nanostructured polyaniline - palladium nanoparticles (Pd/PANI(NS)) composites were prepared by seed induced chemical oxidative polymerization utilizing MCM-41 loaded Pd/PANI(NS) as the seed. The morphology of Pd/PANI(NS) was investigated by field emission scanning electron microscopy. The presence of Pd NPs in Pd/PANI(NS) was confirmed by EDAX measurement. Fourier transform IR (FTIR) and UV-vis spectroscopy were used to characterize the structural features of Pd/PANI(NS). Cyclic voltammogram was recorded to evaluate the electrochemical behavior of Pd/PANI(NS). Pd/PANI(NS) was used reduce 4-amino phenol in cyclic voltammetry.

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Fabrication of a novel cytochrome c immobilized biosensor for electrochemical detection of nitrite ions

Shanmuga sundaram Komathi, *A.Gopalan, *이광필

*경북대 화학과 *경북대 화학교육과*

A novel cytochrome c immobilized biosensor was fabricated by modifying the surface of indium tin oxide coated glass (ITO) electrode using Silica- chitosan - multi wall carbon nanotube- Au nanoparticles composite as the matrix for enzyme immobilization. The biosensor is designated as MWNT-Si-CS/Au/cyt c. Firstly, silica- chitosan composite was embedded into MWNT by performing insitu sol-gel reactions in the presence of functionalized MWNT. Further, Au nanoparticles (Au NPs) were electrodeposited onto MWNT-Si-CS coated ITO electrode. The MWNT-Si-CS/Au/cyt c biosensor was tested for the electrochemical oxidation of nitrite ions by cyclic voltammetry and amperometry. For the comparative purpose, MWNT-Si/Au/cyt c, Si-CS/Au/cyt c, MWNT-CS/Au/cyt c, MWNT/cyt c were also fabricated. The ITO/MWNT-Si-CS/Au/cyt c biosensor exhibited enhanced selectivity and sensitivity towards the electrochemical oxidation of nitrite ions.

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Chiral separation of hesperetin and hesperetin-*O*-glycoside by microbial β-1,2-glucans

조은애, 전유경, *정선호

*건국대 생명공학과 *건국대 특성화학부 생명공학과*

Linear β-1,2-glucans branched by β-1,6 linkages are produced from *Escherichia coli*, *Erwinia chrysanthemi*, and *Pseudomonas* species. Also, Unbranched cyclic β-1,2-glucans with phosphoglycerol substituent are isolated from *Rhizobium* and *Agrobacterium* species. In this study, enantioseparations of some flavonoids with these microbial β-1,2-glucans were investigated. Hesperidin (hesperetin-7-*O*-rutinoside) is the main flavanone glycoside in the peels of sweet orange (*Citrus sinensis*) and it releases its aglycone, hesperetin, on digestion. To separate chiral hesperidin and hesperetin, capillary electrophoresis (CE) has been utilized and pH dependent enantiomerization has been observed. Optimal pH of the buffer was determined to be 8.3 and lower temperature led to the better resolution result. Additionally, we suggest that there are specific chiral interactions between β-1,2-glucans and hesperidin or hesperetin, through this work.

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Tobramycin interacted with linear β-1,2-glucans of *Pseudomonas syringae*

조은애, 권용은, *정선호

*건국대 생명공학과 *건국대 특성화학부 생명공학과*

Tobramycin is an aminoglycoside antibiotic used to treat gram negative bacterial infection, and linear β-1,2-glucans are periplasmic glucans of *Pseudomonas syringae*. Compared with the respective compounds, their mixtures were analyzed with the ^{1}H nuclear magnetic resonance (NMR) spectra. The results show that there are some interactions between tobramycin and linear β-1,2-glucans. The stoichiometry of the complexes was determined by Scott's plot to be 1:1, and the association constant (K_a) was calculated to be 136 M^{-1}. Furthermore, the detailed molecular interactions were confirmed on the basis of two-dimensional rotating frame nuclear overhauser effect spectroscopy (ROESY) spectra. Through this work, a potential of antibiotic resistance by periplasmic linear β-1,2-glucans was suggested.

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발표코드: **Ⅳ35P5포**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

The anti-oxidative assay of refined wood vinegar by distillation and indagated the effect in mixing feeds

신장철, 송미선, *윤상호, **김일광

*원광대 화학과 *목초마을 총괄 **원광대 t생명나노화학부*

The wood vinegar were refined by a reduced pressure distillation method and the anti-oxidative assayed with DPPH radical scavenging assay and reductive power method. a natural function additives were commixed with some inorganic minerals composing and the refined wood vinegar. To improved the compositive effect of the feed additives, the garlic extracts and pyroligneous acid were added simultaneity. The natural functional additives are included abundant beneficial mineral elements as Ca K Mg Fe. The additives were decomposed with acid and processed by filtrating depositing and centrifugal treating to determined by a ICP-Mass system. A GC-Mass method was used to analyze the organic compositions of the pyroligneous acid. The manifold food analysis methods were used to evaluated the compositive effect of the feed additives from the fowls and cattles that feeding with the additives.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Compared antioxidative effects of the extracts from Pine needles, Morus alba bark and Acer Palmatum Var amoenum leafs.

신장철, *김일광

*원광대 화학과 *원광대 t생명나노화학부*

The Pine needles, Morus alba bark and Acer Palmatum Var amoenum leafs were extracted with 80% methanol at room temperature and the extracts were separated to four partition by hexane, ethyl acetate, butanol and water. The antioxidative effect of the parts were compared and evaluated by DPPH radical scavenging assay, reductive power and total phenolics method. the yield of the parts were determined with percentage and the standard BHA, BHT, α-Tocopherol were used in antioxidant ability evaluated.

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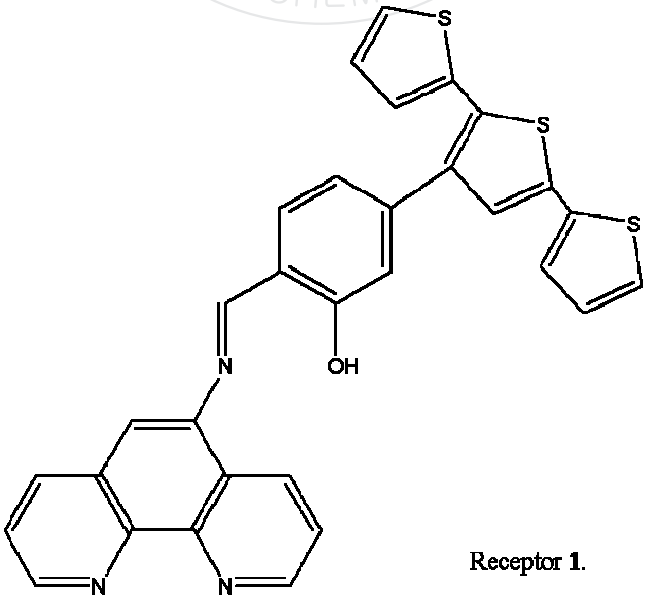
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Selective Optical and Electrochemical Sensing of Copper(II) ions based on 1,10-Phenanthroline-Appended Terthiophene

김동완, 김정환, *황재영, 김재상

*경상대 화학과 *부산대 화학과*

New receptor, terthiophene bearing 1,10-phenanthroline have been synthesized. The binding abilities and stoichiometry of this sensor towards various cations examined by UV–vis and fluorescence spectroscopies. The synthesized receptor showed excellent selectivity for copper(II) ion with respect to the other cations. In DMF, the presence of Cu(II) ion induced the formation of 1:1 (H/G) complex with the receptor. Also, a solid contact copper(II) ion selective electrode was prepared based on the electroploymerization of the ligand. The new sensor show high selectivity to Cu^{2+} ions with a detection limit of 5 x 10^{-5} M.



Receptor **1**.

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장소: 대전컨벤션센터
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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis, Structure and Fluorescence of the Metas Complexes with Bis(pyrrole) Schiff Base Derivative

김동완, 김태호, 김진은, 김재상

경상대 화학과

Schiff Base ligand, bis(pyrrol-2-yl-methanimine)s linked by a *p*-xylene has been prepared. The receptor was characterized with NMR, elemental analysis, spectroscopic studies such as IR, ^{1}H NMR, fluorescence and electrochemical measurement. The binding abilities of this sensor towards various cations examined by UV–vis and fluorescence spectroscopic studies. The structures of the Cu(II) complexes have been determined by single-crystal X-ray diffraction. Self-assemly of the resulting recepotr with Cu(II) gave double-stranded helicates coordination geometry.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of Pd-CNT nanocomposites and investigation of their catalytic properties in the hydrodehalogenation reaction

김자영, 최현철

전남대 화학과

Carbon nanotubes (CNTs) have drawn particular attention on account of both their scientific interest and their potential for technological applications. Recently, CNTs are receiving considerable attention as catalyst supports due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and Fischer-Tropsch synthesis, etc. However, few studies have conducted about the CNTs as catalyst supports for hydrodehalogenation reaction which is very important for the reduction of environmental pollution. In this work, we prepared highly dispersed CNT-supported Pd nanoparticles by introducing thiol groups on multiwall carbon nanotube (MWNT) surfaces. The Pd-CNT nanocomposites effectively promoted the hydrodehalogenation of aryl halides at a low Pd content and in the absence of any ligand. The results suggest that the CNTs could significantly influence the catalytic activities of CNT-supported metal catalysts for hydrodehalogenation.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Preparation & Characterization of Pd-decorated carbon nanotubes for a heterogeneous catalysis

김자영, 최현철

전남대 화학과

Recently, CNTs are receiving considerable attention as catalyst supports in both heterogeneous catalysis and electrocatalysis due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and Fischer-Tropsch synthesis, etc. However, few studies have conducted about the CNTs as catalyst supports for hydrodehalogenation reaction which is very important for the reduction of environmental pollution. In this work, we prepared Pd-decorated CNTs by introducing thiol groups on multiwall carbon nanotube (MWNT) surfaces. The concentration of Pd nanoparticles on the surface of CNTs was about 2.1 atomic % as determined by XPS analysis. Their catalytic performance for hydrodehalogenation reaction was examined, and compared with the reference systems. The electronic structure of theses material of these materials were also examined by high resolution XPS and UPS.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Analysis of 1,3-butadiene using gas chromatography

김윤기, 최성신

세종대 화학과

1,3-Butadiene (BD) is an organic, colourless, flammable hydrocarbon gas. BD is one of the bulk-production industrial chemicals whose commercial production started in the early 1930s. BD is produced from petroleum and used as a monomer in the manufacture of a wide range of polymers and co-polymers such as polybutadiene (BR), poly(styrene-co-butadiene) (SBR), and poly(acrylonitrile-co-butadiene-co-styrene) (ABS). But, due to its toxicity, BD is classified into a hazardous air pollutant. Its cancer risk is more than 25 times higher than benzene. Moreover, BD is the second major contributor to overall risk for chronic exposure to environmental air pollutants. In this work, we analyzed BD using GC-FID and investigated the detection limit and dynamic range. We also analyzed residual BD in BR, SBR, and ABS.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Determination of VOCs using ion mobility spectrometry with corona discharge ionization source

김윤기, 임송희, 최성신, *신명원, *최규섭, *맹석진, *안승건

*세종대 화학과 *(주)우주씨앤티 기술연구소*

Volatile organic compounds (VOCs) include a large of aliphatic and aromatic hydrocarbons, halocarbons, and oxygenated hydrocarbons such as ketone, aldehydes, esters, and alcohols. In ambient air, some of these are potentially explosive or flammable, and the vapors of several common compounds such as benzene, chloroform, and carbone tetrachloride are considered as potential carcinogens or health hazards through inhalation exposure. Analysis of VOCs is normally achieved using GC/MS. However, it is difficult for GC/MS technique to carry on real-time monitoring onsite. Besides, MS instrument must work in a high vacuum environment and the whole GC/MS system is bulky and expensive. Ion mobility spectrometry (IMS) is small and inexpensive equipment running under atmospheric pressure, thus it is excellently suited for on-line selective monitoring of VOCs. IMS distinguishes ions on the basis of their differences in ionic drift velocities through a gas under applied electrostatic field. Ions with different masses or structures possess different movement velocities in a uniform electric field, thus they can be separated. In this study, IMS equipped with corona discharge ionization source was constructed and its performance was tested with various VOCs.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

SPR study on the reaction of poly(diallyldimethyl ammonium chloride), poly(4-styrene sulfonic acid), Nafion and molecularly imrpinted polymer films with gaseous formaldehyde and toluene

장성우, *도영락, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We applied poly(diallyldimethyl ammonium chloride) and poly(4-styrene sulfonic acid) films to sensing of gaseous formaldehyde and toluene using SPR technique.The thicknesses of polymer film were controlled by spin-coating method and the morphology of polymer films were obtained by atomic force microscopy at various thicknesses. The detection limit of formaldehyde and toluene gases tunred out to be of ppb level. The unusual time profile with spikes on top of the normal SPR curve was absorbed and the intensity of spikes decreased as the film thickness increased.The spikes seem to be due to the small binding capacity of the polymer and the modification of surface layers by the reaction with gases. The molecularly imprinted polymer films of SPR chip for the sensing of toluene were synthesized by UV or thermally induced polymerization method and the sensitivity and selectivity were compared with non-imprinted polymer films.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

ABS 중 프탈레이트 함량 분석 불확도 추정The measurement Uncertainty of Phthalate in ABS

이혜진, 김현주, 이웅진, 옥종화

(주)LG화학기술연구원 CRD연구소

전기•전자제품 내 유해물질 사용 제한지침(RoHS)에 따른 유해물질을 분석함에 있어 ISO/IEC 17025 에 따른 체계적인 품질관리 및 보증에 대한 요구가 커지면서 측정 불확도의 표기가 요구되고 있다. 측정 불확도란 시험결과에 대해 측정량을 합리적으로 추정한 값들의 분산특성을 나타내는 파라미터로써 ILAC(국제시험소인정협력체) 등의 국제기구와의 측정 결과에 대한 상호 인정 및 신뢰성 확보에 필수적인 요소이다. 국제적 표준(ISO/IEC17025) 에 맞는 시험 분석 결과의 도출을 위해서는 먼저 소급성을 유지하고 그에 따른 불확도를 산출하여야 한다.ABS 중 프탈레이트 함량을 GC/MSD 로 분석함에 있어 측정 불확도 표현 지침(GUM)에 따라 측정량의 함수의 표현, 입력량의 표준불확도의 계산, 합성표준불확도의 계산, 확장불확도의 계산을 통해 불확도를 산출하였다.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Determination of Ascorbic Acid in Pharmaceuticals Based on $KMnO_4$-Na_2SO_3 Chemiluminescence Detection

서연숙, 김고은, 이상학, *최종하

*경북대 화학과 *안동대 화학과*

For the quantitative determination of ascorbic acid in pharmaceutical formulation, a flow-injection chemiluminescence (CL) method is described. In this study, it was observed that ascorbic acid could enhance the CL emission of the $KMnO_4$-Na_2SO_3 system and this enhancement effect was dependent on the concentration of ascorbic acid added to the system. Based on this phenomenon, a CL system was established for the determination of ascorbic acid. Under the optimum experimental conditions, the linear range and detection limit are 3.6×10^{-6} M to 2.3×10^{-4} M and 1.0×10^{-7} M, respectively. The relative standard deviation (RSD) for 10 repeated measurements of 1.0×10^{-5} M ascorbic acid was 1.27%. The method was applied to the determination of ascorbic acid in pharmaceuticals and the results obtained were in reasonable agreement with the amount labeled.

Reference:

1) Waseem, A.; Yaqoob, M.; Nabi, A. *Luminescence*. **2007**, *22*, 349.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

자동차용 소재의 VOCs 분석법 비교

김해영, *이혜진, *옥종화

*(주)LG화학기술연구원 CRD연구소 *LG화학기술연구원 분석센터*

최근 실내 공기질에 대한 사회적 인식이 높아지면서, 자동차 실내 공기질에 대한 규제도 강화되고 있다. 이에 완성차업체에서도 고분자 소재에 대한 VOCs 규제를 강화하고 있는데, 대표적인 평가 방법으로 유럽 자동차업체(Volvo, GM, Volkawagen 등)에서 정한 VCS1027,2739 방법[120℃/300min Headspace-GC/FID, EG(total carbon emission) 측정]과 GM 의 worldwide 규제 방법인 GMW8081 방법[120℃/60min Headspace-GC/MS, Relative emission 측정]이 있다. 이에 자동차 소재로 널리 사용되는 ABS(Acrylonitrile-Butadiene-Styrene copolymer), PC/ABS, PC/ASA 에 대해 두 가지 규제 방법으로 VOCs 를 평가하여 두 방법간의 상관성을 알아보았다. 또한 Detector 및 Headspace 평형 시간에 따른 차이점도 비교해 보았다.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

A Micelle Enhanced Fluorimetric Method for the Determination of Carbaryl

김고은, 이상학, *최종하, 서연숙

*경북대 화학과 *안동대 화학과*

A simple, rapid and sensitive fluorimetric method was developed for the determination of carbaryl. The use of surfactant sodium dodecyl sulfate (SDS) was investigated. The method is based on the enhancement of fluorescence intensity of carbaryl by the addition of sodium dodecyl sulfate. Under the optimized experimental conditions, the enhanced fluorescence intensity was linearly proportional to the concentration of carbaryl in the range of 0.01-20 μg/ml and the detection limit was found to be 2.3×10^{-3} μg/ml. The effect of the potential interfering substances was optimized. The method was successfully applied to the determination of carbaryl in real-samples.

Reference:

1) Silvaa, R.A.; Wangd, C.C.; Ferna´ndez, L.P., Masi, A.N. *Talanta*. **2008,** *76*, 166.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Highly sensitive detection of dopamine using Bioluminescence immunoassay

류지은, 박호영, 전옥금, 이인숙

서울여대 화학과

Dopamine (DA) is one of the important neurotransmitter molecule of catecholamines. In the presence of abnormal concentration of DA in biological system, it causes neurological disorder such as Parkinson's disease and Schizophrenia. Thus it is essential to develop suitable analytical technique enable to detect DA sufficiently. Bioluminescence immunoassay (BLIA) has developed using components of bioluminescence reaction as a label such as Aequorin. The advantage of BLIA are low background, large dynamic range, high sensitivity, and no need of substrate or enhancer in immunoassay systems. In this work, the Avidin/biotin mediated BLIA for determination of DA was performed for signal amplification.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Characterization of encapsulated silica-alginate micro-hybrid with some cosmetic compound

강상혁, Tara Sankar Pathak, 윤정호, 팽기정

연세대 화학과

Alginate is a natural bio-polymer that can be extracted from algae. silica-alginate hybrid (micro size bead form) can be prepared from a mixture of sodium alginate and sodium silicate using calcium chloride as a cross-linker. After that cosmetic compounds were encapsulated onto the micro size silica-alginate hybrid bead. The blank and encapsulated beads were characterized by using Fourier transform infrared spectroscopy (FT-IR), scanning electron microscope(SEM), porosity, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC).

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Preperation of Mg-Al hydrotalcite by hydrothermal Urea method in aqueous alcohols.

최보라, 김동호, 권수한

충북대 화학과

Mg-Al hydrotalcite 의 Urea 방법으로 합성을 진행하며 용매로는 alcohol 을 일정 비율로 첨가한 용액을 사용한다. 합성의 진행에 따른 pH 변화와 첨가 비율에 따라 합성된 입자의 크기및 크기분포도를 조절한다.본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Microchip gel electrophoresis assay based on programmed field strength gradients for rapid distinguish of Korean cattle species

오두리, 강성호

전북대 화학과

The microchip gel electrophoresis based on programmed field strength gradients (MGE-PFSG) has developed for the fast identification of Korean cattle species. Specific single nucleotide polymorphism (SNP) markers of Korean cattle were amplified using allele-specific polymerase chain reaction (AS-PCR). Based on the PFSG method, the products of amplified AS-PCR were separated in a glass microchip using 0.5% poly (ethyleneoxide) as a sieving gel matrix. The AS-PCR products with various length of DNA fragments (*i.e.* 165, 170, 207, 240, 308, 422, and 647 bp) were analyzed within only 45 s with excellent accuracy and sensitivity under the MCE-PFSG method. This assay method has advantage of smaller sample volume and faster separation time compared to conventional MGE techniques with constant electric field strength.

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Quality Control of Schizonepeta tenuifolia Briq. by Solid-Phase Microextraction Gas Chromatography / Mass Spectrometry and Principal Component Analysis

천미희, 김은경, *홍종기

*경희대 나노생명과학과 *경희대 약학과*

The chemical composition of Schizonepeta tenuifolia Briq.(Sch.t.Briq) is mainly composed of several volatile substances that affect multiple pharmacological targets and provide clinical efficacy. In this work, a headspace/solid phase microextraction/gas chromatography - mass spectrometry (HS-SPME-GC-MS) method was developed to evaluate the profiles of volatile compounds in Sch.t.Briq. The optimization of SPME conditions was carried out using four kinds of fiber, extraction time and temperature, desorption temperature and time, and sample amount. The GC-MS analysis allowed the tentative identification of 21 compounds, with similarities higher than 85%, in accordance with the NIST/Wiley mass spectral library. Major components such as (+)-menthone (14.32%), (-)-pulegone (47.73%), 2-hydroxy-2-isopropenyl-5-methyl cyclohexanone (5.97%), cis-pulegoneoxide (4.12 %), schizonal (4.28%), and schizonal (5.36%) were identified by comparison of retention time and mass spectral data of isolated standards from Sch.t.Briq. The contents of these compounds were about 78% against total amounts of volatile compounds extracted from Sch.t.Briq. Based on optimized SPME method, 19 different Sch.t.Briq. samples collected from market in Korea and China were analyzed to obtain the profiling data of volatile compounds. In addition, principal component analysis (PCA) was performed on the profiling data in order to classify samples collected from different region. PCA could be possible to visualize the grouping tendencies of the studied varieties of herbal samples, as well as the identification of the volatiles responsible for discriminating the groups.

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A New Strategy to Quantitate Proteins on Biochips Using MALDI-ToF MS

이주희, *유수윤, *곽설진, *민달희, 여운석

*건국대 생명공학과 *KAIST 화학과*

Protein chip has been an important analysis format for studying biochemical functions of proteins and interactions of proteins with other proteins, substrates, and small molecules. The raising issue in the use of protein chips is the determination of protein densities on surface. Although several methods have been reported to provide valuable quantitative information for proteins at solid surfaces such as QCM and ELISA, these techniques require quite a few amount of proteins and materials, and some techniques cannot distinguish between protein types.In this work, we report a novel method to quantitate proteins which are specifically bound on a ligand-presenting biochip by matrix assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometry (MS). The bound protein was digested by trypsin and the resulting peptide fragments were analyzed by MALDI-TOF MS in the presence of an isotope-labeled internal standard (IS). The IS has the same sequence as a representative peptide of the target protein digestion but different molecular weight. The absolute amount of the specifically bound protein on a biochip is then quantitated by comparing the mass intensities between the representative peptide and the IS. The intensities of these two analytes represent the real amounts of analytes on the chip because they have the same molecular milieu. As a model system, we tested GST and GST-fusion proteins which were captured on glutathione-presenting biochips. We observed that the glutathione densities on biochips showed a good correlation with absolute quantity of proteins with excellent reproducibility. We believe our method will be an alternative to current existing tools for the surface-protein quantitation.

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Synthesis of Hydrotalcite-Nickel by Electrolysis

김주현, 김이영, 최보라, 박진호, 김동호, 정용석, 권수한

충북대 화학과

본 연구는 전기분해를 이용하여 하이드로탈사이트에 니켈을 침착시키는 것을 목적으로 한다. 하이드로탈사이트 특유의 구조를 이용하여 층간이나 주변에 니켈의 침착이 가능한지를 보고자 한다. 실험은 일정 온도에서 니켈판을 전기공급장치와 연결하여 하이드로탈사이트가 담긴 용기 안에 일정한 전압을 가해 니켈판의 표면에서 니켈이온을 발생시켰다. 또한 실험 시 발생하는 거품을 제거하였다. 이렇게 하여 생성된 니켈-하이드로탈사이트는 본래의 하이드로탈사이트 기능을 향상시킬 것으로 기대된다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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Ultrasensitive Detection of miRNA Using Am-tag and LDI-TOF MS

김소현, 김재일, 여운석

건국대 생명공학과

We report a simple, fast, and sensitive method that allows attomolar detection of miRNAs without the need of PCR or a labeling by combining self-assembled monolayers (SAMs) on gold and laser desorption/ionization time-of-flight (LDI-TOF) MS with a matrix-free format. Our approach started with SAMs on gold microparticles and gold chip consisting of DNAs. The target miRNA was captured specifically by the immobilized DNAs on the gold microparticles and the gold chip. As a model case, we tested two miRNA, mir-122 and dme-bantam. The mir-122 is a liver-specific miRNA which is known to be linked with lipid metabolism, liver homeostasis, and hepatitis C virus replication. The dme-bantam is associated with cell death, and cell proliferation. We used a small molecule (Am-tag) as a reporter for signal amplification of the target miRNAs. The presence of miRNA in a solution was verified by observing Am-tag utilizing LDI-TOF MS. All the analyses were performed without use of a matrix, presumably because the nanostructures on the microparticle surface would help desorption/ionization of Am-tag molecules. The miRNA in the concentration range of 1 nM ~ 10 aM were exposed to capture DNA-modified gold microparticles and biochips. The subsequent MS analysis showed that our strategy can observe miRNAs in solution at a concentration of subfemtomolar. To verify our strategy is applicable to crude samples, we carried out miRNA detection in the extract of Huh-7 cells. We believe that this strategy will provide an important tool for accurate, sensitive, rapid, and low-cost detection of miRNA.

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Detection of a novel selective F- sensor based on dipyrrolemethane derivatives.

유정민, 김슬기, 전승원

전남대 화학과

AbstractDipyrrolemethane derivatives compound easily made available from aldehyde and pyrrole was found to show a highly selective and sensitive response to F- anion. At the neutral state λmax due to the π-π* transition was found to be 500 nm. The significant changes of absorption bands and color show that chemosensor is selective toward fluoride ion (F-) over other anions such as Cl- , Br- , I- , CH3COO- , H2PO4- , HSO4- ,NO3- , SO42-.

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A new method for the development of microarray and cell chip using chemical reaction induced patterning (CRIP)

서현정, 김소현, 여운석

건국대 생명공학과

Selective surface modification methods are important in microarray fabrication and cell chip development. In practice, such demand was achieved by e-beam lithography, UV-photopatterning, and dip-pen nanolithography. Here, we reported a new method of microscale patterning for the development of microarray and cell chip. Our strategy is based on the surface that is modified with quinone-containing molecules, which reveal amine functionality by a chemical reaction (reduction). First, we demonstrated microscale patterning by applying a reducing agent on the quinone-modified surface using a microarrayer followed by a fluorescence isothiocyanate treatment. The fluorescent image of the substrate indicated that amine functional group was revealed selectively on the reduced regions. Secondly, we verified the fidelity of our approach by demonstrating a cell chip. We prepared monolayers on gold presenting the quinone-containing molecule (QSH) with 1% density amongst 99% of oligo(ethylene glycol)-containing background. Upon a treatment with a reducing agent, the QSH revealed amine functionality which subsequently reacted with a heterobifunctional crosslinker to generate maleimide groups. CGRGDS peptide was then incorporated into the maleimides. All chemical conversions on the monolayer were verified by MALDI-TOF MS. Next, we used micro-contact printing (uCP) method to prepare patterned RGD substrate. The PDMS stamp inked with reducing agent was applied to the QSH presenting monolayer, which was then subjected to a series of chemical conversions as described above. As expected, NIH 3T3 fibroblast selectively adhered to chemically reduced patterned area. We believe that this method will be a useful platform technology for the development of cell chips and cell based assay systems.

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Electrospun TiO_2 nanofiber-based chemoresistive sensors

김대규, 김용신

한양대 응용화학

Poly(vinyl acetate)/TiO_2 composite nanofiber mats were formed onto a pair of interdigitated Au electrodes by electrospinning a solution of poly(vinyl acetate) and titanium tetraisopropoxide. Nanostructured anatase TiO_2 sensing layer was obtained through subsequent hot-pressing at 110℃ and calcination at 500℃ in air for 1h. The active film exhibited n-type semiconducting characteristics, and its sensing capability was evaluated upon exposure of ammonia vapors. Furthermore, the surface of the electrospun TiO_2 mat was decorated with additional gold nanoparticles or conducting polymer. These novel materials were also characterized and evaluated in terms of material and gas-sensing properties.

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Study to Ti deposited Hydrotalcite

박진호, 김이영, 김동호, 김주현, 최보라, 정용석, 권수한

충북대 화학과

본 연구는 티타늄을 하이드로탈사이트에 전기분해를 이용하여 침착시키는 것을 목적으로한다. 일반적인 하이드로탈사이트는 기본적으로 이중층의 수산화물 구조로 이 연구에서는 티타늄이온의 침착이 가능한지 연구하고. 가능하다면 최적이 조건이 어떻게 되는지에 대하여 수행하였다. 티타늄판을 전기 공급 장치와 연결하여 하이드로탈사이트가 담긴 증류수안에 일정한 전압을 가해 티타늄판의 표면에서 발생하는 티타늄 이온을 통한 하이드로탈사이트의 표면에 침착시키는 것을 수행하였고 분석기기를 통하여 침착이되었는지 확인하였다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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Study to Fe deposited Hydrotalcite

김이영, 김동호, 박진호, 김주현, 최보라, 정용석, 권수한

충북대 화학과

Hydrotalcite 가 분산되어 있는 용액에 Fe 을 전기분해하여 이온을 발생시킨 뒤 Hydrotalcite 표면(층간)에 흡착(치환)시켜 Fe-Hydrotalcite 를 합성해본다. 기기분석을 통하여 합성된 Fe-Hydrotalcite 의 물성을 알아보고 응용가능분야를 모색한다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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Comparison of Guanidination Efficiency of Protein Tryptic Digests Using Various Reaction Conditions

구건모, *박수진, *김진희, *김정권

*KAIST 무학과 *충남대 화학과*

In the qualitative analysis of peptides, O-Methylisourea, which attaches to specific site of an amino acid (e.g. lysine) and improve the peak intensities, is often used for sample's pre-modification. This is called 'guanidination' of the peptides. However, this pre-modification results varies on the reaction conditions. In this research, we have applied microwave and ultrasound to the reaction solutions to optimize the modification results. The result shows that microwave cannot improve but sonication can improve the guanidination efficiency of several peptides.

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리튬 이차 전지내의 발생 가스 분석을 통한 전지의 상태 분석

이성협

(주)LG화학기술연구원 CRD연구소 분석센터

리튬 이차 전지 내부에서 발생하는 가스를 검출하여 전지내의 상태를 분석하였다. 리튬 이차 전지에 사용되는 전해액은 전지 작동 범위에서 불안정하여 충방전 혹은 수분과의 반응에 의하여 다양한 가스를 발생 시킨다. 발생된 가스를 측정하여 리튬 이차전지의 상태를 분석하였다.

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Selective Detection and Qualitative Analysis of Phospholipids in Lipoprotein from Human Blood Plasma by Multiplexed Hollow Fiber Flow Field-Flow Fractionation (MxHF5) and Nanoflow LC-ESI-MS-MS

이주용, 문명희

연세대 화학과

Principal function of lipoproteins is to transport lipids through vascular and extravascular body fluids, and they are assembled with proteins and lipids such as phospholipids, cholesteryl esters, neutral lipids, and triglycerides. Among lipoproteins, it is known that low density lipoprotein (LDL) is closely related to coronary artery disease (CAD), and high levels of high density lipoprotein (HDL) are related to relieve cholesterol levels in the blood. Flow field-flow fractionation (FlFFF), a separation technique for nanosized materials such as nanoparticles, proteins, etc., was utilized in this study for separating lipoprotein particles in blood plasma with the help of selective detection of lipoproteins using Sudan Black B. Multiplexed hollow fiber flow field-flow fractionation (MxHF5) is an evolutional version of FlFFF for the semi-preparative scale separation using parallel connection of six hollow fiber modules and it was employed and the semi-preparative fractionation of HDL and LDL in blood plasma. Phospholipids in collected lipoprotein fractions were analyzed by nanoflow LC-ESI-MS-MS. In this study, dual scan method was used in positive ion mode to detect phosphatidylcholine (PC) and phosphatidylethanolamine (PE), and in negative ion mode to detect phosphatidylinositol (PI), phosphatidic acid (PA), and phosphatidylglycerol (PG).

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Profiling of Phospholipids from Prostate Cancer Cell Line using Nanoflow LC-ESI-MS-MS

정래웅, 문명희

연세대 화학과

Lipidomics is a growing area to characterize lipid molecular species and of their biological roles with respect to expression of proteins involved in lipid metabolism and function, including gene regulation. Lipid is a major component of cellular membrane and their composition as mixtures of various molecular species depending on the type of polar head groups and the degree of unsaturation of the acyl chains.In this study, nanoflow liquid chromatography coupled with electrospray ionization tandem mass spectrometer (nLC-ESI-MS-MS) was employed for the analysis of phospholipids mixture in prostate cancer cell line. Separation of PLs is carried out using a home made reversed phase capillary column (C18) with a pulled tip and the MS experiment of eluted PL molecules is performed at the precursor scan first and followed by data dependent MS-MS scan.In the Positive ion mode, 19 PCs, 3 PEs were identified. And In the negative ion mode, 7 PSs, 7 PIs , 13 PGs, and 14 PAs were identified. The relative abundance of identified PLs from prostate cancer cells were compared with those of cancer cells treated with allose.

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Qualitative analysis of phospholipids in human urine with prostate cancer using nLC-ESI-MS-MS

민혜경, 문명희

연세대 화학과

Phospholipids are essential cellular constituents and their composition is known to be closely related to various diseases. Therefore, it is important to study the changes of phospholipid composition and relative abundance in various biological samples. In this study, nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nanoLC-ESI-MS-MS) was applied for the analysis of intact phospholipids (PLs) mixtures extracted from a small quantity of human urine using a homemade reversed phase capillary column (C18) with a pulled tip at positive and negative ion mode. The urinary PL species are identified by the precursor scan first followed by a data dependent MS-MS scan. In the positive ion mode, phosphatidylcholine (PC) and phosphatidylethanolamine (PE) are identified. Phospatidylserine (PS), phosphatidylinositol (PI), phosphatidylglycerol (PG) and phosphatidic acid (PA) are detected at negative ion mode.

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Characterization of hydroxyethyl Starch by Flow Field-Flow Fractionation and Multiangle Light Scattering

권지혜, 문명희

연세대 화학과

Hydroxyethyl starch (HES) is a modified natural polymer of branched amylopectin, and is one of the most frequently used blood plasma substitutes. An intravenous solution of hydroxyethyl starch is used to prevent shock following severe blood loss caused by trauma, surgery, and so on. It increases the blood volume, allowing red blood cells to continue to deliver oxygen to the body. The physical and chemical characteristics of HES are mainly defined by the degree of hydroxyethylation and the molecular weight distribution. In this study, the on-line frit inlet asymmetrical flow field-flow fractionation (FI-AFIFFF) / multi-angle light scattering (MALS) was utilized to study the molecular weight distribution of hydroxyethyl starch along with the structures. Size exclusion chromatography (SEC) has been commonly utilized for the separation of HES, however SEC had some difficulties in obtaining an accurate molecular weight value due to the possibility of chain degradation caused by the shear or sample adsorption at the surface of packing materials. This often causes errors in the accurate determination of molecular weight distribution. FI-AFIFFF is an elution based separation technique that is a useful alternative to SEC for the separation and size characterization since separation in FFF channel is carried out in an unobstructed channel. This study demonstrates the application of field programmed FI-AFIFFF to the separation of HES and the simultaneous analysis of FI-AFIFFF with MALS for the characterization of MWD.

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Effect of Channel Geometry on Particle Separation using Asymmetrical Flow Field-Flow Fractionation.

안지연, 문명희

연세대 화학과

Field-flow Fractionation (FFF) is a separation technique that only uses a stream of liquid flow without packing materials. FFF can be applied for the separation of macromolecules such as proteins and colloids having sizes ranged from 1nm to 100 ㎛. Flow field-flow fractionation (FlFFF) is the most versatile method among the various FFF techniques. And FlFFF using asymmetrical channel, called Asymmetrical FFF (As-FlFFF), has an inlet flow, which serves as a source for both the migration flow along the channel length and cross-flow through the permeable channel wall. Molecules are separated by these two flows, but there is an axial velocity gradient that affects the separation capability in asymmetrical channel design. By calculating this gradient and experiments, it is already known that a trapezoidal channel has smaller gradient than a rectangular channel. However, the minimized gradient of trapezoidal channel is not sufficient to provide a constant velocity. That is, it additionally requires nonlinear decrease of the breadth. An exponential channel can help us to get the constant mean channel velocity. We designed a series of channels suggested by an earlier theoretical development in literature. We tested the exponential channel with polystyrene(PS) latex particles from 20nm to 222nm, by only changing the channel geometry. Particles were separated within 30 min. and especially, exponential channel provided a better recovery of large particles. For the performance evaluation, resolution and plate height values of experiments were compared among difference channel geometries and experimental retention time values of each channel geometry were compared with theory.

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Separation and Characterization of Phosphorylated Protein by Isoelectric Focusing – Multichannel Asymmetrical Flow Field-Flow Fractionation

김기훈, 문명희

연세대 화학과

Post-translational modification (PTM) of proteins, such as phosphorylation, plays a critical role in cell signaling and other fundamental cellular functions in living organisms. Studies aimed at analyzing signaling pathways require methods that can specifically detect, identify, and quantify phosphoproteins. Numerous efforts are being made for characterize phosphorylation of specific protein involved in diseases and it requires the development of a noble method to separate proteins depending on the number of phosphorylated sites for clinical application. Isoelectric Focusing (IEF) embedded with multichannel asymmetrical flow field-flow-fractionation (AF4) system that has been developed recently in our lab. It is capable of separating proteins as their pI value and Stoke's diameter without using gel within 30 minutes. However, the change of pI value caused by each phosphorylation is very small(< 0.1 pI value). In this study, we used the carrier ampholyte having very narrow pH range (pH 4~5) to separate phosphorylated proteins more efficiently. To demonstrate the performance of this system, ovalbumin with various number of phosphorylation was utilized. As a result, we successfully separated proteins of different levels of phosphorylation with the observation of different peak area and the fractionated proteins were analyzed by nanoflow LC-ESI-MS-MS after tryptic digestion. With database searching, three phosphorylated peptides in ovalbumin fractions were identified. We have also evaluated the performance of separation of phosphorylated protein depending on phosphorylation sites in protein level.

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Analysis of UV absorbers using MALDI-TOFMS: Solvent effect in sample preparation

임송희, 최성신

세종대 화학과

UV absorbers (UVAs) have been utilized to protect polymer from photo degradation caused by sunlight or ultra-violet rich artificial light. In general, polymers are used by adding two or more UVAs. Tinuvin 213 which mixed polyethylene glycol (PEG) and two types of polymeric UVAs commonly applies to PMMA, NR, TPE, and so on. Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOFMS) is a very useful tool for polymer characterization. It can be used to determine average molecular weights and molecular weight distributions of narrow polydispersity polymers. In this study, Tinuvin 213 was analyzed using MALDI-TOFMS. Because Tinuvin 213 absorbs at 337nm, it can be ionized without any matrix. We will discuss a detailed investigation of the solvent effect on MALDI analysis of Tinuvin 213 using various solvents.

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Analysis of UV absorbers and stabilizers by LC/APCI-MS and LC-UV

장중희, 최성신

세종대 화학과

In general, polymeric materials such as cloth, food packaging materials or plastics are protected from UV light by the addition of mixed UV absorbers (UVAs) and stabilizers (UVSs) to ensure an extended durability. As a result of their various applications, UVAs and UVSs can enter the environment by different pathways. These additives are considered potentially toxic and could damage the human. Since these additives are present in the polymer matrix at low concentrations, a sensitive method for quantification is required. UVAs are mostly based benzotriazole, while UVSs are mostly based hindered amine light stabilizer. HALSs are not easily separated from the other additives with LC because of numerous basic amino groups. Thus, determination of separation condition of mixed additives is a very important task. UV detection is a sensitive method for determination of UVAs, but is not suitable method for determination of UVSs. Fortunately, LC/APCI-MS is a suitable method for determination of UVAs as well as UVSs. A mixture sample of commonly used three UVAs and two UVSs was separated using HPLC and was quantified using MS and UV detections.

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Urea Derivatives Containing Anthraquinone as Dicarboxylate Anion Receptors and Sensors

김정환, 김동완, *박종근, 김재상

*경상대 화학과 *경상대 화학교육과*

Urea derivatives containing anthraquinone unit were synthesized and their anion binding and sensing properities were investigated. The recognition ability for dicarboxylates has been established by fluorescence and UV-vis spectroscopic methods. Cyclic voltammetry and square wave voltammetry showed that receptors were able to act as electrochemical sensors for dicarboxylate anions. To further understand selective recognition, theoretical calculation were carried out

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Improved Isoflavones content and it's antioxidant of fruit of *Sophora japonica L.*

양정원, 김동숙, *한승준, 김영순

*동국대 화학과 *서림바이오주식회사*

Oxidative stress is called skin aging which is caused by reactive oxygen species(ROS) but it can be protected by using isoflavone. Isoflavone is an antioxidant. Isoflavones are almost exclusively discovered by the members of the *Leguminous* group. Cosmetic has recently been required of two aspects. One of them is to protect photo-aging using antioxidant and the other is something natural that people always persue of. Therefore, Isoflavones are extracted from fruit of *Flos sophora japonical L.*, a natural material, are a well-known traditional medicine. *Flos Sophora japonica L.* belong to the *Leguminous* family. Isoflavones are extracted from fruit of *Flos Sophora japonica L.* by methanol and water. Genistin is mainly extracted. Genistin is a sort of isoflavone and its form is glycone. In order to get more genistin content, we developed an extraction method. As a result, isoflavone content increased to about 90%. After that antioxidant ability a classified by isoflavone content compared in vivo with in vitro. Isoflavone constituent in extracts are analyzed by HPLC. In addition to activity of antioxidant is confirmed by DPPH(1,1-diphenyl-2-picrylhydrazyl). IC_{50} is calculated through the DPPH result of various isoflavone content of extracts. Also cell toxicity is confirmed by MTT assay with HaCaT cell(horny substance). We generated ROS inside HaCaT cell and ROS scavenging ability is measured by using hydrogen peroxide.

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Comparison of enrichment efficiencies of pentaphosphopeptides using different oxide compounds

김진희, 신성재, 양효직, 김정권

충남대 화학과

Oxide compounds, such as titania (TiO_2) or magnetite (Fe_3O_4), are commonly used to enrich phosphopeptides. In this study, we applied different oxide compounds (titania (TiO_2), magnetite (Fe_3O_4) and silica (SiO_2)) to enrich pentaphosphopeptides which are generated by acid hydrolysis of bovine beta-casein using a domestic microwave oven. Enrichment efficiencies of the pentaphosphopeptides will be compared. Detailed experimental procedures will be presented.

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Ultrasound-assisted protein digestion efficiency using immobilized trypsin onto magnetic nanoparticles

신성재, 양효직, 김진희, 김정권

충남대 화학과

Ultrasound-assisted protein digestion has proven to be very effective in tryptic digestion of protein, which significantly reduces the digestion time to several minutes. In this study, ultrasound-assisted protein digestion method was performed using trypsin-immobilized magnetic nanoparticles. Primary amine functionalized Fe_3O_4 nanoparticles were synthesized. Then, trypsin was immobilized on the nanoparticle surface. The immobilized trypsin was recycled. Different ultrasound-assisted digestion conditions will be compared to find out the optimized condition of trypsin activity. The stability of the immobilized trypsin will be tested to find out how many times the immobilized trypsin can be used.

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Resolution of Proton pump inhibitors(PPI) including omeprazole on a ligand exchange chiral stationary phase in reversed-phase mode

하진주, 현명호

부산대 화학과

Liquid chromatographic ligand exchange chiral stationary phases (CSPs) have been known to be useful in the resolution of racemic bidentate compounds including α-amino acids, β-amino acids and α-hydroxy carboxylic acids. However ligand exchange CSPs have not been used in the resolution of omeprazole and/or its analogues.Omeprazole contains a sulfur atom in a pyramidal structure and therefore can exist in equal amounts of both the S and R enantiomers. Because S-form is more effective, separation of the omeprazole is important. Omeprazole and its analogues were resolved quite successfully on the ligand exchange CSP with the use of alcohol-water mixture containing CuSO4, acetic acid and tri-ethylamine modifier as a mobile phase. The chiral recognition behavior of the CSP was found to depend on the content and the type of organic and acidic modifiers in aqueous mobile phase.

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Resolution of 1,4-Benzodiazepines as Inhibitors of Respiratory Syncytial Virus using various Pirkle-type CSPs.

박제영, 현명호

부산대 화학과

Respiratory Syncytial Virus is the cause of one-fifth of all lower respiratory tract infections worldwide and is increasingly being recognized as a serious threat to patient groups with poorly functioning immune systems. 1,4-Benzodiazepine analogues were found to show antiviral activity for respiratory syncytial virus. 1,4-Benzodiazepine analogues contain one chiral center and two stereoisomers are possible. However, the separation of the two stereoisomers(enantiomers) have not been resolved. In this study, we demonstrate that Pirkle-type CSPs can be successfully utilized in the resolution of various racemic 1,4-benzodiazepine analogues which were synthesized in our laboratory.

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Development of Compact Semi-Continuous Aerosol Sampler for Korean Atmospheric Heavy Metal Analysis

엄지원, 이동수

연세대 화학과

A compact semi-continuous atmospheric aerosol sampler has been developed for the determination of heavy metals in atmospheric aerosol including large sized mineral dust, loess. The sampler consists of a aerosol growth chamber, an aerosol/gas separator, and a liquid fraction collector. Sample air is withdrawn into a PTFE mixing chamber into which steam vapor is also continuously injected. Resulting moisturized air is then directed into water cooled glass condenser where most water vapor is removed. The air stream is finally introduced into a glass particle impactor where moisturized aerosol is separated from air stream as aqueous solution. The solution is periodically sampled by a fraction collector. This sampler, being significantly smaller and compact than any existing commercial samplers, has better aerosol collection efficiency and wider range of aerosol sampling size. It also gives more uniform aerosol condensate volume. This sampler has been successfully used for Seoul air analysis for several months. Heavy metal analysis results by inductively coupled plasma mass spectrometry showed good agreement with those by methods including realtime XRF analysis. Experimental details and Seoul air analysis results will be presented.

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PM2.5 중 무기이온과 총 유기산 음이온의 동시 모니터링법 개발과 서울대기분석 응용연구

안희진, 이동수

연세대 화학과

서울대기 중의 기체상과 입자상의 수용성 이온 성분의 장기적이고, 연속적인 측정을 통해 종합적인 환경 분석을 시행하고, PM2.5 중 총 유기산 음이온의 동시 모니터링법을 개발하여 서울대기 중에 존재하는 기체상, 입자상의 총 유기산의 농도를 밝힌다.대기 중의 유기산과 무기산을 동시에 분석하는 것은 몇 가지 한계점을 가지고 있다. 용리액을 일반적으로 IC 분석에 사용되었던 Na2CO3 를 사용하였을 경우 유기산의 peak 가 water dip 에 가려 보이지 않아 유기산을 정확히 정량하는데 어려움이 있고, 용리액을 시약제조 하였을 경우 모니터링 기간이 증가 할수록 eluent 가 carbonate 에 오염되기 때문에 water dip 이 커져 유기산의 peak 가 가려지는 현상이 발생하여 정확한 정량이 어렵게 된다. 기존의 본 연구실에서 확립하였던 용리액을 gradient 조건(KOH 0.1-25mM)을 사용한 분석법은 기체상의 분석에서는 적합한 방법이지만 입자상에 도입하기에는 한계점을 가지고 있다. 이에 본 연구에서는 대기 중의 무기산과 유기산의 실시간 동시 모니터링법을 확립하여 장기간의 모니터링 자료를 확보하고, 종합적인 환경 분석을 시행한다. 개발된 분석법은 Eluent generator 를 이용한 isocratic 용리액을 실시간으로 제조(20mM KOH)하여 대기 중의 유기산을 분석하는데, 대기 중 유기물질의 상당량을 차지하고 있는 Formic acid 와 Acetic acid 의 합으로 총 유기산을 정량한다. 유기산 비율 변화에 따른 농도 결정을 위한 표준용액을 Formic acid 와 Acetic acid 를 1:1 , 1:1.5 , 1:2 의 비율로 섞어 제조하여 이론값과 실험값을 비교한 결과 각 성분의 비율이 달라짐에 따라 농도 정량 오차 범위안의 차이를 보여 Formic acid 와 Acetic acid 의 비율을 1:1 로 제조한 표준용액으로 총 유기산의 농도를 정량하였다.

이로인해 대기 중의 기체상과 입자상의 총 유기산의 정량이 가능하며 기존에 잘 소개되지 않았던 입자상의 유기산의 장시간 모니터링 자료를 확보 할 수 있었다.

대 한 화 학 회
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Graphene Platforms for Laser Desorption Ionization Mass Spectrometry

곽설진, 김영관, 유수윤, *나희경, 민달희

*KAIST 화학과 *한국화학연구원 의약화학연구센터*

Mass spectrometry is an important analytical method for the analyses of small molecules, synthetic polymers, and biomolecules. Among various mass spectrometric instruments, matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-ToF MS) is well-suited for obtaining simple mass peaks corresponding to intact molecular ions with little fragmentation of the analytes through soft ionization. At the same time, MALDI-ToF MS is the one that is compatible with biochip format. Although MALDI-ToF MS has been utilized for the analysis of large biomolecules, inhomogeneous crystallization of analytes with organic matrix and background interference in low mass region make it difficult to analyze small molecules. Recently, nanomaterials were harnessed for laser/desorption ionization time-of-flight MS (LDI-ToF MS) in place of conventional organic matrices. Previous studies showed that various nanomaterials including gold nanoparticles and magnetic nanoparticles effectively induce ionization of analytes, and gave clean and simple mass spectra without interference of organic matrices in LDI-ToF MS. In this work, we investigated thin films of carbon-based nanomaterials—graphene oxide(GO) and multi-walled carbon nanotube(MWNT), specifically— as a substrate for LDI-ToF MS analyses. Thin films of GO and MWNT were prepared and analyte samples were deposited on top of the films before mass analysis. This simple sample preparation process gave clean mass spectra even in low molecular weight regions. The present study provides new possibilities of the application of GO and MWNT in mass analyses of small molecules, and in label-free assay on a biochip by using LDI-ToF MS.

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A Convenient Phospholipase Assay by Using Mass Spectrometry

이지언, 김영관, 유수윤, 민달희

KAIST 화학과

Lipase is an important class of enzymes because they are involved in various biological processes ranging from cell signaling process to metabolism of dietary triglycerides. Among them, phospholipase D (PLD) is an enzyme that hydrolyzes phospholipids to form phosphatidic acid and corresponding head groups. This enzyme also has a unique property known as transphosphatidylation, catalyzing the transfer of phosphatidyl groups to various acceptors. To measure PLD activity, several methods utilizing conductance, fluorescence, chemiluminescence, and radio-labeled lipid substrate are currently available. These assay techniques may require sophisticated skills, expensive reagents, tedious sample preparation or cumbersome purification steps. Moreover, many of the conventional methods require labels, which often interfere enzymatic functions in part. In this report, we describe a label-free and quantitative lipase assay platform by using graphene thin films and matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-ToF MS). Graphene-based substrate enabled surface immobilization of phospholipids and matrix-free mass spectrometric analysis of phospholipids and corresponding lipid products generated by PLD. In addition, this platform is compatible with chip-based assay for high-throughput screening of PLD activity. We believe that this new platform for lipase assay will be an important addition to the lipase assay technology and one of the novel application fields of graphenes.

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The studies on the removal of perchlorate ion in aqueous solutions by applying GAC and IXE resin

박수민, 팽기정

연세대 화학과

Perchlorate (ClO_4^-) is the material that is used as propellants of rockets as a form of ammonium perchlorate salts. Perchlorate is in water because old rockets are demilitarized by the water-jet method. If people take it, it interferes with absorption of iodide which is the substance needed to synthesize thyroid hormone in the thyroid gland so that it derivatively has an bad influence upon disturbing pregnancy and synthesis of growth hormone. Therefore, the effective method is necessary to remove perchlorate in water. In this study, we tried to remove the perchlorate through ion-exchange mechanism used several activated carbons and ion-exchange resins mixed properly. Activated carbons are widely used as an adsorbent for the removal of a wide range of pollutants from various matrices because of their high adsorption capacity, fast adsorption kinetics and ease of regeneration, then we estimated that activated carbons have effect on maximizing the adsorption efficiency from ion-exchange resins. Homogeneous or sequence mixtures that is made up of several ion-exchange resins sold in markets and Norit activated carbons are studied about the removal efficiency and selectivity using batch type experiment. Also, comparison to Purolite bifunctionalized ion-exchange resin that is known for the most effective materice is performed.

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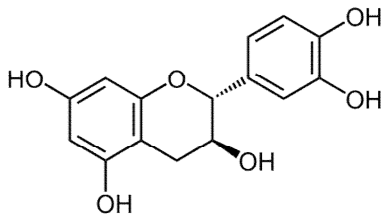
Analysis and antioxidant activity of catechin extracted from green tea

김동숙, 양정원, 송재미, 김영순

동국대 화학과

There are some actions of Catechin upon the human body such as absorbing ultraviolet radiation, suppressing cancer, and sterilizing action, isolating oxygen from harmfulness and preventing age. After extracting catechin taking above effects from a natural substance, we are supposed to make great functional cosmetics. Among others, it is extracted from green tea highly containing catechin. According to this step, we can find out whether producing functional cosmetics is possible or not. First of all, we use various extraction methods to extract catechin from green tea, and then we have to inspect existence and nonexistence of catechin by HPLC that proves those efficacies. Secondly, we confirm how much ultraviolet radiation can be absorbed by using UV spectroscopy. Lastly, the DPPH method is conducted to find out antioxidant activity.



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발표종류: 포스터, 발표일시: 금 14:00~16:00

다성분 혼합가스의 측정 정확성 향상을 위한 유량보정 방법에 대한 연구

김정원, 김정우, 정우찬

대성산업가스(주) 초저온연구소

레이저 발진용 혼합가스 제품과 같이 다성분 혼합가스 제품의 품질보증을 위해서는 매트릭스 영향을 줄이기 위해 같은 조성의 다성분 표준가스를 제조하여 성분별 함량을 측정해야 한다. 중량법으로 제조한 다성분 표준가스는 제조의 정밀성을 확인하기 위해 병간 균질도(homogeneity)를 확인하는 과정뿐만 아니라, 성분별 함량의 정확성을 확인하기 위해 단일성분 표준가스와 비교 검증하는 과정을 거친다.일반적으로 혼합가스의 정량분석에는 가스크로마토그래피가 이용되며, 샘플가스의 정밀한 주입을 위해 열질량유량조절계(MFC) 또는 버블유량계(Bubble flowmeter)의 유량보정법이 사용되고 있으나 매트릭스의 차이에서 기인한 몰분율의 차이로 상대감도차가 발생하게 된다.본 연구에서는 단일성분과 다성분 혼합가스의 정량분석에 있어 다양한 유량보정방법을 통하여 상대감도차를 확인하였다. 그리고 이를 최소화할 수 있는 압력보정방법을 개발하여 보정방법간의 비교를 통해 다성분 혼합가스의 측정 정확성 향상방안을 제시하고자 한다.

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On-line Chiral Analysis with Ultra Performance Liquid Chromatography Coupled with Quadrupole Time-of-Flight Mass Spectrometry by Applying Kinetic Method in Post-Column System.

jinhua, 이용일

창원대 화학과

An on-line ultra performance liquid chromatography-quadrupole time-of-flight mass spectrometry (UPLC-QToF-MS) method has been developed for chiral analysis. The developed method was successfully applied for discrimination and accurate quantification of chiral DL-phenylmercapturic acid and DL-benzylmercapturic acid. The approach was established on Cook's single ratio kinetic method, based on kinetics of competitive unimolecular dissociation of singly charged transition metal ion-bound complexes. Initially, on-line UPLC was used for an achiral separation of two different biomarker chiral compounds and then chiral mass spectrometric detection was successfully used for enantiomeric differentiation. After achiral separation, an appropriate metal ion and reference ligand were pre-mixed and added to target chiral analyte by post-column to produce trimeric M(II)-bound complex ions, $[M^{II}(A)(ref^{*})_2–H]^+$ (M^{II}, divalent transition metal ion; A, analyte; ref^{*}, reference ligand). These trimeric complex ions on collision dissociation produce two dimeric complex ions, $[M^{II}(A)(ref^{*})–H]^+$ and $[M^{II}(ref^{*})_2–H]^+$. The ratio of two dimeric complex ion abundances for one enantiomer expressed relative to that for the dimeric fragments of other enantiomer gives chiral discrimination. Rapid quantitative chiral analysis of DL-phenylmercapturic acid and DL-benzylmercapturic acid was achieved by constructing calibration curves derived from the kinetic method, related the ratio of the branching ratios against the enatiomeric composition of their mixture.

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Application of solid-state ,^{13}C NMR spectroscopy to study organic matter quality in reclaimed boreal forest soils

오세웅, *I. Turcotte, *S.A.Quideau

*목포대 화학과 *Dept of Renewable Resources, Univ of Alberta*

Solid-state ^{13}C NMR has emerged as a key analytical technique to gain insight into soil organic matter composition. Peat organic soils, deciduous and coniferous floors have unique ^{13}C NMR spectral properties that may serve as semi-quantitative tools to evaluate botanical inputs to the soil. Chemical composition of the low density fractions isolated from disturbed and undisturbed sites in the Fort McMurray oil sands region has characterized using solid-state ^{13}C NMR spectroscopy. Differences between disturbed and undisturbed sites reflected influence of different botanical inputs to soil organic matter. Reconstructed soils were characterized by significantly lower alkyl carbon over O-alkyl carbon rates than undisturbed sites. The aromatic and phenolic carbon signals were significantly more important for the undisturbed sites with a contribution of 34.1 % (±3.7), while these averaged at 20.7 % (±3.7) for the disturbed sites.

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Change of polyphenol components in chili pepper infected by anthracnose

김해경, 박세민, 최진영, 신성철

경상대 화학과

Pepper (Capsicum annuum) is one of the most widely cultivated fruit crops in the world and is the most economically important. However, this variety is highly susceptible to major fungal diseases, such as anthracnose, Botrytis cinerea, and powdery mildew. Anthracnose is the first most important disease of pepper and is caused by Colletotrichum fungus species. Polyphenols play a vital role in the growth and propagation of plants and protect plant tissues from damage. A number of phenols are regarded as pre-infection inhibitors, providing plants with a certain degree of basic resistance against pathogenic microorganisms. The objective of our study was to identify the phenolic compounds and generate characteristic chroma-tographic fingerprints of fresh pepper (FP) and infected pepper(IP) by liquid chromatography electrospray ionization mass spectrometry (LC/MS–MS) methods.

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Construction of Solid-state NMR Probe for Bicelle Sample Studies of Membrane Proteins

박태준, 김용애

한국외국어대 화학과

X-ray crystallography and conventional solution NMR spectroscopy techniques are difficult to use for the study of membrane protein structures, because the lipids required for the structural integrity and functionality of the membrane proteins prevent the crystallization of the proteins as well as reducing their rate of overall reorientation in solution. Solid-state NMR experiments on lipid bilayer or bicelle samples are valuable for membrane proteins with a predominantly helical secondary structure. Because these oriented samples takes advantages of the spectral simplifications that result from uniaxial orientation parallel to the direction of applied magnetic field. Especially, the sample preparation of the bicelles is easier and the bicelle samples are more stable than mechanically oriented lipid bilayer samples between glass plates, so that they can be kept for more than a year. So magnetically aligned bicelle samples in recent years are frequently used to determine the structure of membrane proteins by solid-state NMR spectroscopy. In this study, the double resonance probe has been designed to carry out polarization inversion spin exchange at the magic angle (PISEMA) experiments to obtain orientational constraints for the aligned membrane proteins in lipid bicelle environment at 400MHz wide-bore magnet. Here, we present the home-built solid state NMR probe and the preliminary 2D PISEMA and SAMMY spectra of bicelle samples.

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Composition and structure analysis of PE-1-octene using time-domain NMR

박선영, 정민환

LG화학기술연구원 CRD연구소

NMR analysis of olefin is time consuming as the polymer melts at high temperature. However, faster analysis can be achieved with Time-domain NMR (TD-NMR) technique which gives reproducible and non-destructive analysis without the need of a solvent. This poster presents 2 examples where olefin was analyzed with TD-NMR.First is a composition analysis of PE-1-octene. The comparison of FID signals (without FT) led to a calibration curve for PE-1-octene. Because of the different relaxation behavior, hard and soft parts in one sample were distinguished along with their amounts.Second is block PE-1-octene copolymer analysis. Using the least-squared method, hard segment % was measured from FID curve. Difference existed between block and random copolymer.

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A simple electrochemical detection of small molecules and enzyme reaction utilizing oligonucleotides on the gold electrodes

김재일, 박꽃한아름, 김동은, 여운석

건국대 생명공학과

The measurement of enzyme activity and detection of small molecules are one of the major themes in biology for basic researches and in biotechnology for various applications. Recently, many elaborate methods have been reported focusing on simplicity and rapidness of the protocol. In this poster, we present a new method of enzymatic assay and small molecule detection using DNA immobilized biochip and electrochemistry. The strategy was based on the DNA duplex on biochips which was comprised of capture DNA on the self assembled monolayers (SAMs) on gold and the complementary DNA modified with ferrocene. In response to interaction between the small molecule and DNA duplex on the biochip the electrochemical ferrocene signals changed, which verified the presence of small molecules in solution. Secondly, we applied our approach to enzyme activity assay. As a model system helicase, the DNA duplex unwinding enzyme was tested. We observed that the ferrocene signal was diminished as the enzyme reaction proceeded indicating that unzipped DNA strand by helicase was dissociated from the biochip.

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WO_3/SnO_2 based thick film gas sensor for detecting Hydrogen sulfide

김용재, 민병삼, *박영호, 이창섭

*계명대 화학과 *한국국제대 제약공학과*

This study investigates sensitivity of the sensor to Hydrogen sulfide gas with operating temperatures and catalysts. The thick-film semiconductor sensor for Hydrogen sulfide gas detection was fabricated WO_3/SnO_2prepared by sol-gel and precipitation methods. The nanosized SnO_2 powder mixed with the various metal oxide(WO_3,TiO_2,and ZnO) and doped with transition metals(Au, Ru, Pd Ag and In). Particle sizes and specific surface areas of sensor materials were investigated by SEM, XRD and BET analyses. The metal-WO_3/SnO_2thick films were prepared by screen-printing method. The measured sensitivity to Hydrogen sulfide gas is defined as the ratio (Ra/Rg) of the resistance of WO_3/SnO_2 film in air to the resistance of WO_3/SnO_2 film in a Hydrogen sulfide gas. It was shown that the highest sensitivity and selectivity of the sensor for Hydrogen sulfide by doping with 1wt% Ru and 10wt% WO_3 at the optimum operating temperature of 200℃.

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중합 조건에 따른 Poly(lactic acid)의 분자량 변화에 대한 연구

오선옥

(주)LG화학기술연구원

PLA 는 biomass 를 기반으로 한 높은 기계적 능력과 열가소성, 직물능력과 생체적합성을 가지고 있는 선형 지방족 열가소성 polyester 이다. 최근에는 PLA 와 같은 biopolymer resin 을 기존 ABS, PC, PP 등의 수지와 compounding 하여 물성을 보강한 후, 휴대폰 외장재, 자동차 내장재 등의 용도로 사용하려는 노력이 활발해 지고 있다. 이러한 PLA 는 주로 lactic acid 를 lactide 로 제조하고 이를 다시 ring opening polymerization 을 통해 제조하는 방법이 사용된다. 본 연구에서는 반응 온도, 촉매 종류, 촉매 량과 같은 중합 조건에 따른 분자량 변화 및 antioxidant 와 metal deactivator 가 내 가수성에 미치는 영향에 대한 연구를 진행하였다. 이를 통해 최적의 중합 조건 및 최적의 antioxidant 와 metal deactivator 의 조합을 확인하였다.

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Study on the SnO_2/ZnO gas sensor for detecting toluene gas

민병삼, 김용재, *박영호, 이창섭

*계명대 화학과 *한국국제대 제약공학과*

This study investigates the use of ZnO, Ag, Au, Cu, In, Pd, and Ru that greatly improves the sensitivity of the sensor to toluene gas. The metal-SnO_2/ZnO thick films were prepared by screen-printing method onto Al_2O_3 substrates with platinum electrode. The characterization of the sensor meterials were investigated will SEM/EDS, XRD, BET, and FTIR analyze. The sensing characteristics were investigated by measuring the electrical resistance of each sensor in a 1L chmber as a function of detection gas concentration. This was then used to detect toluene, benzene, xylene, ethanol and methanol vapours within a concentration range of 1-2000ppm. The gas sensing properties of metal-SnO_2/ZnO thick films depended on the content and variety of metals. It was found that sensitivity and selectivity of the films for toluene gas at 350℃ showed the best result by dopping with 1wt%Cu and 20wt%ZnO on SnO_2.

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GPC-viscometer를 이용한 Polybutadiene의 구조 분석

유진숙

(주)LG화학기술연구원 CRD 연구소

신발 밑창이나 자동차 타이어, 스포츠 용품, 고무 피복이나 벨트 등 다양한 곳에 사용되는 고무의 한 종류인 polybutadiene rubber (BR)는 중합 시 일반적으로는 1,4- addition 으로 반응이 진행되지만 소량 1,2-addition 으로 진행되기도 한다. 1,2-addition 반응으로 생긴 이중결합의 side chain 이 반응하여 가지형 고분자가 만들어지기도 하는데 선형 대비 가지형 성분이 많아질수록 고무의 물성이 달라진다. 따라서 Gel permeation chromatography(GPC)법을 이용해 고무 시료를 분자량 별로 분리한 후 light scattering 과 viscometer 를 이용하여 분자량에 따라 고무 시료의 구조를 분석하였다.

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Development of compositional analysis method of Polyamideimide (PAI)

송신헌, *유정석, **신은미

*LS전선 분석기술그룹 *LS전선 중앙연구소 분석기술그룹 **LS전선 중앙연구소*

A lot of properties of a polymer, which including thermal, mechanical and physical properties are influenced by the type and the ratio of the components that compose of the polymer. Therefore, structural information makes it possible to develop polymer materials with great properties. We have successfully developed compositional analysis method of polyamideimide (PAI). To analyze the polymer efficiently, PAI, which composed of methylenediamine (MDA) and trimellitic anhydride (TMA), was cleaved by pyrolysis and hydrolysis. The cleaved fragments were exactly detected using gas chromatography/mass spectrometer (GC/MS) and ^{1}H-NMR. The ratio between MDA and TMA was determined by ^{1}H-, ^{13}C-NMR, distortionless enhancement by polarization transfer (DEPT) and 2 dimensional (2D) NMR of PAI.

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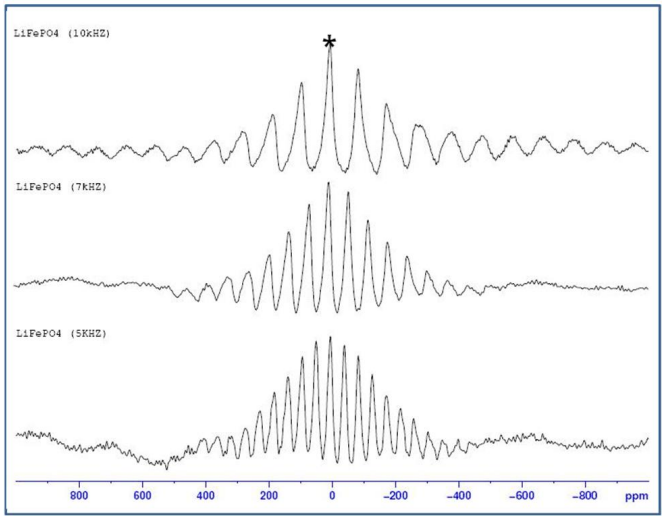
7Li and 31PMAS NMR Studies of OlivineLiMn$_x$Fe$_{1-x}$PO$_4$ (x = 0, 0.6)-Type Materials

박슬아, 송혜영, 이영일

울산대 화학과

Olivines of LiMPO$_4$ (M=Mn, Fe, Co, Ni) have received much recent attention as promising positive electrode active materials for lithium rechargeable batteries. Solid-state NMR study has been performed to understand of relationship of atomic environment and electrochemical performance forOlivineLiMn$_x$Fe$_{1-x}$PO$_4$ (x = 0, 0.6). Magic angle sample spinning (MAS) NMR spectroscopy is a complementary technique which is very sensitive to the atomic and electronic environment at the lithium and phosphorous sites. Successful application of the MAS NMR technique would allow direct observation of Li and P in the bulk of these interesting materials. 7LiMAS NMR of LiFePO$_4$ spectra are characterized by single isotropic peaks and broad spinning sideband manifolds, as expected for paramagnetic materials containing a single type of Li site, as shown in Fig. 1. The 7Li NMR spectra of LiFePO$_4$ yield an isotropic 7Li peak at 5 ppm.



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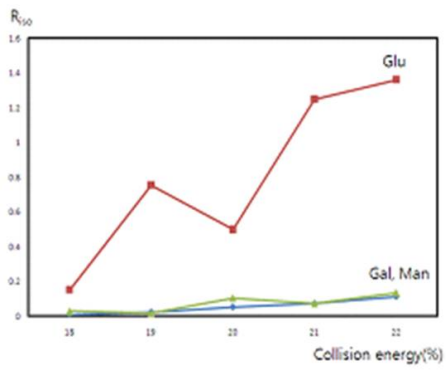
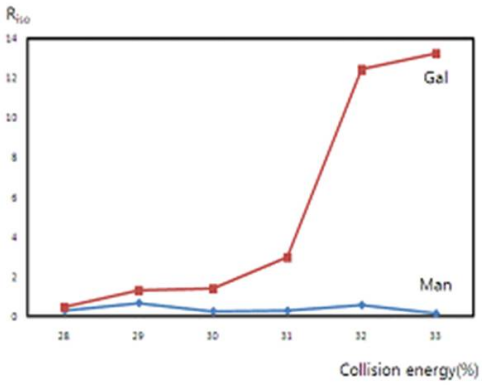
Isomeric discrimination of Oligosaccharides, D-Glucose, D-Galactose, D-Mannose using kinetic method by electrospray ionization ion trap mass spectrometry

신준영, 이용일

창원대 화학과

A rapid distinguished isomeric oligosaccharide, D-Glucose (D-Glu), D-Galactose (D-Gal), D-Mannose (D-Man) is achieved using electrospray ionization and cluster ion dissociation with data analysis by cook's kinetic method. The kinetic method is based on the competitive dissociation of divalent transition metal ion bound to trimeric complex ions in an ion trap mass spectrometer. Present work describes, the optimization of the method and the isomeric discrimination(R_{iso}), ratio of the two fragment ion abuandances. When the complex contains one isomer of the analyte expressed relative to that for the other isomers. Transition metal bound complex ion performed using mixture of Cu(II), D-tryptophan and analyte. The D-Glu was distinguished from D-Gal and D-Man in the MS^2 spectrum(Fig.1). In the MS^3 spectrum(Fig.2) D-Gal and D-Man could be distinguished by the isomeric ratio. Fig.1: Ratio of D-Glu, D-Gal and D-Man in MS^2 spectrum. Fig.2 :Ratio of D-Gal and D-Man in MS^3 spectrum





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Comparison between aptamer-based direct competitive assay and direct and indirect competitive enzyme-linked immunosorbent assay (cELISA) for determination of residual tetracyclines

전옥금, 류지은, 박호영, 이인숙

서울여대 화학과

Tetracycline antibiotics are protein synthesis inhibitors, inhibiting the translation. So that they are widely used for prevention and control of infectious diseases. Also they have been widely used for growth promotion and therapeutic purposes in animal husbandry. However, indiscreet applications of antibiotics can induce an increase of tolerance. To ensure the safety and reliability of food, novel assay designs are still desired. In this work, the three kinds of competitive assays were performed to determine tetracycline. One is an anti-tetracycline aptamer-based competitive assay which has been developed using avidin-biotin system. Aptamers are short, single-stranded, functional DNA or RNA that bind nearly any target molecules, from small molecules to proteins, with high affinity and selectivity. Consequently the aptamer-based competitive assay was suited to the determination of tetracycline. The others were performed to determine tetracycline using anti-tetracycline antibodies with shortened steps than hitherto cELISA designs. As a result, attractive features (for instance, wide dynamic range, low detection limit and high selectivity) were obtained not only in buffer but also in real samples, for instance, milk and honey.

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Development of Enzyme Linked Aptamer Assay (ELAA) for sensitive and selective screening of dopamine

박호영, 전옥금, 류지은, 이인숙

서울여대 화학과

As a new biorecognition element, aptamers are short DNA or RNA oligonucleotides that fold up into unique 3-D structures, allowing them to bind specifically to other target molecules. Aptamers have numerous advantages over antibodies. Aptamers are stable, ease in conjugation to various molecules at desired locations and adaptability to various targets. Also these have low immunogenicity, high specificity and affinity for target materials. Thus, aptamers have become a potential alternative to antibody. In this work, Enzyme Linked Aptamer Assay (ELAA) method was performed to determine dopamine (DA). Dopamine (DA) is one of catecholamine and play a important role in the brain. The assay optimized incubation time, temperature and especially buffer composition. Also it used avidin/biotin system for the signal amplification.

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Determination of Hexavalent Chromium in PCB (printed circuit board) by Ion chromatography coupled with Inductively coupled plasma Atomic Emission Spectrometer

김유나, 남상호

목포대 화학과

PCB(printed circuit board)는 RoHS 규제가 적용되는 광범위한 전기.전자제품 분야 중 하나로 TV, VTR, 컴퓨터, 휴대폰 등 모든 전자제품에 필수적으로 사용된다. 실생활에 직접적으로 사용되기 때문에 PCB 내의 유해물질 분석은 매우 중요하다. 유해물질 중 크롬은 산화상태에 따라 우리 몸에서 필수 영양소로 작용하는 Cr(Ⅲ)와 독성이 매우 강한 Cr(Ⅵ)로 나눌 수 있다. Cr(Ⅲ)는 우리에게 포도당, 콜레스테롤 등을 활성화시켜 지방의 대사를 도와주는 필수적인 영양소이지만, Cr(Ⅵ)는 강력한 산화제로 접촉 시에는 피부궤양 및 피부암을 유발하고 섭취 시에는 세포안으로 침투하여 암을 유발하는 독성물질이다. 이러한 독특한 크롬의 특성 때문에 시료중의 Cr(Ⅲ),(Ⅵ)의 분리는 총 크롬양에 대한 분석보다 더 중요시되어진다. 주로 Cr(Ⅲ),(Ⅵ)의 분리 분석법으로 diphenylcarbazide(DPC)와 착물을 형성시켜 발색정도를 분광 광도계로 측정하는 방법이 이용된다. 이 방법은 높은 검출한계를 가진다는 단점과 시료의 전처리가 완벽하지 못하다는 단점이 있기 때문에 본 연구에서는 IC-ICP-AES(Ion chromatography - Inductively Coupled Plasma - Atomic Emission Spectrometer) 기기를 사용하여 실험하였다. IC-ICP-AES 를 사용함으로써 낮은 검출한계와 Microwave Digestion 을 이용한 완벽한 전처리 등의 장점이 있다.Method EPA 3060a 방법을 사용하여 시료를 전처리하고 Ionpac AS7 column 을 사용함으로써 수용액 중에 음이온으로 존재하는 Cr(Ⅵ) (CrO 나 CrO)를 효과적으로 분리할 수 있었다. Eluent 는 0.25 M (NH)SO, 0.1 M NHOH 를 사용하였다.

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Reduction of the intensities of alkali-metal adducted ions in matrix-assisted laser desorption/ionization mass spectra of peptides using carbohydrate addition

양효직, *박규환, **김현식, 김정권

*충남대 화학과 *한국기초과학지원연구원 질량분석개발팀*
***한국기초과학지원연구원 질량분석기개발팀*

In this study, we applied various carbohydrates to a commonly used MALDI matrix a-cyano-4-hydroxy cinnamic acid (CHCA) to reduce the intensities of alkali-metal adducted peaks. To elucidate the mechanism of reduction of the alkali-metal adducted ion peaks by using carbohydrates, we tried glucose, sucrose, and raffinose to the matrix solution. The addition of carbohydrates to the CHCA solution significantly improved and enhanced the signals and even no interference was observed for tandem MS/MS result.

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UV 경화형 acrylate 점착제 중 잔류 AOI 및 MOI 분석

김노선

LG화학기술연구원

AOI (2-(Acryloyloxy)ethyl isocyanate) 및 MOI (2-(Methacryloyloxy)ethyl isocyanate) 는 점착제 경화를 위하여 점착 수지 중합 시 혼용하여 사용되는 경화 작용기를 포함하는 모노머이다. 수지 중합 후 잔류하는 AOI 및 MOI 는 점착제의 점착력 차이 및 경시 변화에 영향을 미치게된다. 이러한 미량의 잔류 AOI 및 MOI 분석을 위해 우레탄 유도체화하여 GC/FID 분석법을 개발하고, UV 경화형 acrylate 점착제 중 잔류 AOI 및 MOI 분석에 적용하였다. AOI 및 MOI 를 이용한 우레탄 유도체의 반응성 및 분석법의 직선성, 정확도, 정밀도 및 검출 한계와 같은 분석법 유효화 데이터와 점착제 제품에 적용하여 확보한 분석 데이터를 보고하고자 한다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

금속표면 코팅에서의 Cr(VI)의 정량을 위한 유효성 평가

(Evaluation of effectiveness for measuring hexavalent chromium(Cr(VI)) quantity on corrosion-protected metals coatings)

임혜영, *김성일, **신은미

*LS전선연구소 분석기술그룹 *LS전선 분석기술그룹 **LS전선 중앙연구소*

2003 년 2 월에 WEEE(Waste Electrical and Electronic Equipment)에 의해 제정 공포되고 2006 년 7 월 1 일에 발효된 유럽연합의 유해물질 사용제한지침인 RoHS(Restriction of Hazardous Substances Directive)는 해로운 물질을 사용한 전자제품이나, 전기기기를 제한하는 지침으로 Pb, Cd, Hg, Cr(VI), 등 6 개 유해물질을 사용을 제한하고 국제 분석표준을 IEC 62321 로 제정해 KOLAS(Korea Laboratory Accreditation Scheme.한국인정기구)에서 분석시험기관을 선정하고 있다. IEC 62321 규격으로 KOLAS 인정을 받을 경우 Annex 해당부분은 유효화 검증이 필요하다. 그 중 Annex B 는 금속재질에 코팅된 Cr(VI)의 존재확인을 위한 실험방법으로 끓는 물에 용출한다. 관련 CRM 이 존재하지 않으므로 유효화 검증을 위해서 Cr(VI) 표준용액을 고농도, 저농도로 spike 하여 "화학적 시험방법의 유효성 확인을 위한 KOLAS 지침"에서 기술된 절차에 따라 Annex B 의 시험방법의 유효성을 평가해 보았다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Determination of the residual byproducts of a crosslinking power cable insulation using headspace - gas chromatography/mass spectrometry(HS-GC/MSD)

유정석, 신은미

LS전선 중앙연구소

Nowadays, Crosslinked Ployethylene(XLPE) is applied as the insulation from medium voltage(MV) power cables to extra high voltage(EHV) power cables all over the world. LDPE is crosslinked by DiCumyl Peroxide(DCP) to form XLPE. Unfortunately, the reaction produce several byproducts such as methane, water, a-methylstyrene, acetophenone, a-cumyl alcohol. Because these materials, byproducts, are known as one of the causes for the insulation breakdown, so the byproducts should be removed through the degassing process as the last step of work. Therefore, Itis important to measure residual byproducts, a-Methylstyrene, Acetophenone, a-Cumyl alcohol, in power cables insulation. Using Headspace Gas Chromatography/mass spectrometry(HS-GC/MSD), the quantitative analysis were performed. 1,4-dioxane was used an internal standard and linear calibration curve with a correlation coefficient of r2 ≒ 0.99 were generated respectively. For the purpose of verifying the method, we tested for precision, Limit of Detection(LOD), Limit of Quantity(LOQ) and so on. As a conclusion, the analysis using HS-GC/MSD is an effective and correct measurement method for byproducts.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Comparison of the Bench-Top and Portable XRF Methods for the Analysis of Five Hazardous Metals in PE and PP Samples

최수정, 김종혁, 이석근

한국화학연구원 화학분석센터

RoHS and other environmental laws have been enforced in Europe and many countries. Especially, RoHS restricts the use of six hazardous materials such as lead(Pb), mercury(Hg), cadmium(Cd), hexavalent chromium(Cr(VI)) and their compounds, and two types of brominated flame retardants, polybrominated biphenyls(PBB) and polybrominated diphenyl ethers(PBDE) in the manufacture of various types of electronic and electrical equipment. There are several methods for the analysis of six materials, and the first step is screening by x-ray fluorescence spectrometer(XRF) in that it is non-destructive and real-time multi-element analysis. For this reason, it has led to increasing interest towards XRF spectrometry. As a basic research for development of the domestic portable XRF spectrometer, we will discuss the analytical results of bench-top and field-portable XRF methods for five heavy metals such as Pb, Hg, Cd, total-Cr and total-Br in Polyethylene(PE) and Polypropylene(PP) certified reference materials(CRMs) and real plastic samples.

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폴리카보네이트 수지 중 인계 난연제 정량분석

진미경

(주)LG화학기술연구원 CRD연구소

난연제는 고분자 물성 향상에 도움을 주는 물질로 기존에는 할로겐계 난연제가 주로 사용되었으나 최근 할로겐계 난연제의 규제로 인하여 비할로겐계 난연제를 쓰고 있는 추세이다. 비할로겐계 난연제 중 인계난연제가 폴리카보네이트와 같은 수지에 많이 사용되고 있다. 난연제의 함량 및 종류가 수지의 물성에 많은 영향을 주기 때문에 그 종류 및 함량을 측정하는 것이 중요하다. 이러한 이유로 인계 난연제의 정성 및 정량분석법들을 자체적으로 확립하여 활용하고 있다. 정량분석의 중요인자인 전처리에서 용매 및 추출방법을 최적화하였다. 또한 직선성, 정밀도, 검출한계, 회수율을 측정하여 유효성 검증을 하였다.

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The identification of unknown plasticizer in optical film using GC/MS, LC/MS and NMR spectroscopy

권혁주, 김건성, 이귤섭

효성기술원 분석센터

Plasticizers are added to various industrial products such as plastic, cement and film for improving properties like plasticity, elasticity and flexibility. It is important to verify the entity of plasticizer in optical film due to its different effect on physical properties. In this work, unknown plasticizer in optical film was analyzed by GC/MS, LC/MS and ^{1}H-NMR spectroscopy. Besides, the formation of amide and primary alcohol by aminolysis with monoethanolamine was performed to predict the chemical structure of unknown plasticizer.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Sequence Relation and Qualitative Analysis of Various Inks using TOF-SIMS

이지혜, *이연희, 김강진

*고려대 화학과 *KIST 화학분석센터*

Red stamping-ink samples are frequently submitted to forensic laboratories for identification and comparison in a wide variety. Time-of-flight secondary ion mass spectrometry (TOF-SIMS) for the analysis of red stamping-inks on paper surfaces was investigated. TOF-SIMS spectra were employed to identify elements and organic compounds in Korean, Chinese and Japanese red stamping-ink samples. In addition, the documents printed by ink-jet printer and laser-jet printer were discriminated by using TOF-SIMS spectra. And overlapped area of red stamping-ink with ballpoint pen or red stamping-ink with printed letter in the document was also investigated in order to identify the sequence of recording. The sequence relation was also studied as getting mapping image of the character section which a stamp was printed on. Therefore, this study indicates that TOF-SIMS is a useful technique for the non-destructive analysis of questioned documents.

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Monitering of Cartap, Tecloftalm, Cyromazine Pesticide Residues in Agricultural Products by GC, LC

신용운

부산지방식품의약품안전청 유해물질분석과

To monitor pesticides residues of agricultural products circulating in Korea market, we analyzed samples. 152 of the samples (16 kinds of vegetables, cereal grains, potatoes and fruits) have been collected in different 13 provinces (Incheon, Seoul, Gyeonggi, Chungcheong, Gangwon, Busan, Daegu, Gyeongsamg, Jeolla, Gwangju, Deajeon, Ulsan and Jeju provinces) between March and May, 2009. The average recoveries obtained from each sample ranged between 80 and 98% about 0.1 to 2.5ppm concentration. These pesticides were analyzed with linearity of 0.9993-0.9998 by GC/FPD, GC/ECD, LC/PDA. All pesticides (Cartap, Tecloftalam, Cyromazine) were not detected in this period.

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Determination of the Major Elements (Na^+,K^+,Ca^{2+},and Mg^{2+}) in Various Salts by Ion Chromatography (IC)

CUI SHENG, 남상호

목포대 화학과

The major elements (Na^+,K^+,Ca^{2+},and Mg^{2+}) in salts have been determined in this study. Due to the different environments and the forming process, the contents of the major elements in salts from different places are not identical. Ion Chromatograply (IC) has been used for the quantitation of the investigated elements in salts. A number of various salts from Korea and other foreign countries have been studied. The salt samples were prepared by dissolving the salts in water as suitable concentrations, then determined by IC directly. The results for the salts have been compared and discussed in terms of concentrations of the major elements in salts.

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Amine 자성 입자의 표면 특성 평가와 정량 분석

이나래

(주)아스타 연구개발팀

나노 및 마이크로 크기의 자성입자는 단백질, DNA 또는 생물시료를 분리 및 정제하는데 널리 이용되고 있다. 특히 SiO2, Amine, COOH 와 같이 다양한 기능기로 코팅된 자성 입자는 고가의 분석 장비 없이도 목적에 따라 선택적으로 사용될 수 있어 그 수요가 점점 증가하고 있다. 그러나 amine 으로 코팅된 나노 자성 입자의 표면기를 정확하게 정량하는 방법에는 어려움이 있다. 따라서 본 연구에서는 FE-SEM 과 형광 현미경을 이용하여 amine 자성입자의 표면특성을 확인하였고, Ninhydrin 법을 이용하여 정량 분석하는 실험을 수행하였다. 일반적으로 Ninhydrin 은 1 차 amine 과 80~100℃에서 2~5 분정도 반응하여 청남색(Ruhemanns Blue)을 띤다. Standard 로 Glycine 과 Glutamic acid 를 사용하였고, 반응시간, 온도, pH 의 변화에 따른 Ninhydrin 의 영향을 살펴보았다. Ninhydrin 법은 적은 오차 범위 내에서 amine 표면기를 정량할 수 있는 방법이고, 이를 이용하여 정량 분석 하는데 최적의 조건을 찾고자 하였다.

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Characterization of Alumina Nanofibers Synthesized by Sol-Gel and Electrospinning Techniques

조준모, 박주연, 강용철

부경대 화학과

One-dimensional nanostructures such as nanowires have been extensively studied as building blocks for nanoscale electronic devices.The synthesized alumina nanofibers have been fabricated by using electospinning technique between the tap of a needle and the drum collector. The experimental results show that the morphology and crystalline phase alumina nanofibers are influenced by the content of aluminum oxide in composite nanofibres and the calcination temperature.The synthesized alumina nanofibers were characterized by scanning electron microscopy (SEM), diffuse reflectance Fourier transform infrared spectroscopy (DRIFTS), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

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Analysis of small and polar compounds using Hydrophilic Interaction Chromatography (HILIC) with Mass Spectrometry

임영희, 박덕희, 조혜성

LG화학기술연구원 CRD연구소

Detection of small and polar compounds (lactic acid or vitamins) was performed by LC/MS with hydrophilic interaction chromatography. Compared to the reversed phase HPLC, HILIC is increased the amount of organic solvent in the mobile phase and retention time for analysis of the compounds. HILIC has advantages for sensitivity and peak shape of the compounds.

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Effect of carrier viscosity and channel angle on elution of micron-sized particles in gravitational field-flow fractionation (GrFFF)

강다영

한남대 화학화

Gravitational field-flow fractionation (GrFFF) is a useful tool for separation of micron-sized particles. In this study, the effect of the carrier viscosity and the channel angle on retention, zone broadening and the resolution of micron-sized particles in GrFFF were investigated using polystyrene (PS) latex beads as the model particles. The channel angle (angle between the gravitational field and the longitudinal axis of the channel) was varied from 0° to 60°. The viscosity of the carrier liquid was varied by adding various concentrations of (hydroxypropyl) methyl cellulose (HPMC) in water. Then the retention ratio (R), resolution (Rs) were measured at various channel angles and at various carrier viscosities. Results showed the particles migrate faster as the carrier viscosity increases due to increased lift forces. Also the zone broadening decreases at higher carrier viscosity, presumably due to higher focusing effect. As a result, separation was improved in terms of both the separation time and the resolution, as the carrier viscosity increases. It seems that the improvement in the resolution is mainly contributed by reduction in the zone broadening.

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Quantitative analysis of various molecular weight controllers combinated to terminal groups of Nylon 6 by GC/FID and NMR spectroscopy

박민경, 오종하, 이귤섭

효성기술원 분석센터

The polymer yielded by the polymerization of Nylon 6 in the presence of suitable additives contains about 10% of a hydroextractable material composed of caprolactam monomers and cyclic oligomers containing 2 to 7 monomeric units, deteriorating polymer characteristics. They should be as low as possible and it can be acquired by decreasing the contents of terminal group through having control of polymerization kinetics. Accordingly, in the process of caprolactam polymerization, molecular weight controllers such as benzyl amine, amino tetramethylpiperdine(ATMP), terephthalic acid(TPA) and acetic acid etc. are used. The MW controllers terminate polymerization of Nylon 6, forming amide bonds with end groups of Nylon. To promote capability of Nylon 6, it is required to analyze quantity of terminators. In this study, we established the quantitative analysis methods to determine benzyl amine, ATMP, TPA and acetic acid by 1H-NMR and GC/FID with chemical reactions and compared those methods.

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Detection of explosive materials and mono-nitroaromatic compounds with poly(diallyl dimethyl ammonium chloride) film using SPR technique

양승주, *장성우, 유연규, *박찬량

*국민대 생명나노화학과 *국민대 화학과*

We studied the gas detection of explosive materials(2,4,6-trinitrotoluene, 2,4-dinitrotoluene, 2,6-dinitrotoluene) and mono-nitroaromatic compounds (nitrotoluene, nitrobenzene) with poly(diallyl dimethyl ammonium chloride) film utilizing SPR phenomena. The thicknesses of the polymer films were controlled by spin-coating method and the morphology of polymer films were obtained by atomic force microscopy at various thicknesses.The gas flow system for vapor generation of solid and liquid compounds was constructed using the porous solid sample holder and the bubbler chamber, respectively. The concentrations of vapor generation were quantified by the weight loss of samples with the purging the nitrogen gas.The detection limits of nitroaromatic compounds with functional polymer films using SPR technique were tested at several tens of ppb level.

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Large scale synthesis of silica nanoparticles with improved reproducibility and size characterization using sedimentation field-flow fractionation (SdFFF) and electron microscopy (EM)

안세영

한남대 화학과

Silica nanoparticles are usually synthesized by emulsion polymerization, which may not be reproducible in terms of the size distribution. In this study, silica nanoparticles having diameters of about 150 nm were synthesized by using tetraethylorthosilicate (TEOS) as the silica source, and ammonium hydroxide as the surfactant using a new apparatus, which provided much improved reproducibility in the size distribution of the silica nanoparticles. The size distributions of the silica particles were measured by sedimentation field-flow fractionation (SdFFF), dynamic light scattering (DLS), and field emission scanning electron microscope (FE-SEM) and Energy-Filtering Transmission Electron Microscopy (EF-TEM). The size data obtained by different techniques were compared.Two different types of the agitator (type-A and B) were tested. The effects of the agitator type and the agitation speed on the size distribution were investigated. Generally, as the agitation speed increases, the average diameter of silica particles tends to decrease. The use of the agitator type-A at the agitation speed of 400 rpm yielded a large scale synthesis of silica particles having the average diameter of 120 nm with a narrow size distribution.

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On-off Surface Plasmon Resonance Fuel Sensors for Direct Fomic Acid Fuel Cells

심혜림, *김예은, *이재영, 김수희, **Shaikh Nayeem Faisal**, 이혜진

*경북대 화학과 *광주과학기술원 환경공학과*

Formic acid is a highly promising liquid fuel for direct liquid fuel cells (DLFCs) since it both generates energy with high efficiency and possesses very low toxicity towards humans. While there has been extensive efforts in creating portable DLFC devices,[1-3] the design and introduction of fuel sensors to improve fuel cell performance and efficiency has been much less studied. In this presentation, on-off surface plasmon resonance (SPR) sensors measuring reflectivity changes upon the adsorption of formic acid fuels onto a thin gold film is demonstrated. In order to optimize the SPR detection signal specific to changes in formic acid concentration, a wide range of self-assembled monolayers formed on the gold surface featuring hydrophobic or hydrophilic functionalities are investigated. Excellent reproducibility and long-term stability were obtained for monitoring commonly used concentration ranges of formic acid in DLFCs. Finally, micro-SPR sensors are applied to a DLFC single cell unit to investigate on-off controlling of in-situ sensing capabilities.References:1. Uhm, S.; Lee, H. J.; Lee, J. *Physcal Chemistry Chemical Physics*, **2009**, accepted.2. Miesse, C. M.; Jung, W. S.; Jeong, K. J. *Journal of power sources*, **2006**, *162*, 532.3. Ha, S.; Dunbar, Z.; Masel, R. I. *Journal of power sources*, **2006**, *158*, 129.

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Comparison of Thermal Field Flow Fractionation (ThFFF) and Size Exclusion Chromatography(SEC) in analysis of Polysilanes

남유미

한남대 화학과

Thermal field-flow fractionation (ThFFF) is capable of separating various types of polymers having wide range of molecular weight. The ThFFF separation is based on both the chemical composition and the molecular weight (M). For homopolymers, separation is based solely on the molecular weight (or the size). ThFFF is particularly useful for separation of high molecular weight (or large) polymers. As the M decreases, the resolution (Rs) of ThFFF decreases because the retention of the polymers tends to decreases with decreasing M. In this study, the capability of ThFFF was tested for analysis of analysis of polysilanes having diphenyl or methyl phenyl functional groups. Then the ThFFF results were compared with those from size exclusion chromatography (SEC). Also the retention behavior of the polysilanes in THF, n-Hexane and toluene were studied. Polystyrene (PS) and polymethyl methacrylate (PMMA) were used as the calibration standards. Sample solutions were prepared by stirring for 24 hours at 30℃ in HPLC grade solvents.

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Monitoring Sweeteners as "stevioside, aspartame, sucralose and M.S.G" in soju by high-performance liquid chromatography

남윤식, 차기석, 이기수, *박현미, *이강봉

*KIST 특성분석지원단 *KIST 특성분석센터*

High performace liquid chromatography (HPLC) with UV 205nm was developed to monitor sweetener "stevioside, aspartame, sucralose and M.S.G" in soju which was made in Korea. The method is simple for sample preparation due to only use a single dilution.The LC separation was performed on an YMC-pack C18 (2.1 mm x 150 mm) with a mobile phase of acetonitrile and water (35:65).The method was validated. Standard solutions at 5 concentration levels which included range from 1 to 100ppm were prepared for the validation work, including the tests for precision, linearity and recovery.The solutions were prepared in triplicate for each concentration. The relative standard derivation (%RSD) for the precision test was 0.999. The average recovery ranged from 96 to 101% for the spiked soju samples with these standard concentrations. The detection limit for sweetener was estimated at 0.1~10 ppm.The method was used to monitor 11 kinds of soju samples; stevioside was detected range from 6.2 to 25.2 ppm and the other sweeteners were detected below the detection limit.

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Effect of sample loading on fractionation efficiency of a large scale SPLITT Fractionation (SF)

이지연

한남대 화학과

SPLITT Fractionation (SF) has been developed into a useful tool for preparative separation of colloidal particles. SF can be operated both in a batch mode (injection of a finite amount of sample) and in a continuous mode, where sample is fed continuously, thus allowing separation in a preparative scale. Conventionally, SF is carried out in a thin ribbon-like channel equipped with splitters at the inlet and the outlet of the channel, across which an external field is applied. In the current study, the external field is the gravity.In this study, the effect of the sample loading (the amount of the sample that can be processed in a unit time period, g/hr) on the fractionation efficiency (FE, number% of particles that are predicted by theory) of a large scale splitter-less SF system that was specially designed to operate in the full feed depletion mode (FFD) was investigated. In the FFD mode, there is only one inlet through which the sample is fed, thus the sample dilution is prevented. The sample loading of 3.0, 6.0, 9.0, and 12.0 g/hr were tested with polyurethane latex beads (PU). Then the large scale FFD-SF was tested with sea-sediment. For determination of the size distribution and FE of each SF-fraction, an optical microscopy (OM) was used.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Size-controlled synthesis of silica nanospheres and characterization by sedimentation field-flow fractionation (SdFFF) and dynamic light scattering (DLS)

김재훈

한남대 화학과

Silica particles are used widely as a particle standard, an enzyme of the bio-center in various fields such as a sieve in a semiconductor material, a membrane material, and environmental particle analysis. The characteristics, effects and the role of the silica particles vary according to the particle size. The purpose of this study is to develop a method for synthesis of silica nano-spheres having narrow size distributions in a large quantity. Like in a conventional emulsion-polymerization, tetra ethyl orthosilicate (TEOS) as a silica source, ammonium hydroxide, H2O, and ethanol were used. The reaction mixture is then stirred at room temperature for 6 hrs. The produced silica nanoparticles are then allowed to settle by centrifugation at 1600 rpm for 4-8 hrs. In this study, a specially manufactured reaction apparatus was manufactured for a large quantity synthesis of silica nano-spheres. Various reaction parameters (the agitator shape and size, stirring speed, and composition of the medium, etc.) were carefully tested for optimization of the synthesis. Then sedimentation field-flow fractionation (SdFFF) and dynamic light scattering (DLS) were used to characterize the silica particles. Silica spheres having the mean diameter of about 500 nm and relatively narrow size distribution were obtained at the stirring rate of 180 rpm.

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Characterization of whey proteins in raw milk using flow field-flow fractionation (FlFFF)

문재미

한남대 화학과

Whey proteins represent approximately 20% of the original milk proteins. The utilization of whey proteins is limited because there still exists a large variability in the composition and functional properties of commercial whey proteins. It is possible that the incongruence of physico-chemical and functional performance of whey proteins reported from different laboratories might result from the compositional variations arising from different whey resources or processing conditions in commercial whey products. In order to clarify this problem, how to obtain whey protein in its native form free from any denaturizing becomes of utmost importance.A simple and economical method to isolate whey proteins from fresh raw milk was developed by de-fatting, casein-eliminating, and then lactose-removing. The isolated whey proteins were analyzed using gel filtration chromatography (GPC) and flow field-flow fractionation (FlFFF). Four major whey components, including immunoglobulin (Ig), bovine serum albumin (BSA), -lactoglobulin (-Lg) and α-lactalbumin (α -Lac), and a non-protein of low molecular mass (～1.7 kDa) were detected simultaneously. FlFFF showed some unique advantages in protein analysis. First, there is very little (if any) mechanical stress on the sample components as the channel is open. Second, FlFFF is so versatile that various carrier liquids can be used. Third, the diffusion coefficient of sample components can be directly determined from the retention measurement.

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Multiresidue method for determination of 52 pesticide in cucumber and cabbage with comparison of extraction MSPD and QuEChERS using LC-MS/MS

박세민, 김해경, 최진영, 신성철, *정원영

*경상대 화학과 *경상대 자연과학대학*

Residues of 52 pesticides in cucumber and cabbage were analyzed by liquid chromatography-tandem mass spectrometry (LC/MS-MS). Pesticides were extracted by MSPD (matrix solid-phase dispersion) and QuEChERS method. The detection limit for the pesticides were varied from 0.4 to 1.7 μg/kg. The recoveries in MSPD methods were compared to those of the QuEChERS extraction.

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Determination of molecular weight and structure of carboxymethyl starch using asymmetrical flow field-flow fractionation coupled multi angle light scattering (AsFlFFF/MALS).

김선태

한남대 화학과

Carboxymethyl starch (CMS) is a water-soluble polysaccharide which is widely used as an additive in the paper industry or as a thickener in the formulation of textile printing pastes. The application of CMS in enhanced oil recovery is also growing. CMS is obtained as a product of the reaction of starch (St-OH) and sodium monochloro acetate in the presence of sodium hydroxide. The water solubility of CMS is reported to increase as the degree of substitution (DS) increases, and thus the change in DS will likely result in change in the molecular weight distribution.Cross-linked CMS has been used for the extraction of metals. By cross-linking and carboxymethylating, the corn starch becomes an active and relatively insoluble metal scavenger, useful for extraction of toxic metals. By increasing the degree of carboxymethylation and cross-linking, metal scavenging activity of the starch could be increased up to the level required for industrial applications. Cross-linking of CMS is achieved by irradiating CMS with γ-rays or electron beam. The dose needed for cross-linking depends on the degree of substitution. Also the radiation-induced cross-linking depends on the molecular weight. The larger the molecular weight, the lower the dose required to obtain the predetermined degree of cross-linking [1]. AsFlFFF-MALS has shown its applicability to determine the molar mass distribution of ultrahigh polymers such as starch [2]. This study deals with (a) carboxymethylation of native corn starch using sodium chloro-acetate and its molecular weight characterization using AsFlFFF-MALS, (b) modification of carboxymethylated starch derivatives by cross-linking with electron beam radiations and the estimation of their gel contents, and (c) evaluation of the cross-linked carboxymethyl starch derivatives for extraction of metals in water.

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Tandem gravitational split Fractionation (GSF)

문윤정

한남대 화학과

SPLITT Fractionation (SF) provides separation of particles into two subpopulations. Separation into more than two subpopulations requires repeated SF operations on the SF fractions. In this study, two SF channels were coupled online (SF/SF) to obtain separation into three subpopulations in one operation. Conventionally in SF, the sample suspension is fed through the top inlet, while the carrier liquid is fed through the bottom inlet to force the sample to form a narrow layer near the top of the channel, which results in about 10 times dilution of the sample. In this study, each SF was operated in the full-feed depletion (FFD) mode to prevent the sample dilution. Either the fraction-a or b from the first SF channel was fed into the second SF channel. When the fraction-b from the first channel (fraction-1b) was fed into the second channel, the fractionation efficiency (FE) of the fraction-b of the second channel (fraction-2b) was increased by about 10-15% compared to that of the fraction-1b.

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Surface-enhanced Raman Spectroscopy Using Stable Silica-Void-Triangular Silver Nanoparticles[발표취소 9-28]

고재윤, 정세훈, 김승빈

포항공과대 화학과

Metal nanoparticles, especially silver and gold, can be good controlled size and particle shape and are distinguished applications in catalysis, biosensors, surface-enhanced Raman scattering (SERS), etc. However, metal nanoparticles are easily aggregation and these phenomena make the damaged on catalysis and SERS effect. So, to maintain the consistent electromagnetic properties and prevent aggregation, metal nanopartic[illegible]ilica has lots of advantages for the capsulation of metal nanopa[illegible]oparticles have not affected any environmental or chemical char[illegible]ggregation, electromagnetic coupling and so on. Moreover, silica coating allow the easy attachment of functionalizing ligands and is inexpensive and rich in material that can produce much of coated particles in manufacturers. Therefore, we synthesized silica capsulated shape controlled triangular silver nanoparticle, and it is applied in SERS. If we get the great enhancement factor in Raman spectrum using this particle, it can be useful for the quantitative analysis.

발 표 취 소

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Surface-Enhanced Raman Scattering between Gold Nanocore and Nanoshell[발표취소 9-28]

허성우, 정세훈, 김승빈

포항공과대 화학과

For over 30 years, Surface-enhanced Raman scattering (SERS) has been known and investigated. Various types of metal nanoparticles such as Metal core with Silica shell and silica shell and metal shell have been extensively studies as SERS su [illegible] d and characterized the metal-silica-metal nanoparticles as SERS s [illegible] rough reduction of $AuCl_4^-$ and silica shells that entrap the core. Next [illegible] re covered by thin metal shell. Silica interlayer as probe-doped dielectric layer is synthesized by TEOS and probe-labeled organic silane. We controlled Metal core size and thickness of silica interlayer and metal shell. And change the metal of core and shell.

발 표 취 소

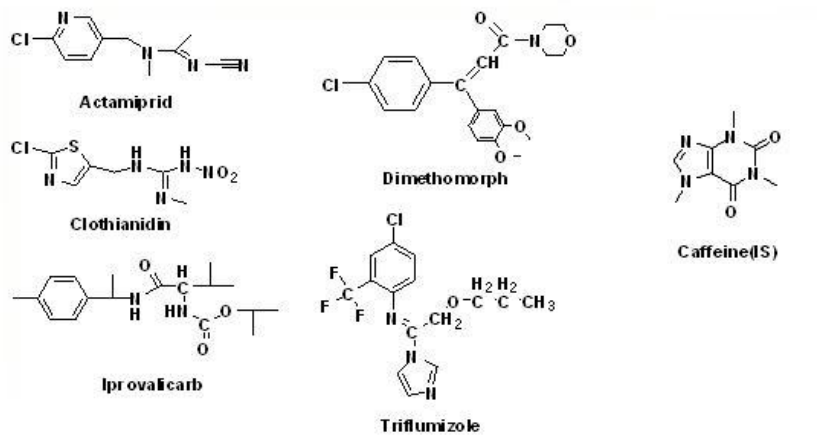
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅳ35P98포**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Method development of rapid and sensitive determination of pesticides in five cucumber species by liquid chromatography-electrospray mass spectrometry(LC/ESI/MS/MS)

박형진, 박세민, 최진영, 정원영, 김해경, 신성철

경상대 화학과

In this work, a new multi-residue methodology using liquid chromatography, ion-trap tandem mass spectrometry (LC-MS/MS) for the quantitative (routine) analysis of pesticide residues in cucumber species was evaluated for different types of vegetables of cucumber family- pumpkin, cucumber, watermelon. The Analytes were extracted by MSPD (matrix solid-phase dispersion) method. Mass spectrometric detections were performed in the multiple reaction monitoring (MRM) mode. The most sensitive transitions were used for the quantification of the analytes and the second transitions for confirmation. Mean recoveries were in the range from 80 to 93%. LOQ values fall into the range from 5ug/kg to 100ug/kg



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Separation of PAMAM dendrimers of various generations by using Asymmetrical Flow Field-Flow Fractionation (AsFlFFF)

Sachin Nehete

한남대 화학과

Asymmetrical-flow field flow fractionation (AsFlFFF) was successfully applied for separation of polyamidoamine (PAMAM) dendrimers of various generations (G4-G9), which have molecular weights ranging in 14-467 KDa and the radius of gyrations ranging in 17.87-46.47Å. A wide variety of analytical techniques have been tested for characterizing dendrimers: size exclusion chromatography (SEC), low angle laser light scattering, infrared (IR) spectroscopy, capillary electrophoresis, Mass spectrometry (chemical ionization and fast-atom bombardment), laser desorption, electro-spray ionization, matrix-assisted laser desorption/ionization-time-of-flight (MALDI-TOF), and 1H, 2H, 13C NMR. The performance of all those techniques tends to decline as the size of the dendrimer increases (1). It was reported that in SEC at neutral pH (7.2) due to strong electrostatic interaction with the column packing material, dendrimers (Generation-5) were not able to elute from SEC columns.(2) AsFlFFF, due to its open channel geometry, was able to separate and characterize the dendrimers without sample degradation. AsFlFFF was also applied to study the interaction of the PAMAM dendrimer (generation-5) and bovine serum albumin (BSA). It was found that higher order aggregates were formed at relatively higher dendrimer concentration. Results suggest AsFlFFF is useful for the separation and characterization of large charged molecules such as PAMAM dendrimers.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of Fe-type birnessite in presence of Hoffmeister anions

강광철, 백민훈, *황성주

*한국원자력연구원 방사성폐기물기술개발부 *이화여대 화학·나노과학과*

본 연구에서는 Hoffmeister 음이온인 Cl^-와 SO_4^{2-}이온이 Fe-type birnessite 의 합성시 구조 및 morphology 에 미치는 영향을 고찰하였다. 분석방법으로는 XAS(X-ray Absorption Spectroscopy) 분석으로 합성된 Fe- type birnessite 에서 Mn 및 Fe 의 산화 상태를 확인하였으며, 그 결과 $Mn4^+$와 $Fe3^+$ 의 산화수를 가짐을 확인하였다. Morphology 를 확인하기위해 FE-SEM(Field Emission-Scanning Electron Microscope)으로 합성된 Fe-type birnessite 의 표면 상태및 입자 크기를 확인하였으며, Hoffmeister 음이온의 영향으로 결정크기및 표면의 상태가 다르게 합성됨을 알 수 있었다. 또한 77K 에서 질소 흡탈착을 이용하여 BET 를 측정하였고, 측정결과 Cl^-에 의해 합성시 227.98m^3/g 으로 측정되었고, SO_4^{2-}에 의해 합성시 95.66m^3/g 으로 측정되었다. 이러한 비표면적의 차이는 양이온의 흡착에는 관여하나, 음이온 흡착에는 영향이 없는것으로 판단 된다.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

HPLC(Ion Pair)-ICPMS를 이용한 농산류 식품 중의 셀레늄 화학종 분리

장희영, 도미송, 정지선, 박용남

한국교원대 화학교육과

High performance liquid chromatography-inductively coupled plasma mass spectrometer(HPLC-ICPMS)를 이용하여 마늘 시료 중의 셀레늄 화학종을 분리 분석하였다. 다원소 이온종들과 공존 원소들에 의한 분자들의 방해를 제거하기 위하여 octapole reaction cell(ORC)의 reaction gas 로 H_2 gas 를 사용하였다. 표준시료를 이용하여 주요 셀레늄 화학종인 SeIV(selenite), SeVI(selenate), SeMet(selenomethionine), SeCys(selenocystine), SeMC(Se-methyl selenocysteine)을 C8 컬럼(Symmetryshield^{TM} RP8, 3.5 ㎛, 4.6 × 150 mm)을 사용하여 분리하고 최적 조건을 찾고 이를 바탕으로 마늘 시료 중의 셀레늄 화학종을 분리하였다. 마늘 시료의 추출 방법으로는 마이크로파를 이용한 추출, 물을 이용한 추출, 효소를 이용한 추출을 사용하였고, 각각의 셀레늄 화학종 분리 분석 결과를 비교하였다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Determination of major elements in low alloy steel by laser-induced breakdown spectroscopy

정세훈, 김승빈

포항공과대 화학과

Laser-induced breakdown spectroscopy (LIBS) should be useful technique for quantitative and qualitative analysis in steel. The technique is based on atomic emission spectroscopy. The LIBS provides numerous advantages such as rapidity, multi-elemental analysis, minimal sample preparation and low cost. The plasma on sample has been created with Q-switched Nd:YAG laser in air. The plasma emission is detected using an Echelle spectrometer of wide spectral range (200 ~ 780 nm) combined with an intensified charge coupled device camera. In this study, the concentration of major elements such as Al, Si, P, S, Cr, Mn, Ni and Mo in low alloy steels is studied by LIBS. 7 kinds of certified reference materials were used to calibrate concentrations of each element. Fe lines were used to internal reference for the elimination of matrix effects. The results of steel samples were good agreements compare to their certified values.

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Characterization of flavonoids in the four different tissues of Agrimonia pilosa using Liquid Chromatography coupled by Tandem Mass Spectrometry[발표취소 10-15]

최진영, 박세민, 박형진, 김해경, 정원영, 신성철

경상대 화학과

Agrimonia pilosa is a plant of rose [illegible] nds in trunk, flower, root and leaf were analyzed by liquid chromato [illegible] ctrometry. Flavonoid compounds that belong to a type of secondary [illegible] d shows numerous biological and pharmacological actives.

발 표 취 소

일시: 2009년 10월 28~30일(수~금) 3일간
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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

수소화물 발생 HPLC-ICPMS를 이용한 셀레늄 화학종 분석의 감도 개선

지하나, 정지선, 도미송, 박용남

한국교원대 화학교육과

High performance liquid chromatography-inductively coupled plasma mass spectrometer(HPLC-ICPMS)에 수소화물 발생 장치(hydride generation, HG)를 연결하여 시료 중에 포함되어 있는 미량의 셀레늄 화학종을 분리 분석하였다. 분광학적 동중 간섭을 제거하기 위하여 octapole reaction cell(ORC)의 reaction gas 로 H_2 gas 를 사용하였다. 수소화물 발생 장치의 조건은 3 mol L^{-1} 의 HCl 과 2.5%(w/v) NaBH4 을 사용하였고, 주요 셀레늄 화학종 표준시료를 이용하여 감도를 측정하였다. 또한 개선된 감도를 바탕으로 곡류 시료 중의 셀레늄 화학종을 분리 분석하였다.

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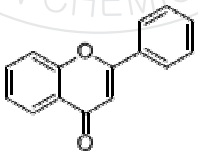
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

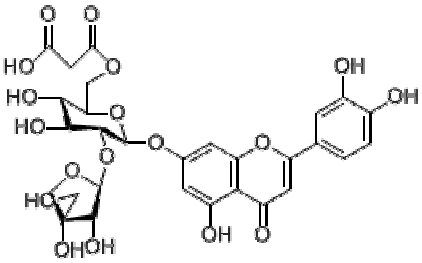
Analysis of phenolic components in bell pepper leaf (Capsicum anuum L.) infected by powdery mildew (Leveillula taurica) employing LC-MS/MS

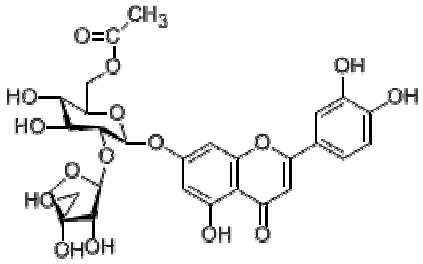
정원영, 박형진, 신성철

경상대 화학과

Powdery mildew of Paprika caused by Leveillula taurica has been a serious problem in greenhouse cultivation. The powdery mildew forces the change of the phenolic component distribution in bell pepper leaf. A number of phenols play an important role as pre-infection inhibitors, providing plants with a certain degree of basic resistance against pathogenic microorganisms. In this work we identified the phenolic compounds and compared characteristic chromatographic fingerprints of the fresh pepper with infected one by liquid chromatography electrospray ionization mass spectrometry (LC/MS–MS) methods.







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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Application of Diffusion NMR Spectroscopy in Polymer

박희용, *정민환

*(주)LG화학기술연구원 CRD 연구소 *LG화학기술연구원 CRD연구소*

Over the last decade, pulsed field-gradient(PFG) NMR spectroscopy has become the method for measuring the diffusion coefficient. However, it is hard to measure the diffusion in polymer due to low gradient strength. Recently, high field gradient NMR system with a maximum strength of more than 1,000G/cm and new pulse sequences make it possible to measure the diffusion in polymer. It is expected that this technique plays an important role in the interpretation of the polymer NMR spectrum. We will present this PFG-NMR technique for the analysis of polymer spectrum using the spectral editing with gradients and the separation of mixtures. In addition, we will demonstrate the application of diffusion NMR for the analysis of polymer terminal structures with DOSY pulse sequence and the result was confirmed by Mass spectrometry.

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Electrochemical Studies for glucose using new the nickel-coated ITO electrode

장지혜, 최영봉, 김혁한

단국대 화학과

An enzyme-free measurement of glucose has been developed using a nickel-coated ITO electrode obtained by electrochemical deposition of NiCl2 solution on the ITO electrode and KOH solution. The nickel-coated ITO electrode were characterized by scanning electron microscopy (SEM) and cyclic voltammetry(CV).The electrochemical oxidation of glucose was first investigated at the activated nickel-coated ITO electrode in KOH solution. As can been, upon glucose addition, there is an increase in the anodic peak current together with a decrease in the cathodic peak current. Also, potential becomes shift as add glucose's quantity.

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Electrochemical characterization of polymer-liganded Osmium Complex

박초롱, 이예림, 강연지, 김혁한

단국대 화학과

A series of novel, electro-active complexes of osmium were prepared and then characterized using electrochemical techniques. The osmium complex contain 4,4'-Dipyridyl, 2,2'-Dimethyl-4,4'-bipyridyl and Poly vinyl imidazol. Synthesize osmium complex of PVI-Os(bpy)2Cl, PVI-Os(dme-bpy)2Cl that 5 coordinations and 6 coordinations exist at the same time. The electrical signals were measured by voltammetry technique. Also, catalytical current was amplified by GOx and HRP which are electrically mediated by new osmium redox film. Redox complexes for horseradish peroxidase-mediated reduction of H2O2 coupled to glucose oxidase-mediated oxidation of glucose.

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Hydrodynamic separation of giant unilamellar vesicles using microfluidic device

우영준, 허유희, *이기라, **신관우

*서강대 화학과 *한국기초과학지원연구원 물성과학연구부 **서강대 화학과 및 바이오융합과정*

Giant unilamellar vesicle (GUV) consisting of single phospholipid membranes, are fascinating model cellular systems for studying the dynamics and structural features of many cellular processes, including endocytosis, reconstitution of membrane proteins, and DNA-lipid adsorption, etc.. Due to its considerable size (a diameter on the order of 10 um to 100um), it can be easily resolved and manipulated while being monitored by using on optical microscope Among various GUV preparation methods, electroformation method, where external electric field is applied to lipid deposited on an electrode, is commonly used to produce GUVs without a complicated procedure. However it is technically difficult to obtain homogeneous GUVs with a narrow size distribution. Prevously, we tested the feasibility of the size dependent separation of GUV mixtures in a microfluidic chip. In that experiment, the microfluidic chip had two channels connected trough slits and we applied pinched flow fractionation segment into the chip to locating all vesicles near slits. However, back flow in the narrow channel was inevitable. In this experiment,, we modified the microfluidic chips, by adding extra channels to reduce the pressure in the secondary channel. In this presentation, we will present newly designed microfluidic devices for size-dependant separation of GUVs and compare the size distribution of the GUVs formed by initial electroformation to one from the microfluidic channels.

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Application of Polydimethylsiloxane Mini-Disk Extraction to the Analysis of Floral Aroma by Gas Chromatography and Mass Spectrometry

장혜진, 이동선

서울여대 화학과

This paper reports application of a novel sampling method called headspace polydimethyl-siloxane (PDMS) mini-disk extraction (HS-PDE) combined with GC/MS for the analysis of floral aroma from *Prunus mume*, *Lantana camara*, and *Albizia julibrissin*. The technique uses a prototype PDMS mini-disk (diameter: 8 mm, thickness: 0.157 mm, weight: 9.4 mg) as a sorption device and very small volume (0.03 mL) of acetonitrile as an organic solvent for extraction. The relative extraction efficiencies of proposed method have been compared with other sampling techniques based on headspace solid phase micro-extraction (HS-SPME) and mulberry paper bag micro-solid phase extraction (MPB-μ-SPE). This new HS-PDE method is very simple to use, inexpensive, rapid, requires small sample amounts and solvent consumption.

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Vibrational spectroscopy to study the difference between natural and Beryllium-diffused sapphires

이상욱, *박지민, 정회일

*한양대 화학과 *한양대 공학대학원*

The diffusion of Beryllium is a common way to improve the color quality of sapphire. By the diffusion of Beryllium into low quality sapphire, the resulting color is close to that of natural sapphire. Since market values of natural and Beryllium-diffused sapphires are quite different, there is a strong demand of analytical method that can non-destructively identify the structural differences. For this purpose, we employed Raman, IR and NIR (near-infrared) spectroscopy since these methods are fast, easy for spectral collection with non-destructive nature. The spectra of natural and Beryllium-diffused sapphires were collected using each spectroscopic method and resulting spectra were examined. The detail spectral features will be discussed in the presentation.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Antimicrobial activity of a chalcone glycoside from Sorbus commixta Hedl

Lok Ranjan Bhatt, *김보미, 채규윤

*원광대 화학과 *원광대 생명나노 화학과*

Sorbus commixta Hedl.(Rosaceae), have long been traditionally used as a tonic for the treatment of cough, asthma, and other bronchial disorders in East Asian countries, including Korea, China and Japan. Despite a long history of use, little is known about the chemical constituents of this plant. We, herein report the isolation and identification of Chalcononaringenin -4 methoxy 6' –O- β glucopyranoside and its in vitro antimicrobial activity. The structure of the compound was elucidated using various spectroscopic methods viz. IR, UV, NMR and MS. The antimicrobial activity of the compound was evaluated against Escherichia coli, Salmonella typhimurium, Pseudomonas aeruginosa, Staphylococcus aureus, Staphylococcus epidermidis, Enterococcus faecalis and Candida albicans, using microdilution method.

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Ultrasensitive Detection of IgE Proteins using Nanomaterial-enhanced SPR Biosensors

김수희, 심혜림, Shaikh Nayeem Faisal, 이혜진

경북대 화학과

This poster describes the development of an ultrasensitive surface-based method for the detection of IgE proteins using surface plasmon resonance (SPR). The detection principle is based on the combined use of biofunctionalized nanoparticles and surface enzyme reactions at the surface of a functionalized gold thin film. The analysis of IgE proteins in biological samples is extremely important since the concentration of IgE can be used as a marker for the diagnosis of allergic diseases. SPR is an excellent method for protein detection as it does not require the chemical labeling of target molecules. The detection scheme proposed for the measurements of IgE proteins involves three major steps; i) design of bio-probe molecules specific to IgE proteins (e.g. antibody & aptamer) and their surface immobilization chemistry, ii) nanoparticle-enhanced surface sandwich assays, and iii) surface polyadenylation reactions utilizing an IgE specific RNA aptamer. We expect that the newly proposed ultrasensitive detection scheme can powerfully be applied to the direct measurements of IgE proteins in biological samples at femtomolar concentrations.

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Determination of Aceclofenac Concentration in Suspension Formation using Raman Spectroscopy

신가영, 정희일

한양대 화학과

We have determined the concentration of aceclofenac (2-[[2-[2-[(2,6 dichlorophenyl)amino]phenyl]-acetyl]oxy], non-steroidal anti-inflammatory drug, Clanza STM) in a turbid pharmaceutical suspension using Raman spectroscopy. For reliable quantitative analysis, we employed WAI (Wide Area Illumination) scheme for spectral collection. The WAI scheme allows to cover wide sample area (6mm laser spot, area : 28.3mm2, focal length : 248mm) for Raman spectral collection. Raman spectra collected by the WAI scheme were much more reproducible and better representative of sample compared to a traditional small-spot scheme. We prepared the pharmaceutical suspensions containing different concentrations of aceclofenac in gel capsules. The relative concentrations of aceclofenac varied from 70 to 130% based on the target concentration. The concentration for each sample was expressed as the percentage relative to the amount of aceclofenac in a suspension. A suspension containing 100mg/100mL was designated as 100% aceclofenac. Partial least squares (PLS) regression was used to determine the concentration of aceclofenac. Comparing with HPLC (conventional method of determining aceclofenac), Raman spectroscopy is much faster and non-destructive in pharmaceutical analysis.

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New stationary phases with improved ligand morphology prepared by polymerizationof styrene upon initiator-attached silica particles

황동국, 이승미, 정원조

인하대 화학과

In this study, peculiar stationary phases have been developed by attaching a new radical initiator onto porous silica particles followed by polymerization of styrene upon them. Silica particles of different shapes (spherical vs. irregular) were reacted with (3-chloropropyl) trimethoxysilane followed by sodium diethyldithiocarbamate to yield initiator attached silica particles. The dried porous initiator silica particles were allowed to undergo radical polymerization with styrene under optimized reaction conditions. The stationary phases were packed in glass-lined stainless steel micro columns (300X0.5mm). We investigated separation performance of the prepared stationary phases in HPLC. The performance of the polystyrene bound initiator silica was found to be better than that of corresponding C18 modified silica particles. This may be attributed to the particular morphology of the polystyrene thin layer of the new stationary phases.

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Surface Characterization of Plasma Polymerized Fluorocarbon Thin Films

김영수, 이지혜, *이연희

*고려대 화학과 *KIST 특성분석센터*

Plasma polymerization is a thin film deposition process and may be uniformly coated onto any substrate. Plasma polymers generally have different properties from those of conventional polymers due to their unique properties. Plasma polymer films have been used in a variety of applications including barrier coating, protective coating, anti-scratching coating, and dielectric layer in microelectronics. In this study, plasma-polymerized films fabricated by inductively coupled plasma (ICP). Two kinds of fluorine-containing gases such as C3F8 and C4F8 were investigating their effect on the films. Also, process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, and processing time were investigated. Surface analytical instruments such as Auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), and time-of-flight secondary ion mass spectrometry (TOF-SIMS) were used to provide useful information about the chemical properties such as surface composition and functional groups. And, also, Field-Emission Scanning Electron Microscope (FE-SEM) and Atomic Force Microscope (AFM) were used to provide growth mechanism such as surface morphology and thickness.

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Preparation of open tubular MIP capillary columns with various templates by a generalized procedure and their chiral and non-chiral separation performance in capillary electrochromatography

shabiabbas, 황동국, 정원조

인하대 화학과

A generalized preparation procedure of open tubular (OT) molecule imprinted polymer (MIP) columns is proposed for a number of templates with acidic functionality such as profen drugs and others. The template (S-enantiomer) was mixed with methacrylic acid (MAA), ethylene glycol dimethacrylate (EDMA) and 4-styrenesulfonic acid (4-SSA), dissolved in a porogen mixture of acetonitrile/ 2-propanol (9/1), and incubated in a pretreated and silanized fused silica capillary by the thermal non-covalent polymerization procedure. The whole preparation procedure was exactly the same for all the MIP capillaries except for the selection of template. Nevertheless, the morphologies of the MIP layers were markedly variant depending upon the choice of template. The separation efficiency of each OT-MIP column for chiral separation of R- and S- enantiomers was examined and tuned to obtain the best separation efficiency by changing the chromatographic parameters such as eluent composition and pH. Different optimized conditions were obtained for different OT-MIP columns although a unified eluent could be used to obtain still quite satisfactory results. Non chiral separation of the MIP columns were also examined in the unified eluent with two sets of test mixtures, that is, a mixtures of alkylbenzenes and a mixture of small polar solutes. The chiral and non-chiral separation of this study resulted in very good separation efficiencies. This work is the very first study for the generalization of preparation of OT-MIP columns for a number of templates.

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The Preparation and Certification of Glucose Certified Reference Material

이화심

한국표준과학연구원 바이오/임상센터

lucose, a monosaccharide, also known as grape sugar, blood sugar, or corn sugar, is a very important carbohydrate in biology. The living cell uses it as a source of energy and metabolic intermediate. How blood sugar works during the digestive process, much of the food that is eaten is converted into glucose, commonly known as blood sugar. Glucose circulates in the bloodstream and is used as food for the body's cells. The level of glucose is regulated to a normal level by insulin. The high level of glucose is lead to Diabetes. Diabetes mellitus is a disorder that affects the body's ability to efficiently utilize blood glucose. people with diabetes must monitor their blood sugar levels. In order to measure the level of glucose, Certified Reference Material of glucose is required. Then the preparation and certification of glucose CRM were performed in this study. The serum used in this study were gathered from the healthy korean that were proved as negative through the tests of HIV, HVB and HVC. The certification of five kinds of glucose CRM were performed by isotope dilution liquid chromatography-mass spectrometry. The expanded uncertainties were below 1.5% in all items.

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혈액내 헤마토크릿 측정을 위한 평면형 소형 센서에 대한 연구

김민수, 이용석, 강태영, 신정원, *남학현, *차근식

*(주)아이센스 부설연구소 *광운대 화학과*

헤마토크릿(Hematocrit)은 혈액내의 적혈구 용적율을 의미한다. 헤마토크릿의 측정은 임상학적으로 환자의 탈수, 빈혈 및 적혈구 증가증 등의 상태를 진단하는 척도가 된다. 기존 헤마토크릿의 측정법으로는 혈액을 모세관 튜브에 채취한 후 원심 분리를 통하여 전혈구 분리 비율을 산출하는 마이크로 헤마토크릿 측정법과 일정량의 혈액을 현미경을 사용하여 직접 세어 측정하는 방법 등이 있다. 본 연구소에서 개발한 헤마토크릿 센서는 전기 전도도법을 통한 측정법으로 혈액 중 혈구가 고유저항체로 작용하므로 혈구의 용적량에 따라 혈액의 전기 전도도 값이 상관관계를 가지는 원리를 이용하였다.헤마토크릿 센서는 스크린 프린팅 방법으로 제작된 Ag 전극 위에 2 개의 백금흑(Platinum black) 전극을 형성하여 전도도를 측정하였다. 전도도 측정 전극은 여러 개의 전기화학 센서와 함께 평면형 소형 센서 위에 제작되었다. 스크린 프린팅 방법의 사용은 제조 시 마다 모든 전극이 균일하게 형성되므로 센서의 성능을 일정하게 유지시킬 수 있으며 대량생산에 용이하다는 장점을 가진다.본 연구에서 제작된 헤마토크릿 센서는 2 주 이상의 일정한 감응성을 유지하였으며, 마이크로 헤마토크릿 측정법과 상용화된 기준장비(Radiometer 사 ABL835)와 측정값을 비교해 본 결과 매우 우수한 상관관계를 나타냈다.

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혈액 자동분석을 위한 평면형 타입 소형 전기화학 센서

김현숙, 최병현, 하정한, 신정원, *남학현, *차근식

*(주)아이센스 부설연구소 *광운대 화학과*

혈액 내 생체시료 분석은 현대 의료진단에서 중요한 부분을 차지하고 있으며 따라서 보다 쉽고 정확하게 그리고 경제적으로 검출하기 위한 소형 화학센서의 개발이 활발히 진행되고 있다.본 연구에서는 혈액 내에 여러 가지의 화학종을 동시에 자동으로 분석하기 위한 전기화학 센서(electrochemical sensor)들을 평면의 작은 플라스틱(polyethylene terephthalate, PET) 위에 여러 전극을 스크린 프린팅 방법으로 제작하였다. 스크린 프린팅 방법은 제조 시 마다 모든 전극이 균일하게 형성되므로 센서의 성능을 일정하게 유지시킬 수 있으며 대량생산이 매우 용이하다는 장점을 가진다.기본적으로 스크린 프린팅 방법으로 Ag 전극을 형성하였고, 전위차법(potentiometry)의 작동전극(working electrode)은 분석하고자 하는 이온종에 따라 최적화된 내부겔과 외부막을 분주하고 건조함으로써 각각의 이온센서를 구성하였다. 전류법(amperometry)의 작동전극과 보조전극(counter electrode)은 백금흑(platinum black) 전극을 형성하여 사용하였다. 기준전극(reference electrode)은 내부 기준용액과 시료가 일정하게 흐를 수 있는 흐름계(flow system)을 구성하여 액간 접촉전위(liquid junction potential)가 일정하게 유지되도록 하였다. 이와 같이 제작된 전기화학 센서를 혈액 자동분석기에 적용하였으며 그 결과 2 주 이상의 우수한 감응성, 직선성 및 재현성을 유지하였다. 또한 상용화된 타사의 분석기(Radiometer 사 ABL835)와 혈액시료에 대한 측정값을 비교해 본 결과 매우 유사한 성능을 나타냈다.

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Quantitative Surface Analysis of Binary Alloy Thin Films by Depth Profiling of TOF-SIMS and Dynamic SIMS.

임원철, *이지혜, 이연희

*KIST 특성분석지원단 화학분석센터 *고려대 화학과*

TOF-SIMS and Dynamic SIMS have been widely used in an elemental analysis and a depth-profiling for trace materials existed on the surface because they are highly sensitive to detect elemental ions as much as ppm or ppb. However, matrix-dependent secondary ion yields limit the capability of the SIMS technique to obtain a quantitative information and there are so many efforts to improve the quantitative analysis due to different matrix effect according to having a different composition. Therefore, we have used TOF-SIMS, Dynamic SIMS, AES and XPS to determine the suitable quantitative analysis of thin layer of homogeneous binary alloys such as Fe-Ni, Co-Pt and W-Si. We obtained calibration curves for their results to give comparison of quantitative analysis information.

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GC-MS analysis of organic residues in archaeological oil lamps from Baekje

강소영, 홍종욱, 지상현

국립문화재연구소 보존과학연구실

The study of organic residues in archaeological artifacts has mainly focused on lipid due to their relative stability. The fatty acid compositions can trace the origin of biological species compared with modern plant and animal references. Deungjan (oil lamps) remains were applied to 18 samples excavated from Neungsa temple site of Buyeo. The surface lipid residues preserved in Deungjans were analysed by gas chromatography-mass spectrometry (GC-MS). The ratios of fatty acids were shown that fat in terrestrial mammals and seeds were used as a fuel sources for the ancient lamps. However, types of fuel source were rarely affected significantly by the substyle of lamp. The results provide evidence for understanding of life style in Sabi period of Baekje.

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Enantiomer separation of N-hydrazide derivatives of chiral acid drugs on crown ether derived chiral stationary phase

김경옥, 황호, 이원재

조선대 약학대학

The chromatographic enantiomer separation of N-hydrazide derivatives of NSAIDs (non-steroidal anti-inflammatory drugs), one of important chiral acid types was performed on crown ether type chiral stationary phases (CSPs) derived from (+)- and (-)-(18-crown-6)-2,3,11,12-tetracarboxylic acid (18-C-6-TA). After preparation of the corresponding N-hydrazide derivatives to introduce amino moiety to the chiral acids of NSAIDs, the indirect enantiomer separation was performed using the mobile phase of 80% methanol containing 10mM sulfuric acid with UV detection at 210 nm and, in general, the enantiomers of N-hydrazide derivatives of the examined analytes except ketoprofen were well resolved. It was shown that the elution orders on CSP 1 derived from (+)-18-C-6-TA were reversed on CSP 2 derived from (-)-18-C-6-TA. Using the analytical method applied in this study, liquid chromatographic enantiomer resolution of other chiral acids as their N-hydrazide derivatives is expected to be used on crown ether derived CSP.

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Chromatographic enantiomer resolution on a covalently immobilized chiral column derived from polysaccharide derivative under reversed and normal phase conditions

황호, 김경옥, 이원재

조선대 약학대학

In this study, liquid chromatographic enantiomer resolution of N-protected α-amino acid was performed on a covalently immobilized chiral column based on polysaccharide derivative under reversed and normal-phase conditions. The effect of the reversed mobile phase on the chromatographic parameters of the enantioselectivities, resolution factors and retention times using the covalently immobilized was shown. Also the enantiomer separation of N-protected α-amino acid in the reverse and normal phase was compared and the results obtained in aqueous acetonitrile solution of the former mobile phase were generally lower than those in the latter mobile phase. However, the enantioselectivities obtained in aqueous methanol solution of the reversed mobile phase were higher than those in the normal mobile phase.

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Validated LC-MS/MS method for determination of propiverine in human plasma

배현진, *정선경, *조경희, *나숙희, *이희주

*바이오코아 신약개발지원부 *바이오코아(주) 신약개발지원사업부*

The concentration of propiverine in human plasma were measured using liquid chromatography tandem mass spectrometry and examined stabilities of propiverine. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using protein precipitaion. The separation was performed on a C18 column (2.0 x 150 mm, 3 m). The mobile phase was composed of 10 mM ammonium formate and acetonitrile (50/50, v/v) and total run time was 3.5 min. The LC-MS/MS system was equipped with an electrospray source operating in the negative ion mode. Using multiple reaction monitoring (MRM), the transition m/z 368→116 and m/z 267→193 were used for quantitation of propiverine and internal standard. The standard curves were linear ($r \geq 0.99$) over the concentration range of 2-50 ng/mL. Validation experiments, runs were generated at the plasma concentration of 2, 10, 100 and 500 ng/mL on 5 consecutive days, showed good precision and accuracy over a wide concentration range. Also stability procedures was evaluated the recovery, short term temperature, long term, freeze-thaw and post preparative stability including stability in stock-solution for low and high concentration separately. Validation experiments, satisfied requirement of 15% less than anticipatable theory value, have shown that the assay was validated and found to have acceptable accuracy, precision, linearity, sensitivity and selectivity. Therefore this sensitive, simple and rapid analytical method by LC-MS/MS had been successfully applied to a pharmacokinetic study of propiverine in human plasma.

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Validated LC-MS/MS method for determination of Terbinafine in human plasma

황보승희, *정선경, *조경희, *이희주

*바이오코아 신약개발지원사업부 *바이오코아(주) 신약개발지원사업부*

The concentration of terbinafine in human plasma were measured using liquid chromatography tandem mass spectrometry and examined stabilities of terbinafine. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using liquid-liqude extraction. The separation was performed on a reverse phase column (Ph, 2.0 x 150 mm, 5 m). The mobile phase was composed of 5 mM ammonium acetate and acetonitrile (20/80 in 0.1% formic acid. v/v). The LC-MS/MS system was equipped with an electrospray source operating in the positive ion mode. Using multiple reaction monitoring (MRM), the transition m/z 292→ 141 and m/z 260→ 98 were used for quantitation of terbinafine and internal standard. The standard curves were linear ($r \geq 0.99$) over the concentration range of 2.5 - 1000 ng/mL. Validation experiments, runs were generated at the plasma concentration of 2.5, 25, 250 and 1000 ng/mL on 5 times for 1 day (Intra-day), 5 times for 5 days (Inter-day). Also stability procedures was evaluated the recovery, short term temperature, long term, freeze-thaw and post preparative stability including stability in stock-solution for low and high concentration separately. Validation experiments, satisfied requirement of 15% less than anticipatable theory value, have shown that the assay was validated and found to have acceptable accuracy, precision, linearity, sensitivity and selectivity. Therefore this sensitive, simple and rapid analytical method by LC-MS/MS had been successfully applied to a pharmacokinetic study of terbinafine in human plasma.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Preparative LC를 이용한 ABS내 첨가제 분석 방법 연구

이현정, *옥종화

*LG화학기술연구원 CRD 연구소 *LG화학기술연구원 분석센터*

ABS 수지는 Acrylonitrile, Butadiene, Styrene 의 3 성분으로 되어 있는 열가소성 수지로 광택과 성형성, 내약품성, 내충격성등이 좋은 종합 Engineering Plastics 의 일종으로 다양한 곳에 사용되고 있다. 각 특성을 더욱 강화하기 위해 다양한 첨가제를 사용하게 되는데 이를 분석하기 위해서는 전처리 과정을 거치게 된다.일반적으로 ABS 내 첨가제 분석을 위해서는 Chloroform/Methanol 재침법을 사용한다. 재침법의 경우, 시료를 고농도로 녹여야 하며, 재침 후 원심 분리 및 농축이라는 일련의 과정을 거쳐야 한다. Preparative LC 는 천연물에서 추출한 시료나 합성 원료를 분리하고자 할 때 사용하는 기법으로, 최근 고 분리능 column 이 개발됨에 따라 그 적용 분야가 늘어나고 있는 추세이다. 재침법에 비해 시료의 농도가 상대적으로 낮고, automation 이 가능하며, 첨가제의 recovery 문제를 해결할 수 있을 것으로 예상되는 preparative LC 를 이용하여 ABS 내 첨가제 분석을 진행하여, 재침법과 비교해 보았다.

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PO 수지 중 첨가제의 Soxhlet 추출법 최적화

한수연, 옥종화

LG화학기술연구원 CRD연구소

PO 수지에서 첨가제의 종류 및 함량은 수지의 특성과 큰 연관성을 가진다. 따라서 첨가제 분석은 고분자 분석에서 매우 중요하다. 첨가제 분석은 수지 내 첨가제의 추출과 분리된 물질의 구조분석 및 함량분석으로 대별된다. 각 수지에는 다양한 첨가제들이 광범위하게 사용되고 있으며 수지의 종류, 가공조건, 사용조건에 따라 다르게 선택되어진다. PO 수지내의 첨가제 추출 분리를 하기 위해서 일반적으로 Soxhlet 추출법을 사용한다. 이 추출법은 추출용매, 추출시간, 시료상태 등 여러 조건에 따라서 추출 효율이 달라지는데 여기서는 최적의 Soxhlet 조건을 찾고 연구하였다. 본 연구는 PO 수지의 첨가제 추출 시 Soxhlet 추출법에 대한 체계를 확립하는 것을 목표로 한다.

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Determination of Epinephrine by Ethylenediamine Condensation System

타스리마펄도우스, 김고은, 이상학, *최종하, 서연숙

*경북대 화학과 *안동대 화학과*

The oxidized product of epinephrine with mercury (II) nitrate was condensed with ethylenediamine (EDA) which formed a strong fluorescence compound. For the enhancement of the fluorescence intensity acetone was added. The influence of buffer solution on the fluorescence intensity was investigated. The measurement was carried out at 504 nm with excitation at 398 nm. In order to obtain better response, several operational parameters have been investigated. Under the optimum conditions, the fluorescence intensity of the epinephrine-mercury nitrate-acetone-EDA system is linearly proportional to the epinephrine concentration in the epinephrine concentration range of 5×10−4 – 1×10−3 M. The correlation coefficient for the calibration curve was 0.93467. The limit of detection as defined by IUPAC, C LOD=3S b/m (where S b is the standard deviation of the blank signals and m is the slope of the calibration graph) was found to be 9.624×10−6 M. The proposed method was also applied for the determination of epinephrine in pharmaceutical preparations. The reaction mechanism was also described.Reference:1) Karim, M. M.; Alam, S. M.; Lee, S. H. J. Fluores. 2007, 17, 427.

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Fluorimetric Estimation of Levodopa in Pharmaceutical Preparations Using Silver Nanoparticles

세이크 마피즈 알람, *서연숙, *김고은, *이상학, **최종하

*경북대 화학과 *경북대 화학과 **안동대 화학과*

A simple and sensitive fluorimetric method for the determination of levodopa using silver nanoparticles as emission reagent has been investigated. In this study, silver nanoparticles were prepared based on aqueous-gaseous phase reaction of silver nitrate solution and ammonia gas. The nanoparticles were water soluble, stable and have narrow emission band. Silver nanoparticles were used as fluorimetric assay of levodopa (1). It was found that levodopa can greatly quench the emission intensity of silver nanoparticles. Under the optimum conditions the quenched fluorescence intensity was linear with the concentration of levodopa in the range 3.7×10-8 to 3.5×10-6 M and the detection limit was 1.0×10-8 M (s/n=3). The relative standard deviation of the proposed method calculated from 11 replicate injection of 1×10-7 M levodopa was 2.9 %. The proposed method was applied to the determination of levodopa in commercial pharmaceutical formulations.Reference:1) Madrakian, T.; Afkhami, A.; Mohammadnejad, M. Talanta. 2009, 78, 1051.

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수분에 의한 전해액 내 $LiPF_6$의 분해 메커니즘 연구

이민정, 안정애, 옥종화

LG화학기술연구원 CRD연구소

수분에 의해 이차전지 전해액 내의 $LiPF_6$ 는 LiF, HF, PF_5, POF_3, $PO_2F_2^-$, PO_3F^{2-}, PO_4^{3-} 등으로 분해되며 $LIPF_6$ 의 분해물에 의해 carbonate 계의 용매가 쉽게 분해되므로 전해액 내의 수분의 함량은 이차 전지 성능에 중요한 요인으로 작용한다. 본 연구에서는 수분뿐만 아니라 알코올 함량에 따른 $LIPF_6$ 의 분해 산물들의 조성을 IR, NMR 등을 이용하여 확인하고자 한다.

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소형챔버법 대용 Headspace-GC TVOC평가법

원정혜, 이혜진, 이웅진, 옥종화

(주)LG화학기술연구원 CRD연구소

환경오염에 따른 실내공기질 문제에 대한 사회적 관심이 커짐에 따라 실내 환경의 중요성이 강조되고 있다. 특히, 새집증후군의 원인으로 알려진 휘발성 유기화합물(VOC) 노출이 가장 큰 문제로 인식되고 있으며, 이에 대한 제도나 규제 등이 엄격해 짐에 따라 환경친화적 제품을 생산하는데 각 기업체들이 주력하고 있다. 이에 따라 VOC 평가의 중요성이 증대되고 있으며, 다양한 VOC 평가법이 있다. 현재 TVOC 분석법에는 Dynamic headspace 법(Purge&Trap, Thermal Desorption) 및 Static headspace 법(Headspace, SPME)과 소형챔버법를 이용한 분석방법이 있다. 이 중 소형챔버법의 경우 제품의 VOC 분석으로 ISO16000-9 에 명시되어 있으며, 환경마크 등에 규제 기준치가 제시되어 널리 활용되고 있다. 그러나 소형챔버법의 경우 분석 시간이 오래 걸리는 단점이 있어, 1 차적으로 Headspace-GC 를 이용하여 낮은 TVOC 수치를 대상으로 Screening 한 후, 2 차적으로 소형챔버법을 통해 최종적인 분석 평가를 하는 방법이 효율적이다. 본 연구에서는 건축자재로 사용되는 벽지 및 도료의 TVOC 측정 Data 로 두 방법간 상관성을 파악하여, 소형챔버법 대용 Headspace-GC TVOC 평가법을 제시하였다.

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Determination of streptomycin residues in Environmental Samples by LC/ESI-MS/MS

이종혁, 명승운

경기대 화학과

Streptomycin(STR) is an aminoglycoside antibiotic widely used in medical and animal origin, like meat, milk and honey. The effective and sensitive method for the determination of streptomycin in environmental sample by LC/ESI-MS/MS was developed. Streptomycin was extracted and cleaned through a Mixed Cation-eXchange (MCX) catridge from environmental aqueous sample. Chromatographic separation was achieved on a Eclipse Plus C18 column (2.1x100mm, 5μm), using gradient elution with 20mM HFBA in water and acetonitrile. As a result, calibration curve showed good linearities (above r2=0.99) in the concentration range of 0.25-1.0 ng/mL. The limit of quatitication (LOQ) was 0.12 ng/mL. Recoveries from the blank surface water were grater than 70%. The established method can be used to determine pg/mL levels of streptomycin from aqueous samples.

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TIMS Measurement of Uranium Standards in Ultra Trace Levels

최인희, *박종호, *송규석

*충북대 화학과 *한국원자력연구원 원자력화학연구부*

The precise isotopic ratio measurement of uranium using a thermal ionization mass spectrometry (TIMS) is of importance in the analysis of nuclear samples. In case of the analyses for the ultra-trace amount of uranium samples, it is essential to define the backgrounds such as from filaments, reagent blank, and room blank followed by minimizing the unwanted effects from filaments due to the low instrumental intensities of the uranium isotopes, especially minor isotopes, such as 234U and 236U. In a thermal ionization source a double filament system evaporates, and then, immediately ionizes samples by high temperature (~1800℃). We varied the conditions for degassing filaments prepared with zone-refined rhenium ribbons to determine the most efficient heating current and duration time, which were 3.5A and 60min, respectively. The TIMS measurement combined with isotope dilution mass spectrometry (IDMS) technique showed that the uranium backgrounds were measured to be negligible for the reagent blank and room blank under the operating conditions.Additionally, the modified total evaporation technique was used to measure the isotopic ratios of uranium standards (NIST U005 and KRISS natural uranium) showing that the analyzed isotopic ratios reasonably agreed to the certified value within the typical accuracy. Based on this study, the TIMS system is considered to be adequate to analyze trace-amount nuclear materials in swipe and environmental sample with high precision.

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Ga-68 생산을 위한 Ge와 Ga 원소의 분리에 관한 연구

이홍래, *김상욱, 최상무, *양승대

*한국원자력연구소 방사선공업환경연구부 *한국원자력연구원 방사선공업환경연구부*

현재 국내에서는 Ge-68/Ga-68 방사선 발생장치의 개발에 대해서 전무한 상태이다. 이번 연구에서는 Ga-68 을 생산하기 위한 방법에 관한 연구에 대하여 보고하고자 한다. 과량의 Ga 이 존재하는 시료에서 소량의 Ge 만을 염산과 사염화탄소를 이용한 용매추출법을 통하여 분리하였다. 이때 Ge 의 회수율은 90% 이상이었으며, Ga 의 잔존량은 0.02%임을 확인하였다.소량의 Ga 과 Ge 존재한 시료에서 순수하게 Ga 만을 추출하기 위하여 Tio_2 와 음이온 수지 등을 이용하여 분리하였다. 이때 Ga 의 추출율은 80% 이상이었으며, Ge 는 10^{-3}% 미만으로 관찰하였다.

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Polydimethylsiloxane Mini-Disk Extraction as a Novel Sampling Technique

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*KIST 도핑콘트롤센터 *서울여대 화학과*

A novel sampling method called headspace polydimethyl-siloxane (PDMS) mini-disk extraction (HS-PDE) was developed, optimized, validated and applied for the GC/MS analysis of flavors for the first time. A prototype PDMS mini-disk (diameter: 8 mm, thickness: 0.157 mm, weight: 9.4 mg) has been designed as a sorption device. The technique uses a small PDMS mini-disk and very small volume of organic solvent. This new HS-PDE method is very simple to use, inexpensive, rapid, requires small sample amounts and solvent consumption. Because the acetonitrile for extraction is reduced to a very small volume of only 0.03 mL, there is minimal waste or exposure to toxic organic solvent and no further concentration step. Linearities of calibration curves for α–pinene, β-pinene, limonene and γ–terpinene by HS-PDE combined with GC/MS were generally good. LOD and LOQ showed very low values, and dynamic ranges were 6.00 ng~3500 ng. This method exhibited good precision and accuracy. The overall extraction efficiency of this new method was evaluated by using partition coefficients (K_{fg}) and concentration factors (CF) for several characteristic components from nutmeg and mace. Partition coefficients were in the range from 2.04 x 10^4 to 4.42 x 10^5, while CF values were 0.88~15.03. HS-PDE was applied successfully for the analysis of flavors compositions from cumin, nutmeg and mace. The HS-PDE method is a very promising sampling technique for the characterization of volatile flavors

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Chiral separation and discrimination of catechin by sinorhizobial octasaccharides in capillary electrophoresis and ^{13}C NMR spectroscopy

권찬호, *정선호

*건국대 생명공학과 *건국대 특성화학부 생명공학과*

Succinoglycan, sinorhizobial exopolysaccharide produced by *Sinorhizobium meliloti*, is composed of an octasaccharide subunit. *S. meliloti* produces both high-molecular-weight and low-molecular-weight (M_r ^{13}C NMR spectroscopy. The chiral separation of catechin took place when sinorhizobial octasaccharides (M2 and M3) were added to the background electrolyte (BGE) in CE. NMR signal splittings were also observed on the interactions of sinorhizobial octasaccharides with the enantiomers of catechin. The chiral separation and discrimination of catechin depend on the presence of succinate substituents of the linear monomeric octasccharide in CE and NMR spectroscopy, suggesting that succinylation of sinorhizobial octasaccharide is decisive for the effective chiral separation and discrimination of catechin.

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Chiral Separation of FITC-amino Acids by CE-LIF Combined with In-line Single Drop Microextraction

양국동, 최기환, 정두수

서울대 화학부

D-Amino acids, free and peptide-bound, have been found in a variety of biological systems. However, analyses of D-amino acids are usually difficult due to the large abundance of the corresponding L-amino acids, thus requiring both high resolution and high sensitivity. In this report, single drop microextraction based on liquid-liquid-liquid extraction was coupled in-line with capillary electrophoresis (CE) for a sensitive analysis of amino acid enantiomers. In SDME, a drop of an aqueous acceptor phase covered with a thin organic layer is formed at the tip of a capillary by simple combination of sample-handling sequences of a CE apparatus. Then analytes in a donor solution are enriched into the drop through the organic layer. Although this SDME scheme is quite simple and powerful, it was difficult to apply SDME to the analysis of amino acids due to their zwitterionic properties even at the isoelectric points, which hinder them from being partitioned in the middle organic phase. The amino acids were thus derivatized with fluorescein isothiocyanate (FITC) in order to block the amino groups and to enhance the sensitivity. The FITC-derivatized amino acids from the donor phase of 0.10 M HCl were extracted into the basic acceptor phase of pH 9.3. With 10 min SDME, the FITC-derivatized amino acids (Leu, Ala, Glu, and Asp) were enriched about 200-fold. The enriched enantiomers were then baseline resolved using an 80 mM sodium borate buffer of pH 9.3 containing 12 mM CD and 18 mM sodium taurodeoxycholate as chiral selectors. The detection limits with laser induced fluorescence for the FITC-derivatized enantiomers of Leu, Ala, Glu, and Asp were 5×10^{-11} M, 5×10^{-11} M, 1.25×10^{-11} M, and 1.25×10^{-11}M, respectively. This scheme enabled chiral analysis of amino acids in a 99.4% enantiomeric excess mixture.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Adsorption of tetracycline from aqueous solution on hyroxyapatite

유구용

삼육대 화학과

In this work, the hydroxyapatite prepared by chemical precipitation methode was used as the adsorbent and the potential of hyroxyapatite for tetracycline adsorption from aqueous solution was studied. The effect of adsorption time, tetracycline concetration, pH, equilibrium parameters were investigated. The results showed that the hydroxyapatite possessed good adsorption ability to tetracycline. The adsorption isotherm studies showed that the Langmuir isotherm was the best choice to describe the adsorption behavior.

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Sensitive Chiral Analysis using pH junction and Sweeping between a Analyte and a Selector in Capillary Electrophoresis

김정연, 최기환, 장서봉, 최정미, 정두수

서울대 화학부

In this report, sensitive chiral analysis based on the combination of pH junction and sweeping was performed in capillary electrophoresis. By employing the efficient stacking techniques, the sensitivity of detection could be improved and chiral analytes could be separated using a chiral selector. The zwitterionic analytes diluted in low pH buffer are concentrated at the boundary of low pH and high pH zones due to the changing of electrophoretic mobility of analytes. Then, stacked analytes were swept with 18C6H4. Since 18C6H4 was interacted differently with the enantiomers, chiral separation was achieved simultaneously. The experimental parameters such as plug length, buffer concentration, and 18C6H4 concentration were optimized. The enrichment factor was more than three orders of degree and the value of chiral resolution was 3.2.

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Evaluating bone collagen extraction methods for radiocarbon dating

임은수, 이병철

충청문화재연구원 한국고고과학연구소

Archaeological bone can show marked and complex alterations, both structural and chemical, depending on the environment in which it was buried. Those structural and chemical alternations have an important effect on the result of radiocarbon dating. Our study was based on well-preserved skeletal material from the Ocnam-ri cultural site in Seocheon. In this study we tested by three different collagen extraction methods (improved collagen extraction by modified Login method). Our study shows that there is a difference in the data consistency among the three methods. To our understanding of chemical and physical properties of bone collagen, we tried various analysis such as HI (histological) index, EA (Elemental Analyzer), FT-IR (Fourier transform infrared).

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Effect of Heavy Metal on Single Strain DNA immobilized on PDMS microchip and dye doped silica bead

구진아, 고정아, 임홍빈

단국대 화학과

Recently, we have been exposed to many pollutants, for example, heavy metals, ultraviolet, chemicals, and so on. Particularly, heavy metals like Hg, Cd, Pb accumulated in organ such as lung and kidney, occur many symptoms. In this experiment, the cause of diseases due to the exposure was studies in the point of view of the reaction between DNA with heavy metals. Two different model systems, PDMS microarray-chip and FITC doped silica beads were setup for the reaction. For the PDMS microarray chip, fluorophore-tagged DNA was immobilized on the chip through the attachment of linker. In case of silica beads, about 50 ~ 80nm size of the beads doped with FITC(fluorescein isothiocyanate, Emax for absorption=494nm, Emax for emission=521nm) were synthesized by microemulsion method. Before metal reaction silica beads of NH2 modified and one end cy5, the the other end carboxylic acid labeled DNA reacted, then checked the reaction of fluorescent-tagged DNA with several heavy metals(Cd,Pb) by determining the fluorescent emission cleaved from the DNA immobilized chip or silica beads. For quantitative measurement, fluorescence quenching due to the presence of metal was studied as well.

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Determination of fluorescent whitening agents of paper and paperboard packaging materials by ion-pair high performance liquid chromatography

김정수, *김윤미, 김건

*고려대 화학과 *한솔제지(주) 기술연구소*

Stilbene-type fluorescent whitening agents (FWAs) are used to enhance the "whiteness" and "brightness" characteristics of paper and paperboard materials. Ion-pair high performance liquid chromatographic method was developed for separation and determination of the seven stilbene type FWAs used in paper and paperboard packaging materials. Mixtures of methanol-citrate buffer containing tetrabutylammonium bromide as the ion-pair reagent were used as the mobile phase. This method was applied to the determination of FWAs in paperboard for take-out food packaging.

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Simultaneous analysis of pharmaceuticals in environmental sample by liquid chromatography coupled with electrospray ionization tandem mass spectrometry

박미선, 조현우, 명승운

경기대 화학과

Pharmaceutical substances are used extensively in human and veterinary medicine. The drugs that human and animal take are not entirely absorbed by bodies, and are excreted and passed into water and treated water. Therefore, it required rapidly and certainly analysis method for pharmaceuticals which are existed in environment. Increased attention is currently being paid to pharmaceutical substances as a class of environmental contaminants. In this study, we established the simultaneous analysis method of pharmaceuticals substances (Erythromycin, Tylosin, Virginiamycin and Cimetidine) from aqueous environmental sample. Effective sample clean-up and extraction by solid-phase extraction (SPE) prior to LC-MS/MS analysis were performed. Liquid chromatography/tandem mass spectrometry (LC-MS/MS) with electrospray ionization (ESI) was used to the qualification and quantitation of five pharmaceuticals. The developed method gave good precision, accuracy, LOD and LOQ. A linear correlation observed in the calibration curves for water over the range of 0.01～3.0 ng/mL showed above r2=0.99. Absolute recovery was the range of 56.8%～106.0%. Limit of detection (LOD) and limit of quantitation (LOQ) were the range of 6.6～60.0 pg/mL and 22.0～200.0 pg/mL respectively. The established method can be used to determine low pg/mL levels of pharmaceutical substances from the water and treated water.

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Novel supported nanocatalyst based on carbon nanotube – A facile approach for the preparation using gamma radiation

이세희, *A.Gopalan, *이광필

*경북대 나노과학기술과 *경북대 화학교육과*

The capability of supported palladium (Pd) nanoparticles to catalyze many reactions has attracted intensive research during the last few years. There is a demand for innovative approach to find newer methods for the preparation of Pd supported nanocatlaysts. Carbon nanotubes (CNTs) have attracted as catalyst supports due to their special structures as compared to traditional supports. In the present work, a facile method has been adopted for the preparation of the novel functionalized multiwalled carbon nanotubes supported Pd nanoparticles based nanocatalysts (F-MWNT/Pd) catalyst. In this method, MWNTs were functionalized and loaded with Pd nanoparicles to prepare F-MWNNT-Pd nanocatlyst by - radiation induced reduction of Pd ions.. Field emission scanning microscopy and transmission electon microscopy were used to understand the morphology of F-MWNNT support and the dispersion of Pd nanoparticles into F-MWNT support. The electrocatalytic activity of F-MWNNT-Pd nanocatalyst was tested towards electrochemical oxidation of methanol. Further, the stability of the F MWNNT/Pd nanocatalyst was tested. The new supported Pd catalyst is expected to show promise for the use as catalyst in direct methanol fuel cells.

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Layer-by-layer assembly of poly(diphenylamine)/phosphotungstic acid modified electrode for electrocatalytic oxidation of ascorbic acid

D. Ragupathy, *A.Gopalan, *이광필

*경북대 일반대학원 화학과 *경북대 화학교육과*

Layer-by-layer assembly is a unique technique for the fabrication of composite films with nanometer precision. The attractive feature of this approach is its ability to assemble complex structures from modular components, and integrate them into self-assembling constructions for a wide range of applications such as drug delivery, molecular sensing, batteries and membranes. In the present work, we fabaricate a multilayer films consisting of oxidized poly(diphenylamine) (PDPA) and phosphotungstic acid (PTA). Electrochemical polymerization was used to deposit oxidized PDPA layer (PDPA(+)). A layer of negatively charged PTA was formed over the layer of PDPA(+). The processes of electrochemical polymerization and treatment with PTA were repeated to obtain the multilayer LbL film (PDPA/PTA)n, where n = number of layers of PDPA/PTA. Cyclic voltammetry and amperometric studies was used for the electrochemical property as well as the electroactivity of the (PDPA/PTA)n LbL film electrode towards AA oxidation were investigated. The enhanced electrocatalytic activity of (PDPA/PTA)n LbL film is attributed to the existence of tungsten atoms in the interlayers of PDPA.

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TiO_2 Nanoparticle Coating by HfO_2 ALD

허진국, 박주연, 조준모, 강용철

부경대 화학과

Nanoparticles have been studied for a wide range of applications in nanotechnology from drug delivery to emerging device fabrication. The Nanocoating can change the optical, chemical, and mechanical properties of nanoparticles. Since the size of nanoparticles is very small, their coating requires precise thickness control as well as high uniformity. Thus, ALD is an ideal coating technique.The TiO_2 particles were pressed into a copper grid using polished stainless steel dies and a manual press. The grid had 3.05mm diameter and 200 mesh. The TiO_2 particles were coated with HfO_2 atomic layer deposition. The ALD process carried out using tetrakis ethylmethyl amino hafnium and H_2O at 200 ℃. TEM images revealed TiO_2 particles encapsulated by conformal HfO_2 films with a thickness of ~ 16nm after 300 cycles. These TEM images are consistent with a HfO_2 ALD growth rate at 200 ℃ of 0.5 Å/ cycle.

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Novel polymer nanobiowebs for biocatalytic application

A.Gopalan, 이광필, *Shanmuga sundaram Komathi, **김태경

*경북대 화학교육과 *경북대 화학과 **경북대 나노과학기술학과*

New membranes based on multicomponent and multifunctional hybrid nanofibers are finding potential application in biosensor, batteries etc. Recently, the preparation of composite nanofibers has become an important area of research. In the present work, new functional nanofibrous polymer membranes were prepared and used for biocatalytic application. In a typical approach, poly(vinylidene fluoride) nanofiberous membranes (PVdF-NFMs) were prepared via electrospinning. PVdF-NFMs were then loaded with functionalized silica and gold nanoparticles. Thus, new functional nanofibrous polymer membranes, PVdF-silica@AuNP-NFMs, were prepared. The surface morphology and structural aspects of PVdF-silica@AuNP-NFMs were investigated using scanning electron microscopy, Fourier transform infra-red spectroscopy and wide-angle x-ray diffraction analysis. PVdF-silica@AuNP-NFMs were immobilized with horseradish peroxidase (HRP) to generate the nanobiowebs.. The biocatalytic role of PVdF-silica@AuNP-NFMs/HRP nanobiowebs was evaluated towards the detection of hydrogen peroxide.

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Dispersive solid-phase extraction followed by LC-MS/MS spectrometry for the multi-residue analysis of antibiotics in meat

이경준, 이계호

충남대 화학과

가축의 생산성 및 질의 향상을 증가시키기 위한 목적으로 동물의약품이 과다 사용되어지고 있다. 이는 가축뿐만이 아니라 최종 소비자인 인간에게도 생리학적인 장애 또는 내성이 생기는 문제를 야기 시킬 수 있다. 이러한 문제가 발생하는 것을 예방하기 위해 최대잔류허용량을 규정하고 있으며, 더 효율적이고 정확한 결과를 얻기 위한 방법이 연구되어지고 있다. 이 실험에서는 C18 을 이용한 Dispersive-SPE 방법을 사용하여 경제적이며, 빠른 분석을 할 수 있었다. 또한 매트릭스의 영향을 적게 받고 단시간 내에 분석할 수 있는 HPLC-MS/MS 를 이용함으로써 다성분 동시분석을 할 수 있는 새로운 분석법을 확립하였다. 돼지고기 시료에 표준용액을 첨가하여 분석하였으며, 최적화된 전처리 방법과 기기조건을 찾아내었다. 회수율 및 검정곡선의 직선성, 재현성에서 만족할 만한 결과를 얻을 수 있었다. 본 실험을 통하여 최적화된 전처리 방법을 개발하여 여러 가지 시료와 분석 물질에 적용함으로써 유해 물질의 분석과 여러 분야에 쉽게 응용될 것이다.

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배 추출물(Pyrus pyrifolia fruit Extracts)의 Tyrosinase 저해활성 실험과 HPLC를 이용한 화합물의 정성분석

안진영, 한정우, 김유근, 이상경

경상대 화학과

우리 고유의 배로부터 다양한 효능을 체계적으로 밝히고 그 효력을 검증함으로써 우리고유의 배가 포함하는 우수한 성분물질을 밝히며, 기능성 화장품의 개발과 제약산업의 원료를 공급하고자 한다. 경남 진주 문산 지역의 지역특산물 중 낙과 등 저장이 불가능한 부산물인 하품 배를 활용하여, 유용성이 있는 배추출물(pyrus pyrifolia fruit extract)을 부위별(껍질, 과육, 핵, 전체)로 얻어낸다. 각 부위별로 함유한 성분물질의 함량을 HPLC 로 조사하고 이들 중에서 tyrosinase 저해물질이 가장 많이 포함된 추출물을 이용하여 tyrosinase 저해활성효과를 알아보았다. 또한, 선택한 조건으로 HPLC 를 이용하여 화합물을 정성분석하고 추출물의 함량(w/w%) 설정 후 미백 기능성 화장품으로서 개발할 수 있는지를 실험하였다.

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Specific MicroRNA Are More Produced by Dicer Nuclease in the Presence of Tryptophan-Containing Amphiphilic Peptides

현순실, 한아름, 유재훈

서울대 화학교육과

Dicer converts pre-miRNA to linear ~22 nt single-stranded miRNAs in cytosol. Even though Dicer is potentially important to control availability of mature trans-acting RNAs in cytosol, the enzyme itself does not seem to be the suitable target controlling miRNA processing due to the lack of its substrate specificity. Nature, however, might be intelligent enough to differentiate a variety of pre-miRNA, so that a certain specific pre-miRNA is converted to mature miRNA in case it needs. Therefore, other component(s) in the enzyme complex could be involved in recognition of auxiliary proteins from out sources to give extra specificity. We have synthesized Trp-containing amphiphilic peptides against several pre-miRNA. Peptide 2b showed a picomolar binding affinity and a keen specificity against pre-let7a-1. In vitro miRNA processing, Dicer activity was also selectively enhanced in the presence of this peptide. On treatment with this peptide on hct116 colon cancer cell line, mature let7a-1 miRNA exists in more increased level than reference miRNAs.

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Development of RNA Aptamers against Buckminster fullerene C_{60}

이경현, 현순실, 유재훈

서울대 화학교육과

Buckminsterfullerene C_{60} is the one of famous nanomaterials. It has many potential benefits and useful biological activities in medicine and nanotechnology. But it also shows general toxicity and adverse effects that are poorly understood. To understand those positive and negative biological effects, we are trying to develop specific RNA aptamers against C_{60}-fullerene. SELEX (Systematic Evolution of Ligands by EXponential enrichment) was carried out. After 9 cycles of selection, a pull-down assay showed that C_{60}-specific RNA aptamers were enriched during selection cycles. Enriched pool was subjected to be cloned and sequenced. Some clones showed vary high affinity (near nanomolar affinity) and keen specificity against the cognate fullerene, suggesting that RNA aptamers could be used as tools to detect C_{60} in biological and environmental aspects as well.

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Identification of target RNA with photoMet containing amphiphilic alpha-helical peptides

현순실, 유재훈

서울대 화학교육과

RNA–protein interactions are important interactions among biological molecules as well as protein–protein interactions. RNAs function intimately connected with RNA binding proteins (RBP) in biological systems. The identification of the counterpart RNA of proteins has been considered to be valuable to understand the roles of RNA molecules and discover new therapeutic targets. Photo cross-linking method is a useful way to explore the direct RNA-protein interactions. The cross-linking and immuno-precipitation (CLIP) method has been used to elucidate unknown RNA sequences that interact with RBP. However, this method leads indiscriminately to cross-linked adducts between almost all bases and many amino acids and requires specific antibodies to RBP. Thus, the development of specific cross-linking is demanded for the identification of RNA and protein or even small molecules. Recently, we have developed photoMet containing amphiphilic alpha-helical peptide library and shown that photoMet containing peptide can crosslink with RNA in moderate yield. The diazirine group of photoMet was selectively crosslinked to the plausible base of RNA. The photoMet containing peptides were biotinylated to avoid the use of antibodies, since specific biotin-streptavidin interaction allows stringent purification steps. Here, we present the identification of RNA interacting with photoMet containing peptides.

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Sequencing-By-Synthesis based on mass tags

김다래, *신동윤, **안대로

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The next-generation sequencing (NGS) technology developed recently has begun to contribute a wide range of life sciences. Although the current NGS technology is based on highly cost-effective and rapid processes, compared with the conventional Sanger method, it still needs more improvement to achieve so-called '$1000 sequencing'. In this context, we studied a novel DNA sequencing method based on SBS (Sequencing by Synthesis) using mass tags.

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Sequencing-By-Synthesis based on fluorescent tags

김다래, *신동윤, **안대로

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The next-generation sequencing (NGS) technology developed recently has begun to contribute a wide range of life sciences. Although the current NGS technology is based on highly cost-effective and rapid processes, compared with the conventional Sanger method, it still needs more improvement to achieve so-called '$1000 sequencing'. In this context, we studied a novel DNA sequencing method based on SBS (Sequencing by Synthesis) using fluorescent tags.

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Enhanced cell permeability of kojic acid-phenylalanine amide with metal complex

곽선영, 서효석, 이윤식

서울대 화학생물공학부

Tyrosinase is a critical enzyme in the melanogenesis by catalyzing oxidation of L-tyrosine and L-dihydroxyphenylalanine (L-DOPA) to melanin. Although kojic acid which is a well known tyrosinase inhibitor has been widely used in cosmetic industry, they showed insufficient activity and stability. Thus, we modified kojic acid with amino acids to enhance the tyrosinase inhibitory activity. Kojic acid-phenylalanine amide (KA-F-NH2) showed much higher tyrosinase inhibitory activity compare to kojic acid itself [1], however, it did not show any activity in melanocyte due to the low cell permeability. To enhance its cell permeability, we prepared metal coordination compounds of KA-F-NH2 to increase the lipophilicity. We characterized them by FT-IR and ICP analysis. The metal complex of KA-F-NH2 sufficiently inhibited mushroom tyrosinase as much as KA-F-NH2 and reduced melanin contents in melanocyte efficiently as well. This accomplishment may provide useful information in the fields of whitening agents and drug delivery system.

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Kinetic measurement of nucleic acid unwinding by Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) helicase

이나라, 이아람, *김동은, **정용주

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Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) helicase catalyzes double-stranded (ds) nucleic acid unwinding. Because it is reported that SARS-CoV helicase can unwind dsDNA with 5'-overhang, we performed steady state dsDNA unwinding experiments by using a series of dsDNA with different length of 5'-overhang to find out optimal dsDNA substrate. We also performed dsDNA unwinding experiments to determine whether SARS-CoV helicase can recognize the gap. SARS-CoV helicase showed unwinding activity when dsDNA has minimal 5 ~ 10 bases overhang or gap. Additionally, DNA-RNA hybrid substrates were also tested. The results show that SARS-CoV helicase has low processivity and its unwinding activity is dependent on the length of 5'-overhang.Acknowledgment: This work was supported by Seoul R&BD Program (10580).

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Amphiphilic alpha-helical peptides with acridine and its analogues are promising pharmocophores against RNA hairpin targets

나지영, 유재훈

서울대 화학교육과

Acridine intercalates paired bases or interacts electrostatically with negatively charged phosphate backbone in various RNA targets. By using this moiety, we have demonstrated that amphiphilic alpha-helical peptides containing acridinylated lysine(s)(K*) display picomolar affinity toward RRE and TAR RNA of HIV-1. Encouraged by this result, we are developing an amphiphilic peptide library containing both acridine and its analogues. Synthesized peptides with different position of acridine and its analogues showed totally different binding affinities against RNA targets. For an example, a peptide with 6-chloro-2-methoxy acridine(K**) at position 1 and acridine at position 4 (LK**KLLKLLK*KLLKLKG) showed 30 pM affinity against HBV RNA while a peptide with opposite position (LK*KLLKLLK**KLLKLKG) showed 110 pM affinity (4-fold difference in affinity). Data suggested that position(s) and choice of proper acridine analogues are essential for interactions with counterparts RNA. By identifying important position(s) and proper analogues of acridine, one could generate anti-viral amphiphilic peptides with picomolar affinity and keen specificity.

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PHD2 inhibition by peptide inhibitor

권혁성, *안대로

*KIST 의과학센터 *KIST 생체과학부*

PHD2 is an enzyme which deactivates HIF-1a through hydroxylation. Activation of HIF-1a resulting from inhibition of PHD2 could be a potential target for treatment of ischemic diseases. In this presentation, we designed a peptide inhibitor of PHD2 and studied effects of the peptide inhibitor at both in vitro and cellular levels.

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Dihydroxychromone derivatives selectively inhibit duplex DNA-unwinding activity of Severe Acute Respiratory Syndrome Coronavirus NTPase/Helicase

이진무, 유미선, *정용주

*국민대 화학과 *국민대 생명나노화학과*

Severe Acute Respiratory Syndrome coronavirus (SARS-CoV) Helicase/NTPase is the central catalytic enzyme of viral replication and is an attractive target for antiviral therapy. Aryl diketoacids have been identified as the first SARS-CoV NTPase/Helicase inhibitors with a distinct pharmacophore featuring an arylmethyl group attached to a diketoacid core. Then three classes of dihydroxychromone derivatives were prepared. We purified SARS-CoV Helicase/NTPase for High-throughtput screening (HTS) assay and performed HTS assays to find out inhibitors using a FRET-based duplex DNA unwinding and a colorimetric ATP hydrolysis assays, respectively. The compounds 4a and 4c represented IC_{50} values of 4.1 μM and 2.7 μM for SARS-CoV Helicase duplex DNA unwinding, respectively. Finally, the dihydroxychromone derivatives showed potent and selective inhibition against the SARS-CoV helicase duplex DNA-unwinding activity but not against helicase ATPase activity. We hope that the dihydroxychromone derivatives will potentially useful in vitro for the development of antiviral agent against SARS-CoV.

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Studies of interaction between RIG-I and NS1 in the presence and absence of nucleic acids

조성제, *심희섭, **정용주

*국민대 화학과 효소화학 연구실 *국민대 화학과 **국민대 생명나노화학과*

Retinoic acid–inducible gene I (RIG-I) is known as an intracellular sensor of virus infection. The ATPase RIG-I, an IFN-inducible protein that consists of caspase recruitment domains (CARDs) and a helicase domain, has been identified as double-stranded RNA or 5'-triphosphates single-stranded RNA detector. RIG-I senses various types of viruses, Hepatitis C virus, Sendai virus, influenza virus, vesicular stomatitis virus, rabies virus, and Japanese encephalitis virus. RIG-I is imperative for induction of IFN-I in response to Influenza A virus (IAV). NS1 protein of AIV suppresses induction of IFN-I by targeting and inactivating the RIG-I–dependent signaling pathway. So we studied the interaction between RIG-1 and NS1 of Influenza A virus by Enzyme-Linked Immunosorbent Assay (ELISA). Our results show that RIG-I specifically binds to the NS1 of AIV (K_D = 40nM) in the presence of PolyI:C, but does not bind in the absence of RNA.

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Characterization and isolation of RNA aptamer against Avian Influenza NS1 protein

심희섭, *조성제, **정용주

*국민대 화학과 *국민대 화학과 효소화학 연구실 **국민대 생명나노화학과*

After the outbreaks of Avian Influenza (AI) virus (H5N1) in eastern Asia, it is becoming the whole world-wide's problem due to its high pathogenicity and contagion. AI virus belongs to the family Orthomyxoviridae and consists of eight single-stranded (-) sense RNA segments. NS1 protein is translated by collinear transcript of segment 8. NS1 protein was known for multifunctional protein, which associates with protein-protein and protein-RNA interactions during host cell infection. Because NS1 distracts pathway of IFN-β induction during the infection, it suppresses innate immune response. Therefore NS1 can be a good target for the development of antiviral agent. In the present study, GST-tagged NS1 protein was purified and RNA aptamers against the AIV NS1 were isolated.

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Investigating the Cellular Responses to Graphene Oxide

김미희, 유수윤, 김영관, 민달희

KAIST 화학과

Various nanomaterials are presently under development for diagnostic and therapeutic applications. Specific biomedical applications include drug delivery system, bioimaging, and biosensor. However, little is known regarding the potential adverse effects, immune responses, and cytotoxicity of various nanomaterials which possess high potentials in clinical applications.In this report, we describe important cellular responses of graphene oxide revealed by various bioanalytical assays. Graphene is thinnest carbon based nanomaterial that is recently explored in many research fields including material science and medicine. Graphene derivatives are believed as a promising material for the development of not only transparent conducting films but also of novel drug delivery system. However, cytotoxicity and biocompatibility of graphene oxide are not investigated yet. Here, we quantitatively measured cellular immune response, oxidative stress, and cytotoxicity of graphene oxide using human liver cells. We believe that the present study will give insight on how cells react to graphene oxide and what kinds of cellular processes can be altered by this new nanomaterial.

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Production and NMR Structural Studies of Bovine Lactophoricin

박태준, 김지선, 김용애

한국외국어대 화학과

Lactophoricin (LPcin-I) is a 23-amino acid peptide that corresponds to the carboxyterminal 113 to 135 region of component-3 of proteose peptone (PP3), a minor phosphoglycoprotein found in bovine milk. It has been reported that LPcin-I has antibacterial activity and a cationic amphipathic helical structure, but its shorter analogous peptide (LPcin-II), a 17-amino acid peptide, corresponding to the 119 to 135 region of PP3 does not display antibacterial activity. In fact, it was interestingly known that LPcin-I and LPcin-II have similar charge ratios and identical hydrophobic/hydrophilic sectors, according to their helical wheel projection patterns, and both peptides show cationic amphipathic helical folding and interact with membranes. However, it is known that only LPcin-I incorporates into planar lipidic bilayers by forming voltage-dependent channels. In this study, in order to understand the structure-activity relationship of these peptides, the authors cloned and expressed the two recombinant peptides as fusion proteins inclusion bodies in Escherichia coli. Fusion proteins were purified by Ni-NTA affinity chromatography under denaturing conditions, and recombinant LPcin-I and LPcin-II were released from fusion by chemical cleavage. Final purifications were achieved by preparative reversed-phase HPLC. Using these methods, we obtained several tens of milligrams of uniformly and selectively 15N labeled peptides per liter of growth, which was sufficient for solid-state NMR spectroscopy. Peptides were identified by tris-tricine PAGE, ESI mass spectroscopy, solution and solid-state NMR spectroscopy.

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Protein phosphatase complement of dog genome

Mrigendra B. Karmacharya, 소재원

인하대 화학과

Protein kinases and protein phosphatases which respectively add and remove phosphate group of target proteins, constitute about 2-4% of the genes in a typical eukaryotic genome. Recently, protein phosphatases are evolving as important players in multitudes of cellular processes such as proliferation, differentiation, cell adhesion and motility. Now protein phosphatases are amongst the extensively studied proteins and are reported as potential drug targets of many diseases including cancer and others. In this paper, we identified, classified, and analyzed protein phosphatase complement of domestic dog Canis familiaris. Here, we report at least 177 putative protein phosphatases in dog which include 50 PSTPs, 112 PTPs and 15 Asp-based protein phosphatases. Interestingly, we found at least five novel protein phosphatases in dog, namely DUSP5L, DUSP18L, MTMR9L, MTMR12L, and PPP6CL which are not present in human, mouse, rat and cow. In addition, we found a retro-transposed copy of PTP4A1 gene PTP4A1-rt in chromosome 27. Furthermore, we modeled three dimensional structures of the catalytic domains of these putative protein phosphatases and aligned to see the structural similarities between them.

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Expression and purification of catalytic domain of protein kinase C isoforms using 6xHis tag fusion expression system

권우중, 소재원

인하대 화학과

Protein kinase C (PKC) isoforms are a family of at least 10 serine/threonine protein kinases divided into three subfamilies: classical, novel & atypical, and are important modifiers of several cardiovascular phenomena, carcinogenesis & apoptosis, and are also promising therapeutic target for cancer and other indications. In our present study, we expressed and purified catalytic domain mutants of PKC isoforms. Bacterial protein expression plasmids were constructed by using pBADHisN3 vector. These expression vectors were transformed into TOP10 E.coli strain and expressed by Arabinose induction. Proteins were expressed as His tag protein and purified by Ni-NTA column. We checked the protein expression levels by SDS-PAGE analysis. We will use these proteins to study the role of PKC isoforms in cell signaling pathways.

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Isolation of Bronchioalveolar Stem Cells in Normal and Lung Cancer Mice by Using M-SERS (Magnetic Surface Enhanced Raman Spectroscopic) Dots

강호만, *전봉현, 김성용, *박주영, *현택환, **정대홍, *이윤식

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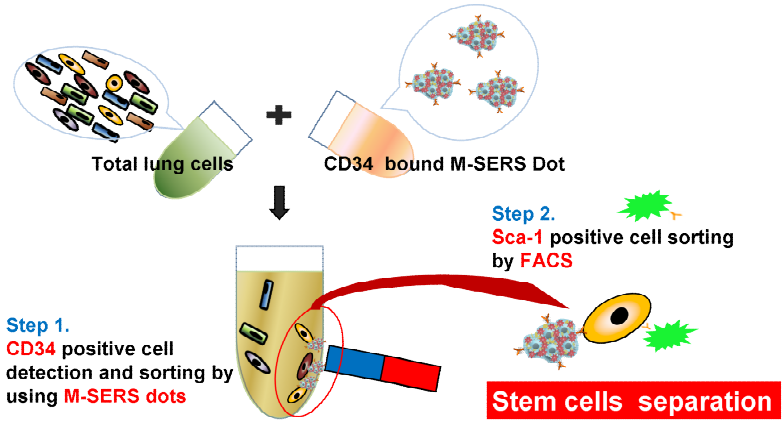
Bronchioalveolar stem cells (BASCs) play a central role in the development of lung cancer. BASC, localized bronchioalveolar duct junction, contain Clara cells and alveolar type II cells. To study the fate of BASCs, their isolation and purification are important. However, the available methods of isolating BASCs are limited, because the cells are very rare in tissues.In this study, we tried to isolate BASCs in the murine lung using magnetic nanoparticle-based surface-enhanced Raman spectroscopic dots (M-SERS Dots). We used K-*ras*^{LA1} mice, a laboratory animal model of non-small cell lung cancer of human, and C57BL/6 mice having the same age as a control. We compared the BASCs between 2 species by FACS analysis with 4 markers of BASCs, Clara cell specific protein (CCSP), surfactant protein C (SP-C), cell differentiation antigen (CD34), and stem cell antigen-1 (Sca-1). We found that BASCs were more abundant in the K-*ras*^{LA1} mice than in the C57BL/6 mice. Also, the M-SERS Dot-mediated positive selection of the CD34^{pos} cells enabled the BASCs to be enriched to an approximately 4- to 5- fold higher level than that in the case without pre-separation. We proved that M-SERS Dots could play an important role in cancer diagnosis, multiple detection and fast isolation of desired cells and biological molecules.



Isolation system by using M-SERS Dots + FACS

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Receptor-mediated endocytosis of biotinylated somatostatin 14 conjugated to the streptavidin coated fluorescent nanoparticles in Rat pancreatic AR42J cells

김은주, *Andrei Zvyagin, *Jin J. Sun, *Varun K.A.S.

*대구대 과학교육학부/화학교육과 *Macquarie University/Physics Department*

Somatostatin (SST-14) and the N-terminally extended form, SST-28, are important regulator of neurotransmission in the brain as well as hormone secretion from the pituitary gland, the pancreas, and the gastrointestinal tract. Their physiological responses are mediated by one or more of the five somatostatin receptors.As a step towards single molecular trafficking in targeted rostral ventrolateral medulla (RVLM) presympathetic neurons that express somatostatin 2A receptor which is important for maintaining and potentially generating sympathetic vasomotor tone using fluorescent nanoparticles, we constructed biotinylated SST-14 and conjugated it to the streptavidin coated Quantum dot (Qdot). We found that the streptavidin coated Qdots, themselves, could be internalized into the cells under the normal experimental conditions. Furthermore, SSTR 2A is not abundantly expressed enough to give the dramatic difference between Qdots bound to SSTR 2A and control Qdots in the Rat pancreatic AR42J cells. In order to tackle these problems, we developed the method for selective internalization of SST-14 conjugated Qdot through receptor-mediated endocytosis but not internalization of Qdots themselves. Internalized SSTR bound Qdots in AR42J cells were visualized and analyzed using confocal fluorescent microscopic method.

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In-situ fabrication of alendronate loaded hydroxyapatite microspheres as an injectable bone filler

고일환, *장정호, *이진형

*인하대 화학공학과 *한국세라믹기술원 바이오융합팀*

This work describes the in-situ synthesis of hydroxyapatite microspheres at room temperature including an alendronate as an osteophoresis drug. The key process for the fabrication of hydroxyapatite microsphere is the use of urease to adjust the reaction pH upto neutral through the decomposition of urea. The acidic reaction solution is mixed with dissolved hydroxyapatite, urea, urease, and alendronate, and then form the water-in-oil emulsion by addition of the mixture solution into mineral oil. This emulsion is homogenized, and then collected by the centrifugation. Obtained alendronate incorporated hydroxyapatite microspheres are shown the homogeneous particles sizes in the range of 200-300 ㎛. This preliminary result should be applied to biomedical field as an injectable bone filler with the controlled drug release materials.

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New Gd(III) Complex of Cyclic DTPA-bis(amide) as High Relaxivity MRI Contrast Agent

Md.Nasiruzzaman, *김희경, **구성욱, 김태정

*경북대 응용화학과 *경북대 의용생체공학과 **경북대 응용화학과*

Magnetic Resonance Imaging (MRI) is an important non-invasive method for studying the internal structures of the human body. There is a need in developing dose-effective contrast agents (CAs) with higher specificity and relaxivity. A mononuclear cyclic Gd(III) polyaminocarboxylates, $[Gd(FcDTPA)(H_2O)]\bullet nH_2O$ was synthesized and characterized by spectroscopic technique. Hydrophobic moieties, such as Cp rings of ferrocene, are introduced into this complex so as to achieve target-specificity. Potentiality of $[Gd(FcDTPA)(H_2O)]\bullet nH_2O$ as contrast agent for magnetic resonance imaging (MRI CA) was investigated by measuring relevant physicochemical properties and relaxivities and compared with $[Gd(DTPA\text{-}BMA)(H_2O)]$ (Omniscan®). The R1 relaxivities of aqueous solutions of this CAs is in the range of 8.9 $mM^{-1}sec^{-1}$, which is about two fold higher than that of the clinically used Omniscan® (R1=3.3 $mM^{-1}sec^{-1}$). This newly synthesized compound exhibited a increase in the R1 relaxivity in saline water with 4.5% w/v human serum albumin (HSA).The MTT assay performed on this complex reveals cytotoxicity as low as that for Omniscan® in the concentration range required to obtain intensity enhancement in the in vivo MRI study.

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Surface functionalized Gold Nanoparticles as Highly Efficient Bimodal MR/CT Contrast Agent

구성욱, *정희영, **김희경, *Md.Nasiruzzaman, *김태정

*경북대 응용화학과 *경북대 응용화학과 **경북대 의용생체공학과*

Functionalized gold nanoparticles were applied as contrast agents for both in vivo X-ray and magnetic resonance imaging. These particles were obtained by the replacement of citrate coated gold nanoparticles with thiolated Gd(III) complex of DTPA-bis(amide) of penicilamine (GdL). Well-dispersed spherical AuNPs coated with gadolinium complexes, abbreviated as Au@GdL, have been obtained; the mean size of Au@GdL is 11-14 nm, and the numbers of GdL are 3000 per Au NP. Au@GdL exhibits extremely high longitudinal (R1) and transverse (R2) relaxivities of 20.1 and 29.4 mM^{-1} s^{-1}, respectively. This study revealed that these particles suited for dual modality imaging, MRI and CT, freely circulated in the blood vessels of lymph node of mouse.

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장소: 대전컨벤션센터
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발표분야: 생명화학
발표종류: 포스터, 발표일시: 목 16:30~18:30

A Bodipy-based Zinc(Ⅱ) Fluorophore as a Detector of Apoptosis

배세원, 김은하, 김훈준, 박승범, 홍종인

서울대 화학부

A Bodipy-based biomimetic Zinc(Ⅱ)-selective fluorophore has been demonstrated to be a good detector of the apoptosis in cancer cells. The Zinc(Ⅱ) fluorophore is cell-permeable to show weak fluorescence, which forms a strong fluorescent 1:2 Zn complex. When apoptosis in cancer cells is artificially induced by anticancer agent, Zinc(Ⅱ) fluorophore selectively and strongly stains apoptotic cells only at early stages, which was verified by using the conventional apoptosis detection probe, annexin V. Detection of apoptosis by Zinc(Ⅱ) fluorophore was perhaps due to significantly increased free Zinc(Ⅱ) flux at early stages of apoptosis.

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발표종류: 포스터, 발표일시: 목 16:30~18:30

Developing Apo A-I Mimetic Peptides as Therapeutics for Alzheimer's Disease

이경현, 함지예, 김예원, 유재훈

서울대 화학교육과

Apolipoprotein A-I mimetic peptide, D-4F, has been shown to increase high density lipoprotein-cholesterol (HDL-C) complex in blood stream, reversing cholesterol efflux from peripheral macrophages to liver cells. Anti-inflammatory effect is accompanied by reversing cholesterol efflux, affording a reduced incidence of coronary diseases. Encouraged by a recent report indicating that D-4F decreases brain arteriole inflammation and improves cognitive performance, we are trying to use analogues of this peptide as a therapeutic for Alzheimer's disease (AD). A variety of amphipathic peptides has been designed and synthesized as mimicry of D-4F by substitution of the most important amino acids to unnatural amino acids both in hydrophilic and hydrophobic spheres. Each peptide was then subjected to cell-based screen using SH-SY5Y human neuroblastoma cells. Selected peptides not only possessed more improved anti-inflammatory and alleviating effect of amyloid beta-induced neuronal toxicity than those of D-4F. The selected peptide could be used as a potential therapeutic for coronary diseases and AD as well.

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Development of RNA aptamers as Tools for Discriminating Epigenetically Modified Histone H3 N-terminal Tails

이경현, 한아름, 유재훈

서울대 화학교육과

Epigenetic changes by post-translational modifications in histone H3 are used to control the chromatin remodeling and gene regulation in cells. Antibodies to discriminate the epigenetic change on histone proteins are widely used, but their specificity and selectivity are not satisfactory. In order to develop the more specific and selective complimentary molecules for epigenetic changed histone H3, various epigenetic marked N-terminal 18-amino acids peptides with biological relevance were synthesized by a standard Fmoc chemistry. Systematic Evolution of Ligands by EXponential enrichment technology was then carried out to select the most selective RNA aptamers against those epigenetically modified peptides. After repeated cycles of selections, pull-down assays showed that specific and selective RNA aptamers for each peptide were enriched during selection cycles. Enriched pool was subjected to be cloned and sequenced, followed by characterization, resulting in specific and selective RNA aptamers against post-translational modified histone peptides.

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Gold Nanoparticles Coated with Gadolinium Chelate as a New Liver-Specific T1 MR/CT Contrast Agent

김희경, *박지애, **구성욱, ***Md.Nasiruzzaman, ***김태정

*경북대 의용생체공학과 *한국원자력의학원 분자영상연구부 핵의학연구팀*
***경북대 응용화학과 ***경북대 응용화학과*

The synthesis and characterization of gold nanoparticles coated by Gd-chelate (Au@GdL) is described, where L is a conjugate of DTPA and cysteine. These particles are obtained by the replacement of citrate from the gold nanoparticle surfaces with gadolinium chelate (GdL). The average size of Au@GdL is 14 nm with a loading of GdL reaching up to 2.9×10^3 per particles, and they demonstrate very high R1 relaxivity (~10^5 $mM^{-1}s^{-1}$) as well as X-ray attenuation. The R1 relaxivity per [Gd] is as high as 17.9 $mM^{-1}s^{-1}$. The present system also exhibits liver-specific property, as demonstrated by histological images as well as CT and MR, rendering itself as a new class of liver-specific T1 bimodal CT/MR contrast agent.

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Intramolecular photo-crosslinking reactions; the reactivity of peptide side chains with in situ generated carbenes

현순실, 박현선, 유재훈

서울대 화학교육과

Photo cross-linking has been used to characterize protein-protein and protein-small molecule interactions. Recently, photo-labile diazirine containing nonnatural amino acid, photoMet, is incorporated to proteins and peptides. Carbenes form covalent bonds with proximate nucleophiles of amino acid side chains. The reactivity of the side chains with carbenes, however, has not been studied in the biological environment, yet. We designed an alpha-helical peptide library that forms intramolecular covalent bonds between a carbene and a nucleophile of an amino acid side chain. Carbene and nucleophile are located in the i and i+4 position on conformationally rigid alpha-helical peptides. In all cases, a water molecule was inserted to carbine. The relative reactivity of nucleophile compared to water was defined as value of $\log(k/(k_0[H_2O]))$. Phenolic hydroxyl group is shown as the most reactive nucleophile and thiol group of Cys is the second most reactivity in L-form amino acids

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Inhibitory Effects of Protocatechuic acid-Amino acid amides on Mushroom Tyrosinase

노진미, 이윤식

서울대 화학생물공학부

Skin pigmentation occurs in various specialized cells through the synthesis of melanin from L-tyrosine through a series of chemical and biochemical reactions. Critical to these reactions is the presence of an enzyme, tyrosinase, which catalyzes the conversion of L-tyrosine to L-dihydroxyphenylalanine (L-DOPA). By inhibiting the activity of tyrosinase, skin pigmentation can be reduced and, thus, excessive pigmentation can be prevented. Phenolic acid and esters are regarded as one of the groups of dietary polyphenols; they are known for their tyrosinase inhibitory activities and antioxidant activities as well. Among them, protocatechuic acid (3,4-dihydroxybenzoic acid) is known for its potent antiradical activity and tyrosinase inhibitory activity.Previously, our group found that when aromatic amino acids were introduced to kojic acid, their tyrosinase inhibitory activity and storage stability were highly increased[1,2]. In this study, we conjugated protocatechuic acid with aromatic amino acids such as phenylalanine, tryptophan and tyrosine, and examined their tyrosinase inhibitory activity. Furthermore, tyrosinase inhibitory mechanism was studied with protocatechuic acid-amino acid derivatrives.[1] Noh, J.M .; Kwak, S.Y.; Kim, D. H.; Lee, Y.S. Biopolymers.88, 300, 2007[2] Noh, J.M.; Kwak, S.Y.; Seo, H.S.; Seo, J.H.; Kim, B.G.; Lee, Y.S. Bioorganic & Medicinal Chemistry Letters.2009, in press.

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Development of Artificial Chaperone using Poly-γ-Glutamic Acid-Cholesterol Nanoparticle

곽미선, *홍승표, *정동진, 함수정, **임용택, **김철중, 성문희

*국민대 *(주)바이오리더스 **충남대*

An artificial chaperone, which can decrease the protein aggregation and increase the activation yield of denatured protein, was developed using poly-γ-glutamic acid-cholesterol conjugate(γ-PGA-cholesterol conjugate). γ-PGA-cholesterol conjugate is composed of hydrophilic γ-PGA backbone and partly substituted hydrophobic cholesterol, and is capable of forming a nanoparticle by the self-association in water. The γ-PGA-cholesterol nanoparticle have the ability to trap and release protein by host-guest interaction of the cholesterol group and β-cyclodextrin, suggested the molecular chaperone activity for refolding of denatured protein. We studied the artificial chaperone activity of γ-PGA-cholesterol nanoparticle by refolding of M2-HA (W150) fusion protein. HA (hemagglutinin) and M2 (matrix protein 2) are the protein that exist on the surface of AI (avian influenza) virus. M2-HA (W150) fusion protein was over-expressed as an insoluble form in *E. coli*. The insoluble M2-HA (W150) fusion protein was refolded by γ-PGA-cholesterol nanoparticle. The renaturation yield of insoluble M2-HA (W150) fusion protein reached approximately 35%. It is considered that the γ-PGA-cholesterol nanoparticle can be used as an artificial chaperone and can be applied for protein refolding. [This work was supported by Top Brand Project grant from Korea Research Council of Fundamental Science & Technology and KRIBB Initiative program (KGM3110912).]

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Proton NMR and Fluorescence Studies of DNA Binding Domain in Human Heat Shock Transcription Factor 1

박성민, LU MING, CHANG ZIWEI, 강신원, 박장수

부산대 화학과

Human heat shock transcription factor 1 (HSF1) is the master transcriptional regulator in heat shock response inducing the expression of heat shock proteins (HSP). The DNA Binding domain (DBD) in three major functional domains plays the important roles in the formation of hHSF1 trimers. The 3D structures of HSF DBD in *Drosophila* and Yeast have been resolved by X-ray spectroscopy. However, the structure of human HSF1 DBD in solution condition remains unknown. Here, to indentify the structural characterization of human HSF1 DBD, we constructed a new plasmid which contains above special DNA, and expressed it in E.coli C41(DE3). After Purification, DBDs were treated with various stress conditions (such as heat stress, pH), and then examined by using proton NMR spectroscopy. According to our results, environmental stress could induce the structural change. Moreover, fluorescence spectra show that heat stress could induce the DBD to form a more compact one. These results provide new insight for hHSF1 function.

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Spot Array Synthesis of Peptides on Glass Surfaces for Kinase Assays

김재희, 김미라, 이윤식

서울대 화학생물공학부

Compared with common solid supports for peptide synthesis such as polymer beads, plane substrates such as glass chip or cellulose paper have unique properties so that they can be used for the preparation of peptide array for direct bio assay. With the recent advances in micro fabrication and surface modification, peptide arrays were widely used for high-throughput screening (HTS) for drug discovery. In this study, the glass surface was modified for kinase assays, and the spot arrays were prepared through patterning with photoresist followed by perfluorination of the background. The model peptide substrates of $p60^{c\text{-}src}$ kinase, which were previously identified by one-bead one-compound peptide library method, were synthesized on the spots on glass surface *in situ*, and the kinase reactions were performed on the glass surface. By using this method, kinase activities toward model peptide substrates were measured quantitatively, and thus, we could identify the specific peptide substrates of $p60^{c\text{-}src}$ kinase among the model peptides.

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발표종류: 포스터, 발표일시: 목 16:30~18:30

Bacterial over-expression of two Ayrl hydrocarbon receptor (AHR1 and AHR2) from Goldfish (*Carassius auratus*), and their TCDD binding activities

CHANG ZIWEI, LU MING, 박성민, 강신원, 박장수

부산대 화학과

The Ayrl hydrocarbon receptor(AHR) is a ligand-activated transcription factor which mediates xenobiotic signaling to enhance the expression of target genes, such as cytochrome P450s family. The AHR signaling pathway mediates the toxic compound including 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) related planar halogenated aromatic hydrocarbons (PHAHS). Here we obtained two distinct AHRs (gfAHR1 and gfAHR2) from the teleost Carassius auratus (Goldfish). They have a 2445 base-pair open reading frame encoding 815 amino acid and a 3075 bp encoding a 1025 amino acid, respectively. Then two AHRs were subcloned into pGEX-5X-1 vectors, and were over-expressed in an Escherichia coli system. After purification, we examined their binding activity with TCDD and found that they showed different characterization. Furthermore, using these expressed AHRs, we can do further study of detecting AHR expression level in goldfish and may be helpful to detect environmental contaminant.

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Inhibitor screening assay of microsomal prostaglandin E_2 synthase-1 (mPGES-1) using coupled enzyme assay system and mammalian cell assay

최경아, 박성준, 유연규

국민대 생명나노화학과

mPGES-1 catalyzes the conversion of PGH_2 into PGE_2, which induced inflammatory response, fever, and pain. To establish an assay method of searching inhibitor of mPGES-1, a coupled enzyme assay system using mPGES-1 and 15-PGDH has been developed. In this assay, PGH_2 was converted to PGE_2 by mPGES-1 and then PGE_2 was transformed to the 15-keto-PGE_2 by 15-PGDH accompanying the production of NADH. During the reaction, spontaneous decomposition of PGH_2 was prevented by PMA. To test this assay, the Km value of substrate and the IC_{50} value of MK-886 measured (150 μM and 3.4 μM, respectively) and then the result is close to both Km value and IC_{50} value as previously reported. To test the utility of this assay, the 160 compounds were assayed and Z´ factor that reflects both the assay signal dynamic range and data variation was determined. We demonstrated that the coupled enzyme assay system has a high Z' value (0.86 ± 0.03), which is appropriate for a HTS assays. Using the assay system we have screened a fragment chemical library from Korea Chemical Bank and identified a few compounds that inhibit mPGES-1 activity. The inhibitory activity of these compounds was further confirmed by a cell-based assay method using A549 cells.

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Molecular Cloning and Bacterial Overexpression of Goldfish hsp70, and Its Applications for Monitoring the Environmental Pollution

배민지, 오범석, **LU MING**, 강신원, 박장수

부산대 화학과

Heat shock proteins (HSP) are a class of functionally related proteins whose expression is increased when cells are exposed to elevated temperatures or other stress. This increase in expression is transcriptionally regulated. HSPs are found in virtually all living organisms, from bacteria to humans. Here, we obtained the full-length hsp70 cDNA from goldfish liver, and cloned it into pGEX-5X-1 vector. After overexpression and purification, hsp70 proteins were injected into mouse for making anti-hsp70 antibody. Then hsp70 antibody could be used to monitoring the environmental pollution.

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Identification and characterization of novel inhibitors of UDP-N-acetylglucosamine enolpyruvyl transferase(MurA) from *Haemophilus influenzae*.

한성구, *이기인, 유연규

*국민대 생명나노화학과 *한국화학연구원 신약연구단*

Most of Gram negative or positive bacteria contain UDP-N-acetylglucosamine enolpyruvyl transferase(MurA) as the first enzyme of bacterial cell wall synthetic pathway. In the cell wall synthesis, MurA transfer the enolpyruvate moiety of phosphoenolpyruvate(PEP) to UDP-N-acetylglucosamine(UNAG). We have found hit compounds from screening of a Fragment Library from Korea Chemical Bank. Comparison study of structures of derivatives and their 50% inhibitory concentrations (IC_{50}) performed to identify more potent inhibitors, which have IC_{50} values lower than micromolar concentration. The inhibitory mechanisms of the identified inhibitors and their effects on the conformation of MurA have been investigated.

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Effect of Heavy Metal and Endocrine Disruptors on Goldfish hsp70 by Enzyme-Linked ImmunoSorbent Assay (ELISA)

오범석, 배민지, 박장수

부산대 화학과

Heat shock proteins (HSPs) are a family of proteins expressed in response to a wide range of biotic and abiotic stressors. The 70 kilodalton heat shock proteins (Hsp70s) are a family of ubiquitously expressed proteins. The Hsp70s are an important part of the cell's machinery for protein folding, and help to protect cells from stress. To aid environmental monitoring several in-vitro methods have been utilized to test the effects of pollutants on biological processes and some of these assays have been based on fish. In this study, we developed an ELISA for goldfish HSP quantification, using polyclonal antibodies, and the ELISA can apply to evaluate HSP induction effects in goldfish by heavy metal and endocrine disruptors.

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Characterization of dexamethasone conjugated polyethylenimine as an efficient gene delivery carrier with anti-inflammatory effect for gene therapy of acute lung injury

김현아, *최준식, 이민형

*한양대 응용화공생명공학부 *충남대 생화학과*

Acute lung injury (ALI) is characterized by disruption of the lung alveolar-capillary membrane barrier with severe acute inflammatory response in the lung and neurtrophilic alveolitis. Dexamethasone is a potent glucocorticoid and has anti-inflammatory effect. In this study, dexamethasone conjugated low molecular polyethylenimine (2 kDa),PEI-Dexa,was synthesized as a water-soluble glucocorticoid and gene carrier for gene therapy of ALI. To confirm the anti-inflammatory effect of PEI-Dexa, PEI-Dexa/pß complexes were transfected into LPS stimulated RAW264.7 macrophage cells. After 24 hrs, the levels of TNF-α, IL-1ß, and IL-6 were measured by ELISA. The results showed that PEI-Dexa transfected cells reduced inflammatory cytokines, compared to the control cells. However, PEI2K/pß and PEI25K/pß did not show this effect. Then, PEI-Dexa was characterized as a gene carrier. MTT assays showed PEI-Dexa transfected cells had lower toxicity to L2 lung epithelial cells than PEI25K. In addition, PEI-Dexa had higher transfection efficiency then PEI2K. For in vivo study, PEI-Dexa/pß-Luc, PEI 2K/pß-Luc and PEI25K/pß-Luc complexes were administrated into the mice lung by intratracheal injection. Luciferase assay showed that PEI-Dexa had higher delivery efficiency to the mouse lung than PEI 2K or PEI 25K. Anti-inflammatory effect of PEI-Dexa was evaluated in LPS induced ALI mouse model. PEI-Dexa/pß complexes were administered in the lungs. After 24hrs, TNF-α and IL-6 levels were determined in BALF and lung tissues. In the result, PEI-Dexa injected group reduced inflammatory cytokines. Finally, H&E staining showed that PEI-Dexa reduced the inflammation in the lungs. The results suggest that PEI-Dexa is an efficient delivery carrier for acute lung injury gene therapy.

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Screening of RNA aptamer specific to Interleukin 32 involved in inflammatory disease

김세호, 김동은

건국대 생명공학과

Interleukin 32(IL-32) is a newly reported cytokine that belongs to IL-1 family which causes autoimmune and inflammatory disease like Rheumatoid Arthritis. IL-32 upregulates Tumor Necrosis Factor α(TNF-α) which has cytotoxic effect on cancer cells. This research aimed to screen RNA aptamer, oligonucleotide that binds to protein with high affinity (nano molar Kd value), to develop antagonist of IL-32. We used 90 nucleotides of RNA library that contains 40 nucleotides of random sequences to obtain RNA aptamer which specifically binds to IL-32 using SELEX(Systematic Evolution of Ligands by Exponential enrichment) method. We screened 8 RNA aptamers, and these can be grouped into 3 groups based on sequence similarity. To confirm the affinity of RNA aptamers, we performed EMSA(Electrophoresis Mobility Shift Assay) and we found that the one with the highest affinity against IL-32. We named as I32SA. We will further determine Kd value for I32SA. Ultimately, we will test the I32SA as inhibitor of IL-32 cytokine in cells.

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Screening of DNAzymes that inhibit Hepatitis C virus replication by cleaving viral nonstructural gene 3 RNA in human hepatoma cells

이복희, 김경보, *김동은

*건국대 생명공학 *건국대 생명공학과*

Hepatitis C virus (HCV) is an enveloped virus known as main cause of chronic hepatitis, liver cirrhosis and hepatocellular carcinoma. A class of antisense oligodeoxyribozymes, known as 10-23 DNAzyme, has been shown to efficiently cleave target RNA at purine-pyrimidine junctions in vitro. In this study, we have utilized a strategy to identify accessible cleavage sites for DNAzyme in the target RNA, the HCV nonstructural gene 3 (NS3) RNA that encodes viral helicase and protease, from a pool of random DNAzyme library. The screening procedure identified 18 potential cleavage sites in the target RNA. Corresponding DNAzymes were constructed for the selected target sites and were tested for RNA-cleavage in vitro. The selected DNAzymes, when they are transfected to the human hepatoma cells harboring the HCV subgenomic replicon RNA, efficiently inhibited HCV RNA replication in cells by reducing expression of HCV NS3 RNA and protein.

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발표종류: 포스터, 발표일시: 목 16:30~18:30

Sequence Specific Visual Detection of Methicillin Resistant *Staphylococcus aureus*(MRSA)

윤일규, 안영창, 박수민, 조민호, 서재원, 정덕현, 이은영, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Staphylococcus aureus is the most important pathogen in nosocomial infections, including bloodstream infections especially, prompt identification of *S. aureus* from blood cultures and detection of methicillin resistance are essential in cases of suspected sepsis.We have studied a new method for the sequence-specific visual detection of minute amounts of nucleic acids using intercalating reaction by addition of SYBR Green Ⅰ to amplicons of LAMP, and it's a unique gene amplification method in which DNA can be isothermally amplified using only one enzyme.MRSA-LAMP, which targets the *spa* gene, encoding *S.aureus*-specific protein A, and the *mecA* gene, encoding penicillin-binding protein-2' for methicillin resistance, detected MRSA within 1h.The MRSA-LAMP assay allowed easy, rapid, accurate and sensitive detection of infection with MRSA and especially applicable in a resource-limited situation.

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Mutation Analysis of Two High Susceptibility Genes BRCA1 and XRCC1 by DHPLC

이은영, 박수민, 안영창, 조민호, 서재원, 윤일규, 정덕현, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Breast cancer susceptibility gene 1 (BRCA1), a tumor suppressor gene on chromosome 17q21, was identified in 1994 based on its linkage to hereditary breast and ovarian cancer syndromes. Five to ten percent of all breast and/or ovarian cancers arise from an autosomal dominant pattern of inheritance according to segregation analysis studies. A striking feature of the X-ray repair cross-complementation group 1 (XRCC1) is the presence of BRCA1 carboxyl-terminal (BRCT) domains, denoted BRCT 1, that is located centrally and at the C terminus of this polypeptide, respectively. XRCC1 protein plays an important role in base excision repair. A high level of XRCC1 mRNA and/or protein has been found in rat and baboon brains. An increased breast cancer risk with a recessive effect was also suggested for Arg399Gln and Arg280His variant in Asian population only. Mutational screening of BRCA1 and XRCC1 was performed for 30 breast cancer parients of breast disease by denaturing high performance liquid chromatography (DHPLC). Through this study, we identified that Korean breast cancer has mutations of the BRCA1 in exon11 and XRCC1 gene in Arg280His and Arg399Gln amino acid changes.

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Detection of Drug-Resistance HBV Screening

서재원, 박수민, 안영창, 조민호, 윤일규, 정덕현, 이은영, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Hepatitis B virus(HBV) is a cause of chronic hepatitis and liver cancer. Lamivudine is a major drug approved for treatment of HBV infection. That is a specific inhibitor of the viral polymerase and reverse transcriptase. But, in long-term lamivudine therapy, about 6 month ~ 1 year after, over 14% drug-resistant mutations emergence in treated patients. In clinic system, drug-resistant test or screening are very important for therapy. In this study, we propose a useful tool for drug-resistance HBV screening by denaturing high performance liquid chromatography(DHPLC). DHPLC is used for SNP screening or mutation detection. We compared standard HBV DNA with clinical HBV DNA. The clinical HBV samples were isolated from hepatitis B patient's serum. The samples were collected from Dankook UNI. Hospital (Chungnam, Korea). As a result, we could identify wild type HBV DNA and the other types. The other types include drug-resistant mutations such as rtL180M or rtM204V.

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Screening of GCK Gene Mutations in Korean Type 2 Diabetes Mellitus Patients

정덕현, 박수민, 안영창, 조민호, 서재원, 윤일규, 이은영

단국대 화학과

Glucokinase(*GCK*) is a key regulatory enzyme in the pancreatic beta cell acting as a glucose sensor which regulates insulin secretion. Mutations in the *GCK* gene encoding the glucokinase protein are responsible for the autosomal dominant Maturity Onset Diabetes of the Young type 2(MODY2). After clinical examination, 50 Korean patients were selected for their clinical characteristics suggestive for MODY. Molecular analysis of the *GCK* gene was performed by PCR-DHPLC analysis of exons 4-9. We can find an association of these mutations in Korean suspected MODY2 patients with healthy controls.

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Delivery of Heme oxygenase-1 gene using dexamethasone conjugated low molecular weight Polyethyleneimine for gene therapy against ischemic stroke

현혜선, *최준식, **이민형

*한양대 생명공학과 *충남대 생화학과 **한양대 응용화공생명공학부*

Dexamethasone is one of the anti-inflammatory glucocorticoid steroids. It was suggested that Dexamethasone conjugated complex was translocated into the nucleus by the ligand-receptor-mediated transport. Therefore, dexamethasone conjugated low molecular weight polyethyleneimine2K (PEI-Dexa) which has nontoxic and high transfection efficiency may have dual functions as an anti-inflammatory reagent and a gene carrier. Heme oxygenase-1 (HO-1) is an anti-apoptotic protein which can protect cell from apoptosis under hypoxia. In this study, HO-1 gene will be delivered to focal ischemic brain of stroke animal model using PEI-Dexa as a gene carrier. In divided groups of rats (n=9), MCAO Control, empty plasmid pNull/PEI-Dexa, pNull/PEI, pNull/Dexamethasone, pNull/PEI+Dexa simple mixture, HO-1/PEI and HO-1/PEI-Dexa complexes were injected directly into the cortex 1 hr prior to middle cerebral artery occlusion (MCAO) except control group. MCAO was performed for 60 min in male Sprague Dawley (SD) rats (280-320g). Infarct size was evaluated by 2% 2,3,5-triphenyltetrazolium hydrochloride (TTC) staining at 24hr after MCAO. The level of cytokines was measured by ELISA in the infarcted area. Also, we performed ELISA for the HO-1 protein and results showed that PEI-Dexa group reduced infarct size significantly compared with other groups. This suggests that PEI-Dexa protects the brain cells under ischemia-reperfusion condition. Furthermore infarct size of HO-1/PEI-Dexa was appreciably reduced in the group which suggests that HO-1 has synergistic effect with PEI-Dexa in reducing inflammatory response in ischemic brain. Therefore, HO-1/PEI-Dexa complex is a potential candidate for therapeutic gene delivery to ischemic brain.

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Detection of Single Nucleotide Polymorphism in leukemogenic BCR-ABL chimeric (b3a2) mRNA using the T4 RNA ligase 2

박꽃한아름, 김동은

건국대 생명공학과

Chronic Myelogenous Leukemia (CML) results from chromosomal translocation between chromosomes 9 and 22, which creates BCR-ABL fusion gene. A targeted therapy against the BCR-ABL protein as an anti-leukemic drug, Imatinib that is a competitive inhibitor at ATP binding site of BCR-ABL, is currently available and considered a first-line agent for newly diagnosed CML. However, the Imatinib-resistance is caused by several point mutations in BCR-ABL gene, among which T315I mutation is one of the most common mutations found in patients undergoing Imatinib therapy. The major reason of the resistance is the uncontrollable dosage of anticancer drug to the patients in early stage without accurate diagnosis. Therefore, we have designed the method to detect point mutation in BCR-ABL RNA that causes single nucleotide polymorphism (SNP) using T4 RNA ligase 2. T4 RNA ligase 2 can distinguish the primers perfectly matched to the target RNA from the mismatched one in ligation reaction. In the case of single nucleotide mismatch in the RNA template, RNA ligation did not occur. This method has been successfully applied in the identification and quantification of point mutation (T315I) in BCR-ABL RNA.

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Suppression of HCV genome replication in hepatic cells with exogenous shRNA or shRNA expression system

김경보, 이복희, *김동은

*건국대 생명공학 *건국대 생명공학과*

RNA interference (RNAi) is a highly conserved gene silencing mechanism among mammalia. This cellular process requires small duplex RNA to degrade target mRNA in sequence specific manner. At present, RNAi has been appled for functional genomics studies as well as potential therapeutic agent. Short hairpin RNAs (shRNA) are commonly used for RNAi. The shRNA hairpin structure is cleaved by the cellular machinery into siRNA, which is then bound to the RNA-induced silencing complex (RISC). Previous studies in our laboratory discovered DNAzymes that very efficiently cleave hepatitic C viral genome in hepatic cells. We suggested that target sites of the DNAzymes are accessible to antisense oligonucleotide (AON). In this study, we designed shRNA targeting against this accessible site and proved shRNA mediated suppression of hetatitic C viral replication in hepatic cells. We utilized two kinds of shRNAs to eradicate the target in the cells; lentiviral vector system and exogenous shRNA transcribed with T7 RNA polymerase. Recently, many studies have shown that innate immune response is triggered by these kinds of duplex small RNA. The immune response can cause inhibition of gene expression in a sequence-independent manner. Thus, we now have been examining whether our designed shRNA and shRNA expression vector induce the Toll like receptor (TLR) mediated immune response when we transfect the molecule into hepatic cell. Furthermore, we will compare the target silencing ability of these shRNA systems in hepatitis cells containing HCV replicon RNA.

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Activation of SIRT1 by resveratrol inhibits matrix metalloproteinase-9 in HT1080 cells

이수진, *김문무

*동의대 화학과 *동의대 자연대학/화학과*

The aim of this study is to investigate the inhibitory effect of SIRT1 activator, resveratrol, on expression of matrix metalloproteinases (MMPs) involved in metastasis and chronic inflammation. Resveratrol has been reported to be an antioxidant contained in red wine and help to prevent development of cardiovascular diseases such as arteriosclerosis. In gelatin zymography assay, resveratrol exhibited the inhibitory effect on expression of MMP-9 in HT1080 cells with or without stimulation of phorbol myristate acetate. In addition, it was observed that the level of MMP-9 expression was reduced in the presence of resveratrol above 16 uM. Resveratrol inhibited the activation of ERK, a MAP Kinase downregulated by both NF-kB and AP-1 transcription factors in western blot analysis. However p38 was not influenced by resveratrol treatment. The expression level of histone deacetylase, SIRT1 was not changed by resveratrol. These results suggest that the activation of SIRT1 by resveratrol inhibits expression of MMP-9 in HT1080 cells.

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Biotransformation of Geraniol by the Marine-derived Fungus Hypocrea sp.

Alain Leutou, Guohua Yang, Zhile Feng, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

Biocatalysis is a powerful tool for regioselective and enantioselective synthesis of bioactive compounds. It can also be applied to generate new, active, and less toxic derivatives of bioactive natural products, because it produces significant quantities of metabolites that would be difficult to obtain from either biological systems or chemical synthesis. Biotransformation of geraniol was carried out with Hypocrea sp. using a two-stage fermentation protocol. After fermentations of Hypocrea sp. with geraniol (20 mg) for 72 h, the culture broth was harvested and filtered, and extracted with EtOAc to yield crude extracts. The extract was purified by repeated Si gel flash chromatography (n-hexane in ethyl acetate) to yield one oxidized metabolite, 1,7-dihydroxy-3,7-dimethyl-(E)-oct-2-ene. The structure of the metabolite obtained was assigned on the basis of detailed spectroscopic data analyses.

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POLYOXYGENATED MACROCYCLIC METABOLITES FROM THE MARINE-DERIVED FUNGUS PENICILLIUM SPECIES

Zhile Feng, Guohua Yang, Alain Leutou, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

In our studies on the chemistry and biology of fungi, we have investigated secondary metabolite from a marine strain of the fungus Penicillium sp. This strain was isolated from the surface of the drifting cotton clothing collected in Namhae Island, Gyeongnam, Korea and identified based on the morphological evaluation and fatty acid methyl ester analysis (Korean Culture Center of Microorganism, Seoul, Korea, a similarity index of 0.919). Here, we report on the isolation and structural determination of 14–membered resorcyclic acid lactone analogues, hydroxyzearalanone and zearalenone, from a marine isolate of the fungus Penicillium sp.

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NEW DECALIN DERIVATIVES FROM THE MARINE-DERIVED FUNGUS ASPERGILLUS SPECIES

Guohua Yang, Alain Leutou, Zhile Feng, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

Our screening assays were designed to identify antimicrobial compounds that are active against Staphylococcus aureus, methicillin-resistant S. aureus, and multidrug-resistant S. aureus. We investigated antimicrobial activity from the fungal extracts, and a crude mycelium extract of Aspegillus sp. was found to be active in the S. aureus, MRSA, and MDRSA screen. Assay-guided isolation of antimicrobial compounds from the mycelium extract to yield dehydroxychlorofusarielin B, a new antibacterial polyoxygenated decalin derivative, and the previously described fusarielins A and B. The structure and absolute stereochemistry of the new compound was determined on the basis of the physicochemical data and X-ray diffraction. Compounds exhibited a mild antibacterial activity against Staphylococcus aureus, methicillin-resistant S. aureus, and multidrug-resistant S. aureus. The MIC values for each strain were as follows: dehydroxychlorofusarielin B and fusarielin B, 62.5 g/mL for all strains, and fusarielins A, 32.5 g/mL for S. aureus and methicillin-resistant S. aureus, and 62.5 g/mL for multidrug-resistant S. aureus.

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The Yeast *TGL2* Gene Encodes an Active Triacylglycerol Lipase Located in the Mitochondria

함혜진, 신승구, 윤혜주

포항공과대 화학과

The *Saccharomyces cerevisiae* Tgl2p shows sequence homology to *Pseudomonas* triacylglycerol (TAG) lipases, but the role of Tgl2p in yeast remains uncertain. Here we demonstrate that the hemagglutinin (HA)-tagged Tgl2p purified close to homogeneity from a yeast strain overexpressing this fusion protein exhibits high TAG lipase activity towards long-chain TAG. Importantly, mutant $Tgl2p^{S144A}$ which contains alanine 144 in place of serine 144 in the lipase consensus sequence G/A-X-S-X-G carries no lipolytic activity. While cellular TAG hydrolysis is reduced in the tgl2 deletion mutant, overproduction of Tgl2p in this mutant increases TAG degradation in the presence of fatty acid synthesis inhibitor cerulenin. On the contrary, no alteration of the TAG degradation rate was resulted from elevated production of $Tgl2p^{S144A}$. These results demonstrate the lipolytic function of Tgl2p in yeast. Although other yeast lipases are embedded in lipid particle, Tgl2p is detected in the mitochondria. The purified mitochondrial fraction shows a strong Tgl2p-dependent TAG lipase activity. We also find that deletion of the *TGL2* gene in yeast confers sensitivity to anti-mitotic drug, but this sensitivity is suppressed by addition of oleic acid, the product of lipolysis. Our data suggest that the yeast Tgl2p is a mitochondrial TAG lipase involved in the survival of cells under anti-mitotic drug treatment.

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Synthesis of New Tetracyclic 4-Amino-2,3,5,6,7,8-hexahydro-1H-10-thia-9-aza-pentaleno[1,2-b]naphthalen-5-ol and 2,3,5,6,7,8-Hexahydro-1H-10-thia-9-aza-pentaleno[1,2-b]naphthalen-4-ylamine Derivatives As Potential AChE Inhibitors

송양헌, *이한미

*목원대 화학과 *목원대 생의약 화학과*

We report the synthesis of new 2,3,5,6,7,8-hexahydro-1H-10-thia-9-aza-pentaleno[1,2-b]naphthalen-4-ylamine derivatives (6a, 6b) and 4-amino-2,3,5,6,7,8-hexahydro-1H-10-thia-9-aza-pentaleno[1,2-b]naphthalen-5-ol derivatives (7a-g) in two ways as potential AChE inhibitors.

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Synthesis of New 6,7,8,9-Tetrahydro-5H-1-thia -5,10-diaza-cyclopenta[f]inden-4-ylamine Derivatives As Potential AChE Inhibitors

송양헌, *이한미, **김미선

*목원대 화학과 *목원대 생의약 화학과 **목원대 생의약화학과*

The synthesis of 6,7,8,9-tetrahydro-5H-1-thia-5,10-diazacyclohepta[f]inden-4-ylamine derivatives in good yield by four-step procedures starting from 2-aminothiophene-3-carbonitrile and 5-substituted cyclohexane-1,3-dione is described as potential AChE inhibitors.

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Synthesis of New Sulfur-Linked 1,2,4-Triazolothienopyrimidine and 1,2,4-Triazolopyrazolopyrimidine Derivatives

송양헌, 손훈영

목원대 화학과

We now report the synthesis of new bis-heterocyclic compounds by integrating fused heterocyclic pyrimidines such as thienopyrimidines and pyrazolopyrimidines into the scaffold of thienotriazolopyrimidines and pyrazolotriazolopyrimidines through a sulfur-linkage in the hope of obtaining compounds of diverse pharmaceutical activities.

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Synthesis of 8-Phenyl-5H-thieno[3,2-e][1,2,4]triazolo[4,3-a]pyrimidin-4-one Derivatives As Potential Antimicrobial Agents

송양헌, 손훈영, *김성민

*목원대 화학과 *목원대 생의약 화장품학부*

General and facile synthesis of 8-phenyl-5H-thieno[3,2-e][1,2,4]triazolo[4,3-a]pyrimidin-4-one derivatives, which were prepared by oxidative cyclization of 2-(N'-benzylidene-hydrazino)-3H-thieno[2,3-d]pyrimidin-4-one using PhI(OAc)2 is described as novel ring system and as potential antimicrobial Agents.

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A direct approach to 5-hydroxybenzofurans via a platinum-catalyzed domino rearrangement/5-endo-dig cyclization reaction of quinols

김경선, *김익연

*고려대 화학과 *한국화학연구원 의약화학연구센터*

A highly efficient and atom-economical construction of 2-substituted 5-hydroxybenzofurans was accomplished by employing a platinum-catalyzed domino dienone-phenol rearrangement/5-endo-dig cyclization reaction of quinols bearing alkynes

THE KOREAN CHEMICAL SOCIETY

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Facile construction of highly substituted indolizinones via palladium-catalyzed coupling reactions

김경선, *김익연

*고려대 화학과 *한국화학연구원 의약화학연구센터*

Rapid construction of highly functionalized indolizonones was realized by employing palladium-catalyzed coupling reactions of 2-iodoindolizinones which in turn were readily accessed via sequential iodine-mediated cyclization/1,2-shift reactions of propargylic alcohols.

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Synthesis of exoalkylidenetetrahydrofurans via Prins-type cyclization

Ullapu Punna Reddy, *민선준, **이재균, *배애님, ***김유승, *장문호, *조용서

*과학기술연합대학원대 *KIST 생체과학연구본부*
***KIST 응용과학연구부 ***KIST 생화학물질연구센터*

We have developed a novel synthetic procedure to synthesize alkylidenetetrahydrofuran derivativeswhich possess a heterocyclic structure frequently found in biologically active compounds. This novel methodology led to the formation of exomethylene-2-(phenylethynyl)-tetrahydrofuran and exomethylene-2-styryl-tetrahydrofuran derivatives from hydroxyl(allenyl/allyl methyl)silanes with electron rich unsaturated aldehydes under a Lewis acid.

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An efficient synthesis of 2,7-disubstituted oxepane derivatives via Prins-type cyclization

Ullapu Punna Reddy, *민선준, **이재균, *배애님, ***김유승, *장문호, *조용서

*과학기술연합대학원대 *KIST 생체과학연구본부*
***KIST 응용과학연구부 ***KIST 생화학물질연구센터*

We have performed a new synthetic procedure to synthesize exomethylene-2,7-substituted oxepane derivatives by using Prins-type cyclization protocol. This novel methodology led to the formation of alkylidene-2,7-substituted oxepane derivatives such as 3,4-dimethylene-2,7-aryl/alkyloxepanes and 4-methylene-2,7-aryl/alkyloxepanes from hydroxyl(allenyl/allyl methyl)silanes with aromatic or aliphatic aldehydes under a Lewis acid

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Synthesis of Benzopyrane Derivatives as Potassium Channel Activators

Meng Lijuan, 이은영, 김신형, 신동수

창원대 화학과

Potassium channels are exceptionally diverse both in variety and function. They play an important and complex role in the basic electrical and mechanical function of a wide variety of tissues, including smooth muscle, cardiac muscle and glands. With the aim of discovering new molecules with potassium channels activating properties, we have synthesized derivatives of cromakalim (CRK), an important molecule which shows specific affinity towards potassium channels, by replacing the pyrrolidinone-cycle of the reference compound with different hetero-cycles. The biological activities of these compounds will be discussed.

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Efficient Synthesis of (R)-Ethyl 4-cyano-3-hydroxybutanoate

Meng Lijuan, 공춘호, 송정한, 이상길, *문기철, 신동수

*창원대 화학과 *창원대 대학원 화학과*

(R)-Ethyl 4-cyano-3-hydroxybutanoate is an important synthetic intermediate for a variety of chiral compounds. It serves as key intermediate for the preparation of neuromediator (R)-GABOB, L-carnitine, and HMG-CoA reductase inhibitor, atorvastatin(Lipitor). The present disclosure relates to the improvement of the synthetic technology of (R)-ethyl-4-cyano-3-hydroxybutanoate from (R)-ethyl-4-iodo-3-hydroxybutanoate, which can be prepared from commercially available (S) -epichlorohydrin. Raw materials, reaction condition, safety and other factors were considered to make it available to be prepared in a large scale in industry.

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Au(I)-Catalyzed Oxidative Cyclization of β-Keto Esters Across Alkenes: An Elegant Method for the Synthesis of Isobenzofuran Derivatives

윤소원, *Arun R. Jagdale

*부경대 화학과 *이화여대 나노바이오기술연구소*

β-Keto esters are one of the most widely used building blocks in organic chemistry and undergo various types of substitution reactions. Particularly, β-keto esters undergo C-C bond formation reactions in the reaction with carbon elecrophiles. However, C-O bond formation reactions are rare in the literature. More interestingly, transition-metal-catalyzed addition reactions of β-keto esters to olefins have been well reported which usually led to the simple C-C bond formation products.Recently, we have developed a new and elegant method for the synthesis of isobenzofuran derivatives in high yields. Ph_3PAuCl/AgOTf-catalyzes effectively the oxidative cyclization reaction of the olefinic β-keto esters to provide the corresponding isobenzofurans in moderate yields. Control experiments employing only either Ph_3PAuCl or AgOTf as a sole catalyst gave no or lower conversions, respectively.

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Cooperative Catalysis of $In(OTf)_3$ and $Zn(OTf)_2$ for Cascade Reactions: An Novel Method for the Synthesis of Tetracyclic Dihydrocoumarin Derivatives

윤소원, *Arun R. Jagdale

*부경대 화학과 *이화여대 나노바이오기술연구소*

Coumarins exist extensively in a number of natural products and show a wide range of biological activities. Transtion-metal-catalyzed hydroarylation of cinnamic acids or esters with phenols has been emerged as a useful tool for the preparation of dihydrocoumarin derivatives. Moreover, significant scope of cascade C-C bond formation reactions attracted us due to its simple reaction conditions and very high atom economy. Recently, we discovered new cooperative catalytic system comprising $In(OTf)_3$ and $Zn(OTf)_2$ for the sequential coupling/cyclization of diethyl 2-(2-alkynylbenzylidene)malonate with phenols to give the tetracyclic dihydrocoumarin derivatives in excellent yields in a single operation. Mechanistically, reaction proceeded with sequential hydroarylation, lactonization, and cyclization pathway with high chemo- and regioselectivity.

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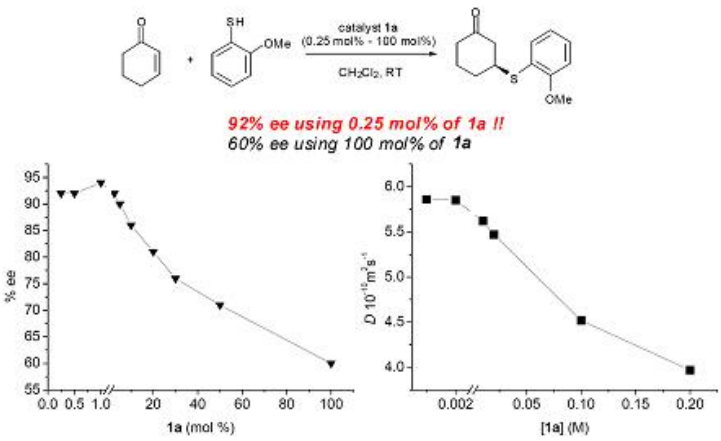
DOSY NMR for Monitoring Self Aggregation of Bifunctional Organocatalysts: Increasing Enantioselectivity with Decreasing Catalyst Concentration

장형빈, *노호식, 송충의

*성균관대 화학과 *아모레퍼시픽 기술연구원 한방과학연구팀*

Thiourea-based bifunctional organocatalysts are of broad interest as they have been shown to catalyze a wide range of organic reactions. However, they suffer from self-aggregation, resulting in a strong dependence of enantioselectivity upon concentration and temperature. We demonstrated for the first time that a DOSY NMR technique is an easy and powerful tool for determining the range of concentrations whereby the bifunctional organocatalysts exist mainly in the monomeric form to give maximum enantioselectivity. Thus, when maintaining substrate concentration, the enantioselectivity of the bifunctional catalysts dramatically increases upon decreasing catalyst loading, strongly indicating that enantioselectivity was only dependent on the concentration of the bifunctional catalysts.



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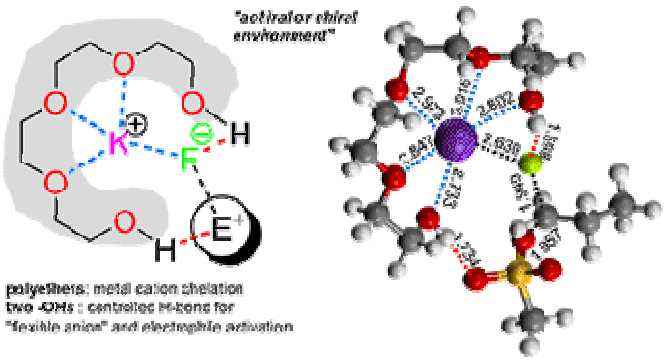
Bis-Terminal Hydroxyl Polyethers as All-Purpose, Multifunctional Organic Promoters

장형빈, yanhailong, *박성우, **이성렬, ***지대윤, 송충의

*성균관대 화학과 *경희대 환경응용화학부 **경희대 화학과 ***서강대 화학과*

In this work, we demonstrate that multifunctional bis-terminal hydroxyl polyethers can phenomenally accelerate a range of chemical reactions via cooperative catalysis, in which readily available alkali metal salts are used as nucleophilic sources. For example, achiral bis-terminal hydroxyl polyether derivatives dramatically facilitate the most difficult process of nucleophilic fluorination with alkali metal fluorides. We believe that this protocol will open up new perspectives in synthetic and medicinal chemistry, e.g. 18F labeling and diagnosing human diseases with positron emission tomography (PET). We also describe the first successful desilylative kinetic resolution of the silyl ethers of racemic secondary alcohols with KF by using the chiral variants of bis-terminal hydroxyl polyether derivatives as catalyst. This certainly creates a new avenue for chiral fluoride catalyzed asymmetric reactions, which have vast synthetic potential in this still undeveloped field. Quantum chemical computations provide a detailed and interesting insight into the origin of the phenomenal catalysis of bis-terminal hydroxyl polyethers, where the terminal -OH groups act as anchors to the nucleophile and the leaving group.



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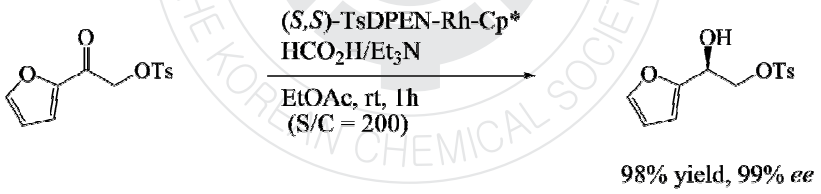
α-Sulfonyloxy heteroaryl ketones: Substrates for Rh-Catalyzed Transfer Hydrogenation

곽세훈, *이기인, *이도민

*과학기술연합대학원대 의약및 약품화학 *한국화학연구원 신약연구단*

Asymmetric transfer hydrogenation of α-sulfonyloxy heteroaryl ketones has been studied. The chiral Rh-catalyst effectively performed in transfer hydrogenation of heteroaryl ketones with an azeotropic mixture of formic acid/triethylamine to produce optically active 1-arylethandiol monosulfonates with excellent enantioselectivity.



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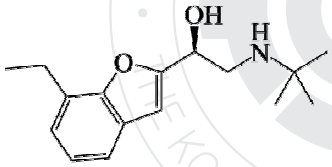
Enantioselective synthesis of (S)-Bufuralol and (S)-Duloxetine

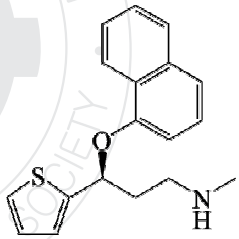
곽세훈, *이기인

*과학기술연합대학원대 의약및 약품화학 *한국화학연구원 신약연구단*

Catalytic transfer hydrogenation of α-sulfonyloxyketone derivatives of benzofuran and thiophene leads to efficient synthesis of (S)-bufuralol and (S)-duloxetine, respectively.



(*S*)-Bufuralol



(*S*)-Duloxetine

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Pd-Catalyzed Oxidative Cyclization Reactions via C-H Activation/C-N Bond Formation for the Synthesis of Carbazoles Under Mild Conditions

윤소원, 빈준형

부경대 화학과

Carbazoles are well-known drug candidates in medicinal chemistry due to of their various biological activities and have attracted much synthetic interest for the multiple applications in material science as well as medicinal chemistry. Recently, a variety of transition-metal-catalyzed syntheses of carbazoles have been reported by many research groups, however, there are still some limitations in their scopes. Therefore, there is great demand to develop more general and mild protocol for the expeditious synthesis of carbazole derivatives. In this report we demonstrate a mild and efficient Pd-catalyzed oxidative coupling reactions of *N*-Ts-2-arylanilines via C-H bond activation and intramolecular C-N bond formation to afford carbazole derivatives. Use of cheap oxidant and mild reaction conditions are the key features of our work.

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Pd-Catalyzed Oxidative Coupling Reactions of *N*-Ts-2-arylanilines with Electron Deficient Olefins via Tandem Directed C-H Activation/C-C Bond Formation/Cyclization

윤소원, 이선영, 빈준형

부경대 화학과

Recently, we developed a mild and efficient Pd-catalyzed oxidative coupling reaction between *N*-Ts-2-arylanilines and electron deficient olefins. Synthesis of 5,6-dihydrophenanthridine-6-acetic acid derivatives has been achieved via directed C-H bond activation, C-C bond formation, and intramolecular nucleophilic cyclization reaction. This reaction was catalyzed by electrophilic Pd complexes under mild conditions such as at room temperature with the use of a cheap oxidant.

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Facile and Convenient One-Pot Synthesis of Dihydroquinolinones via Rh-Catalyzed Tandem Conjugate Addition-Cyclization Reaction

윤소원, 박자옥

부경대 화학과

Quinolinones are pervasive motifs found in biologically active natural products and pharmaceutical agents. Furthermore, 2-quinolinone derivatives have been paid considerable attention due to their use as antiinflammatories, antihypertensives, and analgesics and in the preparation of antipsychotic agents. Recently, we have found that the Rh-catalyzed tandem conjugate addition-cyclization reaction of methyl 3-(2-benzylaminophenyl)acrylate with arylboroxines provides the convenient access to 4-aryl-3,4-dihydro-2(*1H*)-quinolinones. One-pot synthesis of 4-aryl-3,4-dihydrocoumarins was also achieved successfully by using ethyl 3-(2-hydroxyphenyl)acrylate via tandem conjugate addition-cyclization reaction.

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Ru(III)-Catalyzed Sequential C-C and C-O Bond Formations

윤소원, 김병석, 박자옥

부경대 화학과

Both C-C and C-O bond formation reactions have attracted considerable attention from organic chemists. In recent years, transition-metal catalysis plays an important role to achieve these transformations with good chemical yields and selectivity.In this report, we disclose a new Ru(III)-catalyzed sequential C-C and C-O bond formation reaction of alkynyl α,β-unsaturated esters such as ethyl 3-(2-alkynylphenyl)acrylate, to give fused tricyclic compounds. This reaction allows the easy and efficient construction of indene derivatives having a quaternary carbon center.

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Facile and Efficient Synthesis of Quinoline Derivatives via Pd-Catalyzed One-Pot Cascade Reactions

윤소원, 옥수경

부경대 화학과

Synthesis of quinolines has been attracted the considerable attention because they possess a wide range of biological activities such as antimalarial, antibacterial, antifungal, and anticancer properties. Consequently, many classical methods have been developed for the synthesis of quinoline derivatives. However, many of these methods require harsh reaction conditions such as high temperature, prolonged reaction time, and multistep reactions.Herein we report Pd-catalyzed efficient one-pot cascade reaction of 2-alkynylanilines with arylaldehydes for the synthesis of quinolines with the aid of *p*-TsOH as an additive.

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Pd-Catalyzed Unexpected Coupling Reactions Between Sterically Hindered *N*-Ac-2-arylanilines and Electron Deficient Olefins

윤소원, 장충식, 옥수경

부경대 화학과

It has been well known that directed C-H bond activation does not take place at all or only occurs at high temperature in the case of ortho-substituted acetanilides. Recently, we discovered that Pd-catalyzed oxidative coupling reactions between *N*-Ac-2-arylanilines and electron deficient olefins proceeded smoothly under mild conditions via directed C-H activation and C-C bond formation, resulting in the unexpected 6-alkenylation products. This reaction was catalyzed by electrophilic Pd complexes under mild conditions such as at room temperature with the use of a cheap oxidant.

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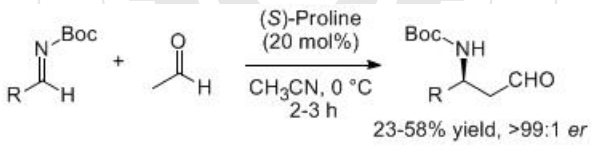
Proline-Catalyzed Mannich Reactions of Acetaldehyde

양정운, *Carley Chandler, *Michael Stadler, *Daniela Kampen, *Benjamin List

*성균관대 에너지과학과 *Max-Planck-Institut für Kohlenforschung*

The proline-catalyzed Mannich reaction between acetaldehyde and *N*-Boc-imines (Boc=*tert*-butoxycarbonyl) gives β^3-amino aldehydes in reasonable yields with extremely high enantioselectivities. The products are useful intermediates in the synthesis of β^3-amino acids and drugs as well as natural products.



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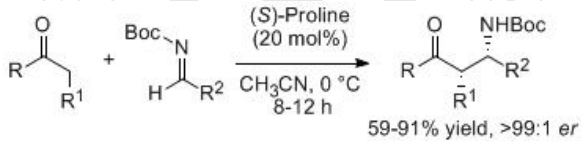
Highly Efficient Organocatalytic Asymmetric Mannich Reaction of Aldehydes with *N*-Boc-Imines

양정운, *Michael Stadler, *Benjamin List

*성균관대 에너지과학과 *Max-Planck-Institut für Kohlenforschung*

The proline-catalyzed Mannich reaction between aldehydes and *N*-Boc-imines (Boc=*tert*-butoxycarbonyl) gives crystalline β-amino-aldehydes in exceptionally high diastereoselectivities and enantioselectivities. The products of this reaction typically precipitate from the reaction mixture and are useful intermediates in the synthesis of α- and β-substituted β-amino acids.



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장소: 대전컨벤션센터
발표코드: **Ⅰ37P257포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Effective Separation of Adamantanediol from a Group of Adamantanols

이영민, 최영화, 박주연, 지기환

울산대 화학과

It is known that adamantane shows distinctive functions because of its three-dimensionally symmetric structure, where each ring is mutually stabilized. Hydroxyl group-containing adamantanes, particularly adamantanols having hydroxyl groups at plural bridgehead positions, are utilized in a broad range of applications. Attempts for the synthesis of 1,3-adamantanediol from adamantane using various catalysts were tried. By oxidizing a substrate such as adamantane, according to this process, adamantanol, adamantanediol, adamantanone and other adamantanepolyols of adamantane can be manufactured at a high conversion and selectivity even under mild condition. However, it is extremely difficult to separate, in an efficient manner, these adamantanol, adamantanediol, and adamantanepolyols among themselves, as each of them has closely similar chemical properties to those of the other. Therefore, an our object of the present work to provide, a process for efficiently separating an adamantanediol from reaction mixture which is obtained by an oxidation reaction conducted in the presence of an imide compound for the production of a group of adamantanols.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Tetrabutylammonium Bromide : Efficient Brominating Reagent of Aryl Amines via Arenediazonium Tosylates

이영민, 황호윤, 차은혜, 지기환

울산대 화학과

A novel and efficient approach to the synthesis of stable arenediazonium salt and subsequent bromination has been developed. Addition of tert-butyl nitrite into a solution of aromatic amines, p-TsOH, tetrabutylammonium bromide (TBAB) and CuBr in an appropriate solvent at room temperature provides a facile and effective method for the preparation of various bromoarenes.The reaction conditions are eco-friendly and match well with the concept of green chemistry because only a catalytic amount (or none) of Cu salts is required. And, the present methodology needs short reaction times and provides good yields. This new, simple and facile method can be successfully applicable for the synthesis of wide range of bromoarenes starting from corresponding aromatic amines. We also tried to use NaBr as a brominating agent instead of TBAB, in order to compare the outcomes under these two conditions. Reaction conditions and results in detail will be discussed in the poster.

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Preperation of β-Aryl-α-thienoylethenes and Their NMR Studies.

전현주, 이창규

강원대 화학과

β-Aryl-α-thienoylethenes were prepared by aldol condensations of 2- and 3-acetylthiophene with m- and p-substituted benzaldehydes in the presence of NaOH in ethanol-water solution. The condensation products were isolated in moderate to good yields depending on the substituents. The NMR spectra of the products were examined in order to evaluate the effect on the 1H and 13C NMR chemical shift by the substituents on the phenyl ring by correlating the chemical shift values with the Hammett σ.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Substituent Effects on Hydride Transfer Reactions of Acridinium Ion with Benzimidazolines

한인숙, *전현주

*강원대 과학교육학부 *강원대 화학과*

The kinetics of hydride transfer reactions of 10-methylacridinium ion (Ac+) with a series of 1,3-dimethyl-5-X-2-(substituted phenyl Y)benzimidazoline (X-BIH: X = CH3, H, F, Cl ; Y = p-CH3, H, p-F, p-Cl, m-F, m-Cl, m,m'-Cl2) have been measured spectrophotometrically in 2-propanol-H2O (4 : 1, v/v) at 25 0.1 oC in order to explore the substituent effect at the 5-position of benzimidazole ring. The reactivity is increased in the order of, Cl < F < H < CH3 as we expected. The rate constants for the reactions of Ac+ with X-BIH are linearly correlated with the Hammett parameters with the slopes of -1.60 -1.67. The reactivity-selectivity principle can be applied to the present system with the reaction constants. This result will be discussed in terms of mechanism and compared with those of other hydride transfer reactions with NADH analogues.

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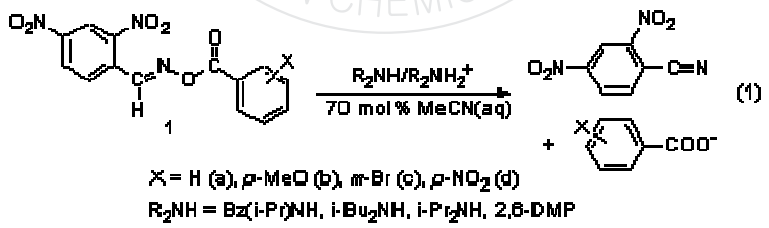
발표종류: 포스터, 발표일시: 목 12:30~14:30

Elimination Reactions of (E)-2,4-Dinitrobenzaldehyde O-Benzoyloximes Promoted by R2NH/R2NH2+ in Aqueous MeCN(aq). Change of the Reaction Mechanism

변상용

부경대 화학과

Ketene-forming eliminations from (E)-2,4-(NO2)2C6H3 CH=N -OC(O)C6H4X (1) promoted by R2NH/R2NH2+ in 70 mol% MeCN(aq) have been studied kinetically. The reactions are second-order and exhibit Brönsted β = 0.27-0.32 and |βlg| = 0.28-0.32. The result can be described by a negligible pxy interaction coefficient, pxy = ∂β/∂pKlg = ∂βlg/∂pKBH 0, which describes the interaction between the base catalyst and the leaving group. The negligible pxy coefficients are consistent with the (E1cb)irr mechanism.



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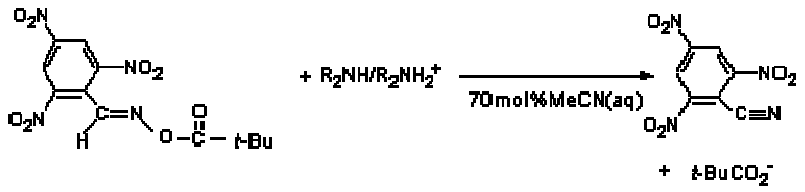
발표종류: 포스터, 발표일시: 목 12:30~14:30

Elimination Reactions of (E)-2,4,6-Trinitrobenzaldehyde O-Pivaloyloxime Promoted by R2NH by R2NH/R2NH2+ in Aqueous MeCN(aq). Effect of β –Aryl Group the Nitrile-Forming Transition-State

변상용

부경대 화학과

Nitrile-forming eliminations from (E)-2,4,6-(NO2)3C6H2CH=NOC(O)(CH3)3 (1) Promoted by R2NH/R2NH2+ in 70mol%MeCN(aq) have been studied kinetically. The reactions are second-order and exhibit Brönsted β = 0.41. The k2 value for elimination from (E)-2,4,6-trinitrobenzaldehyde O-pivaloyloxime promoted by i-Pr2NH/i-Pr2NH2+ in 70 mol % MeCN(aq) falls on a single line in the Hammett plot with the literature data for the β –aryl substituents, which have been shown to react by the mechanism. This result indicates that the reaction mechanism is not changed by the introduction of the 2,4,6-trinitro sunstituents and that the elimination reactions from (E)-benzaldehyde O-pivaloyloximes series proceed by the common E2 mechanism.



1

R_2NH = Bz(*i*-Pr)NH, *i*-Bu_2NH, *i*-Pr_2NH, 2,6-DMP

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The ring-opening of stable aziridinium ions with carbon nucleophiles

김용은, 하현준, *이원구

*한국외국어대 화학과 *서강대 화학과*

Aziridine is a versatile synthetic building block for the synthesis of diverse cyclic and acyclic molecules containing nitrogen via ring opening reactions. The stable methyl aziridinium ions generated form 1-phenylethylaziridines with methyl trifluoromethanesulfonate were reacted with various external carbon nucleophiles to yield synthetically valuable and optically pure acyclic derivatives in a completely regio- and stereoselective manner.

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The ring-opening of stable aziridinium ions with halides

김용은, 하현준, *이원구

*한국외국어대 화학과 *서강대 화학과*

The reaction of enantiomerically pure 2-substituted 1-phenylethyl-aziridines with methyl trifluoromethanesulfonate generated a stable methyl aziridinium ion, whose ring was opened by the external halides ions including fluoride, chloride bromide and iodide to yield synthetically valuable and optically pure halogenated acyclic derivatives. The regio- and stereochemical pathways were dependent to the characteristics of halides.

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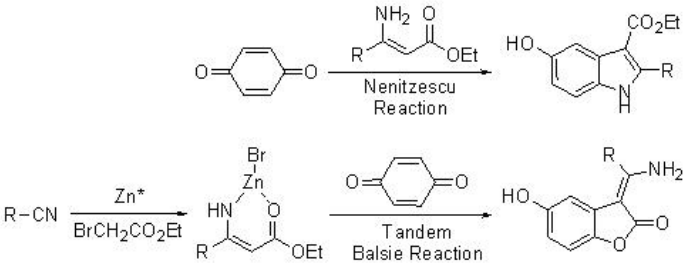
발표종류: 포스터, 발표일시: 목 12:30~14:30

Nenitzescu-type reaction of the Blaise reaction intermediate: A novel method for the synthesis of 3-aminomethylene benzofuran-2-ones

류가연, 전유성, 고영옥, 이상기

이화여대 화학/나노과학과

In contrast to the classical Nenitzescu reaction, reactions of *β*-enaminoester with *p*-benzoquinone affording 5-hydroxyindoles, tandem reaction of the Blaise reaction intermediate, a zinc bromide complex of *β*-enaminoester, with *p*-benzoquinone afforded 3-aminomethylene benzofuran-2-ones in high yields.



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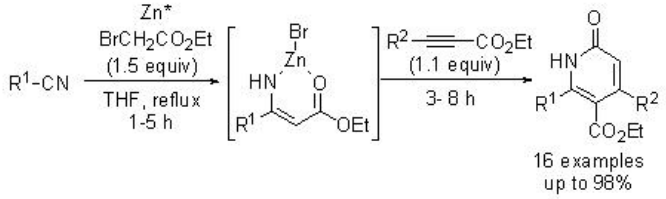
발표종류: 포스터, 발표일시: 목 12:30~14:30

Highly Efficient One-Pot Synthesis of 2-Pyridones *via* Chemo- and Regioselective Tandem Blaise Reaction of Nitriles with Propiolates

류가연, 전유성, 고영옥, 이상기

이화여대 화학/나노과학과

The *in situ* generated Blaise reaction intermediate, a zinc bromide complex of β-enaminoester, possessed ambivalent nucleophilic nature- both α-carbon and β-nitrogen can act as nucleophile, and reacted with propiolates in chemo- and regioselective manner to afford 2-pyridone derivatives in good to excellent yields.



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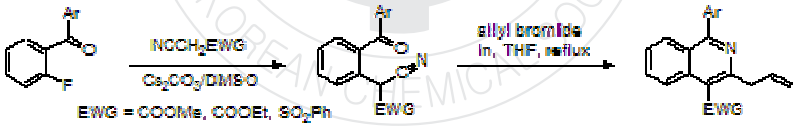
발표종류: 포스터, 발표일시: 목 12:30~14:30

Expedient synthesis of poly-substituted 1-arylisoquinolines from δ-ketonitriles *via* indium-mediated Barbier reaction protocol: Chemoselective allylation of nitrile in the presence of ketone

김성환, 김고훈, 김재녕

전남대 화학과

We developed an efficient synthetic strategy of poly-substituted 1-arylisoquinolines *via* an indium-mediated Barbier type allylation from δ-ketonitriles. Initial attack of allylindium species occurred at the nitrile group selectively to form the enamine intermediate, which reacted with the ketone group intramolecularly to furnish the 1-arylisoquinolines.



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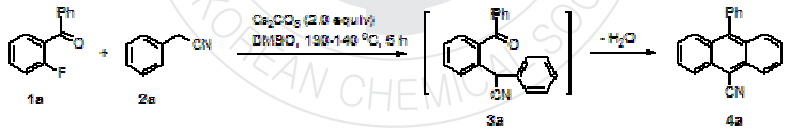
발표종류: 포스터, 발표일시: 목 12:30~14:30

An expedient synthesis of 10-arylanthracenes from 2-fluorobenzophenone and aryl acetonitriles *via* the sequential S_NAr and unusual anionic cyclization process

김성환, 김유미, 김재녕

전남대 화학과

We found an expedient synthetic methodology of 10-arylanthracene derivatives in a one-pot reaction of 2-fluorobenzophenone and aryl acetonitriles under the influence of Cs_2CO_3 in DMSO. The anthracene was formed *via* the anionic cyclization of the intermediate 3a at the *ortho*-position of the arene moiety to the benzoyl group.



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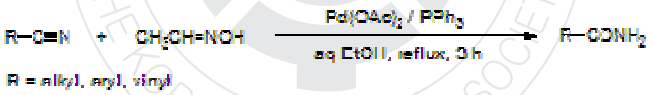
An efficient Pd-catalyzed hydration of nitrile with acetaldoxime: Use of acetaldoxime as a water surrogate

김은선, 이현승, 김재녕

전남대 화학과

An efficient palladium-catalyzed protocol for the hydration of nitriles to amides with acetaldoxime has been developed. A plausible mechanism was suggested involving the first Pd(II)-catalyzed nitrile-oxime coupling and the following disruption of the intermediate into amide and acetonitrile in a concerted manner.



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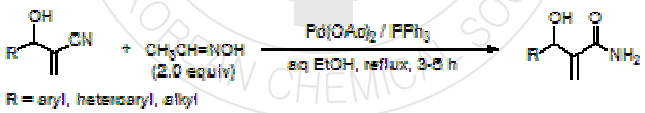
An expedient synthesis of Baylis-Hillman adducts of acrylamide: Pd-catalyzed hydration of Baylis-Hillman adducts of acrylonitrile

김은선, 이현승, 김재녕

전남대 화학과

An efficient palladium-catalyzed two-step protocol for the synthesis of Baylis-Hillman adducts of acrylamide was developed. The method involved the preparation of Baylis-Hillman adducts of acrylonitrile and a Pd-catalyzed hydration of the nitriles with acetaldoxime. Direct synthesis of Baylis-Hillman adducts of acrylamide was known to be very difficult due to sluggish reactivity of acrylamide whereas our two-step procedure afforded high yields of products.



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Electrochemical evaluation of acetylcholinesterase activity and construction of biosensor suitable for anticholinergic compounds assay

Pohanka, *Drobik, **Krenkova, Zdarova-Karasova,
***Holas, Kasalova, *Korabecny, Marek, Kuca, Musilek**

*University of Defense in Hradec Kralove *Charles University in Prague **University of Pardubice*

Biosensors are analytical devices based on two tightly connected parts. Biosensor based on acetylcholinesterase (AChE; EC 3.1.1.7) intercepted on platinum working electrode is described. The AChE based biosensors are suitable for assay of anticholinergic compunds such as nerve agents, organophosphate pesticides, some drugs targeting to AChE and several natural toxins e.g. aflatoxins. Presence of analyte appears as strong inhibition of intercepted AChE. Electrochemical biosensors were found suitable not only for evaluation of AChE activity but also for estimation of basic properties of selected anticholinergic compounds. Due to firm interception of AChE, biosensors would be used for fast estimation whether the inhibition is reversible or irreversible that brings an advantage with the currently available photometrical methods. The Ministry of Education, Youth and Sports, Czech Republic are gratefully acknowledged for project no. ME09086.

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Impact of biological warfare agent Francisella tularensis on oxidative stress and total level of low molecular weight antioxidants in infected host

Pohanka, [*]Bandouchova, Pavlis, Vlckova, Sobotka,
[**]Treml, Musilek, Kuca, Zdarova-Krasova, Marek, [**]Pikula

University of Defence [*]University of Pardubice [**]University of Veterinary and Pharmaceutical Sciences

Bacterial G- microorganism Francisella tularensis is considered as a biological warfare agent of class A according CDC. Microorganism F. tularensis is a causative agent of serious disease tularemia. Though pathology of F. tularensis seems to be partially understood, some aspects of infectious process are not still clear. Especially, factors influencing proliferation of F. tularensis and immune system failure. The study is aimed on assessment of oxidative stress throughout infection in typical hosts: european brown hare, mice and common voles. Fully virulent strain F. tularensis subsp. holarctica was used throughout experiments.The overall impact of tularemia on hares was evaluated by biochemical examination. Though markers for tissue burden were negative, increased level of lactate dehydrogenase appointed at expected proliferation of F. tularensis cells in livers. The present effort is aimed at modulation of cholinergic anti-inflammatory pathway and assessment of its impact on host survivability. The Ministry of Education, Youth and Sports, Czech Republic are gratefully acknowledged for project no. ME09086.

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Synthesis and Characterization of New Iridium Complex with Trimethylsilyl Group for OLEDs

소기호, 안진영, 장상훈, *권순기, 김윤희, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Intense research activities are currently being undertaken on organic light-emitting diodes (OLEDs) because of the potential applications in flat panel displays.OLEDs are solid-state devices composed of thin films of organic molecules that create light with the application of electricity. OLEDs can provide brighter, crisper displays on electronic devices and use less power than liquid crystal displays (LCDs) used today.In this poster, we will present the synthesis of iridium complex with trimethylsilyl group, Trimethylsilyl group can improve the solubility, thermal stability and efficiency due to steric bulkyness via higher volume. Accordingly, the combination of ppy and bulky trimethylsilyl group would be expected to be the best way to achieve an efficient phosphorescent emitter.

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Synthesis, Characterization, and Properties of Well Defined EDOT Containing Hetero Aromatic Oligomers

배영주, 김인태, 이상우, 한우택, 황선우

광운대 화학과

Thiophene based linear π-conjugated oligomers have their potential applications for active materials in organic electronic and photonic devices. 3,4-ethylenedioxythiophene(EDOT) has been used as a building block on several conjugated systems which incorporate unique properties such as electrochromic behavior and low band gap polymers. Herein, we synthesis novel compounds of EDOT-Aryl based materials containing hetero aromatic compounds. The structure of the resulting compounds were characterized by ^{1}H NMR, ^{13}C NMR, and FT-IR. The optical and redox properties of the resulting compounds were measured by UV-vis spectroscopy, PL spectroscopy and CV, respectively.

일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P275포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Kinetics and Mechanism of the Pyridinolysis of ArylDithiocyclopentanecarboxylates in Acetonitrile

이한나, 오혁근

전북대 화학과

Kinetic studies of the pyridinolysis (XC_5H_4N) of aryl dithiocyclopentanecarboxylates (c-$C_5H_9C(=S)SC_6H_4Z$) are carried out in acetonitrile at 60.0°C. A biphasic Brönsted plot is obtained with a change in slope from a large ($\beta_X = 0.69$) to a small ($\beta_X = 0.35$) value at $pK_a^o = 5.2$, which is attributed to a change in the rate limiting step from breakdown to formation of a zwitterionic tetrahedral intermediate, $T^{\pm}$, in reaction path as the basicity of the pyridine nucleophile increases. This mechanism is supported by the change of the cross-interaction constant ρ_{XZ} from a large positive ($\rho_{XZ} = +1.02$) for the weakly basic pyridines to a small negative ($\rho_{XZ} = -0.17$) value for the strongly basic pyridines. The magnitudes of ρ_Z and activation parameters are also consistent with the proposed mechanism.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Nucleophilic Substitution Reactions of ArylDithiocyclohexanecarboxylates with Anilines in Acetonitrile

박선영, 오혁근

전북대 화학과

The aminolysis of phenyl dithiocyclohexanecarboxylates with anilines in acetonitrile proceeds by rate-limiting breakdown of a tetrahedral intermediate, $T^{\pm}$. The unusually large β_X (β_{nuc}) values can be accounted for by a strong localized cationic charge on the nitrogen atom of anilines in $T^{\pm}$, which is lost in the aniline expulsion from $T^{\pm}$ (k_{-a}). The breakdown rate ratio of k_{-a}/k_b is large due to large k_{-a} and relatively small k_b. The proposed mechanism is also supported by a large positive cross-interaction constant, ρ_{XZ} (= 1.68), adherence to the RSP, and low activation parameters. The greater than unity k_H/k_D values involving deuterated anilines suggests a four-center type hydrogen-bonded TS.

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Reactivation of acetylcholinesterase inhibited by nerve agent - Russian-VX (Structure-activity Study)

Kuca, Musilek, Pohanka, Marek, Karasova, *정영식

*Faculty of Military Health Science *한국화학연구원 신약연구단*

Acetylcholinesterase (AChE; EC 3.1.1.7) reactivators are drugs used as treatment in case of organophosphorus pesticide and nerve agent poisonings. According to the recent knowledge, none of the clinically used AChE reactivators is able to counteract every nerve agent poisoning. Due to this, novel candidates for the AChE reactivation are still synthesized. To prepare promising compounds with optimized structure, structure-activity studies are generally used. In this study, structure-activity study of 30 AChE reactivators is shown. Russian VX, extremely toxic nerve agent developed during cold war in Russia, was used as member of the nerve agent family. As resulted, AChE inhibited by Russian VX is easy to reactivate. Structural requirement for reactivators.of Russian VX-inhibited AChE will be presented.This work was supported by the project of Ministry of Education, Youth and Sports (Czech Republic) – No. ME09086.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Monooxime-monocarbamoyl reactivators of OP pesticides with xylene linker

Musilek, *Holas, Pohanka, Kuca, **정영식

*Faculty of Military Health Sciences *Faculty of Pharmacy in Hradec Kralove*
***한국화학연구원 신약연구단*

The reactivators of acetylcholinesterase (AChE, EC 3.1.1.7) are very important components in the treatment of intoxications caused by organophosphate inhibitors such as nerve agents and pesticides [1]. These inhibitors covalently bind to active site of mentioned enzyme and irreversibly inhibit its activity. The reactivator breaks the inhibitor-enzyme covalent bond and restores its activity. Unfortunately, there is no reactivator applicable for every type of inhibitor; it means that every structural change in the molecule of inhibitor needs a specific structure of the reactivator [2].This novel group of compounds was prepared as analogues of former effective reactivator K203 [3]. Their reactivation ability was evaluated on model of paraoxon-, methylparaoxon- and DFP-inhibited AChE in vitro. Several compounds presented effective reactivation of OP pesticides, but did not exceed compound K203. Additionally, the in vitro results showed apparent influence of xylene linker to reactivation ability of prepared compounds.[1] Marrs, T.C.. Pharmacol. Therapeut. 1993, 58, 51.[2] Bajgar, J. Adv. Clin. Chem. 2004, 38, 151.[3] Musilek, K. et al. J. Med. Chem. 2007, 50, 5514.The work was supported by the Grant Agency of Ministry of Education, Youth and Sports (Czech Republic) – grant no. ME09086.

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Pyridinium Oximes Reactivators for Acetylcholinesterases Inhibited by Organophosphorus Agents

정희춘, *박노중, **정영식, ***Musilek, ***Marek, ***Kuca

*충남대 화학과 *한국화학연구원 Bio-Refinery **한국화학연구원 신약연구단*
***University of Defence in Hradec Kralove*

Fluorinated compounds are frequently encountered in modern medicinal chemistry and many of these substances are highly effective drugs. A common beneficial property associated with fluorine substitution is an increase in blood brain barrier (BBB) permeability due to changes in lipophilicity. In order to develop new bis-pyridinium oxime reactivators for the Acetylcholinesterase (AChE) inhibited by organophosphorus toxic agents, we have designed and synthesized a series of fluorinated oxime compounds in order to probe the effect of fluorine substitution on reactivation of inhibited AChE.

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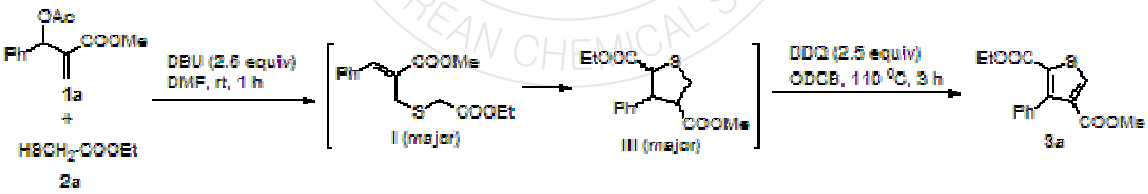
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis of poly-substituted thiophenes from Baylis-Hillman adducts *via* the sequential S_N2'-intramolecular Michael addition-aromatization strategy

이현승, 김세희, 김재녕

전남대 화학과

The reaction of Baylis-Hillman acetates and ethyl mercaptoacetate in the presence of DBU in DMF produced 2,3,4-trisubstituted tetrahydrothiophenes at room temperature as a diastereomeric mixture *via* the sequential S_N2' and Michael addition. DDQ oxidation of the tetrahydrothiophenes produced 2,3,4-trisubstituted thiophenes in good yields. This is the first synthesis of thiophene scaffold from Baylis-Hillman adducts.



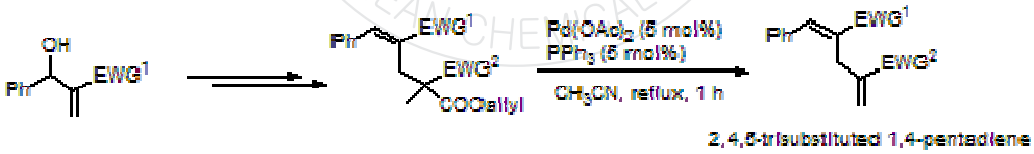
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P281포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

An expedient synthesis of 2,4,5-trisubstituted 1,4-pentadienes from Baylis-Hillman adducts *via* the Pd-catalyzed decarboxylation-elimination protocol

김고훈, 김은선, 김재녕

전남대 화학과

An efficient synthetic method of 2,4,5-trisubstituted 1,4-pentadienes from Baylis-Hillman adducts was developed *via* the Pd-catalyzed decarboxylation-elimination protocol as a key step. In the reaction, β-H elimination occurred in a regioselective manner at the methyl moiety and produced 1,4-pentadienes as the major product. Starting materials were prepared from Baylis-Hillman adducts *via* sequential introduction of allyl ester and methylation.



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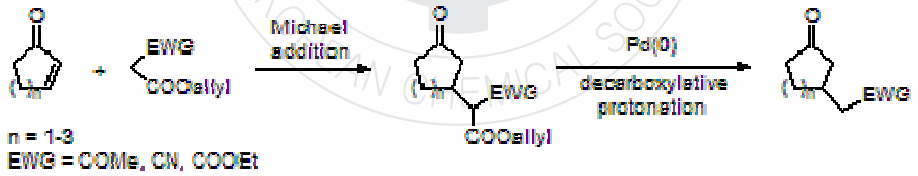
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Expedient synthesis of 3-substituted cycloalkanones *via* a Pd-catalyzed decarboxylative protonation protocol: A good alternative to the Mukaiyama-Michael approach

김세희, 김성환, 김재녕

전남대 화학과

An efficient method for the introduction of -CH_2EWG moiety at the β-position of 2-cycloalkene-1-ones was developed *via* the Pd-catalyzed decarboxylative protonation protocol. This method can be used efficiently as a good alternative to the Mukaiyama-Michael reaction for the synthesis of 3-substituted cycloalkanones.



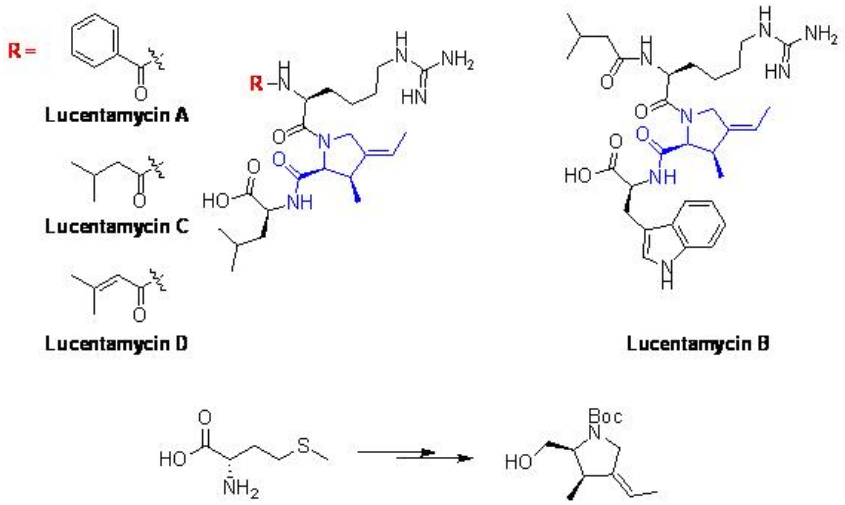
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P283포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

The Chiral Synthesis of The Lucentamacins A-D Core, 3-Methyl-4-Ethylideneproline

유하나, *최환근, 하정미, 심태보

*KIST 생체과학본부 *서강대 화학과*

Lucentamycins A-D were isolated in 2007 from the Marine-Derived Actinomycete Nocardiopsis lucentensis by Cho and co-workers. It turned out that Lucentamycin A and B possess anti-proliferative activity on HCT-116 with IC50 value of 0.20 and 11 M respectively. Interestingly, Lucentamycin C and D did not exhibit growth inhibitory activity against HCT-116, human colon cancer cell even at 150 uM concentration. Our research group has been most recently interested in identifying molecular target protein of Lucentamycin A and B in cancer cells. To achieve this goal we have embarked to synthesize effectively 3-methyl-4-ethylideneproline, the core structure of Lucentamycins starting from (L)-methionine. This synthesis has successfully been accomplished by adopting rhodium catalyzed cyclization reaction of a 1,6-enyne in efficient and stereoselective manner.



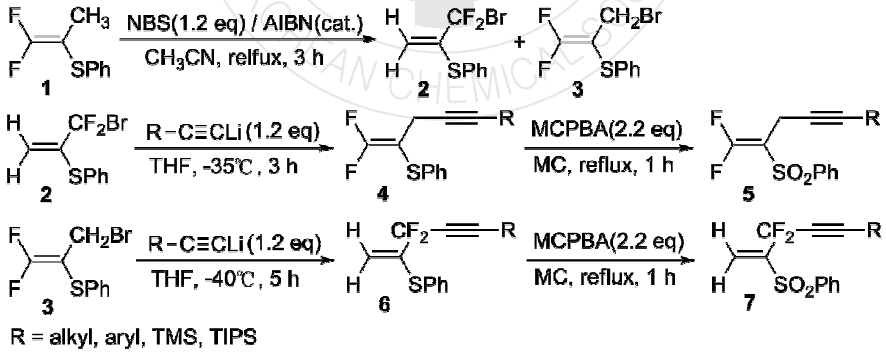
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P284포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

A new approach to *gem*-difluorinated 1,4-enynes and their reactions

황지혜

연세대 화학과

Treatment of 1,1-difluoro-2-phenylthio 1 with NBS(1.2 eq) at reflux in CH_3CN for 3 hour resulted in the formation of regioisomers 2 and 3 in 58% and 24% yields, respectively. Alkynylation of 2 with a variety of alkynyllithium reagents in THF at -35℃ for 3 hours provided 1,4-enynes 4 in 45-85% yields. Further oxidation of 4 with MCPBA gave 1,4-enynes 5 in 80-87% yield. Similar alkynylation reaction of 3 and oxidation of resulting product afforded the 1,4-enynes 6 and 7 in high yields. Synthesis and reactivity of 5 and 7 will be presented.



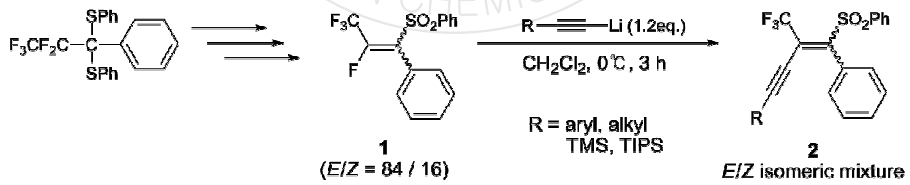
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P285포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

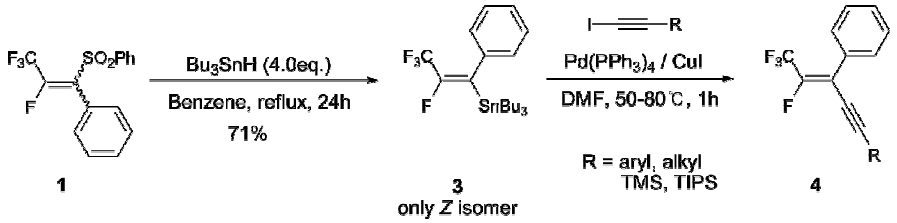
Preparation of novel trifluoromethylated 1,3-enynes and their reactions

정연희

연세대 화학과

2,3,3,3,-Tetrafluoro-1-phenyl-1-phenylsulfonylpropene 1 was prepared in 2 steps from pentafluoroethylated dithioketal. The addition-elimination reaction of 1 with lithium acethylides (1.2eq) in CH_2Cl_2 at 0℃ provided the trifluoromethylated 1,3-enynes 2 in good yields. 1-Tributylstannyl-2,3,3,3-tetrafluoro-1-phenylpropene 3 was prepared in 71% yield from the reaction of 1 with Bu_3SnH at reflux in benzene for 24 hours. The palladium-catalyzed cross-coupling reaction of 3 with a variety of alkynyl iodides afforded the corresponding trifluoromethylated 1,3-enynes 4 in good yields. Preparation and reactions of 2 and 4 will be presented.





일시: 2009년 10월 28~30일(수~금) 3일간
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발표종류: 포스터, 발표일시: 목 12:30~14:30

Reduction of 1-Aryl-4,5,6,7-tetrahydro-4-oxoindoles

권민진, 이창규

강원대 화학과

Reduction reactions of a series of 1-(m- and p-substituted phenyl)-4,5,6,7-tetrahydro-4-oxoindoles to the corresponding indoles were studied. The substituents are -H, -CH3, -OCH3, -Br, and -Cl. The best results were obtained when the reduction was carried out with hydrazine hydrate in the presence of potassium hydroxide in diethylene glycol at 180-190℃. But the reaction with lithium aluminium hydride gave only the corresponding alcohol. On the other hand, sodium borohydride did not undergo any reduction. The results are contrasted to the N-H compound.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Preparation of (2E)-3-Aryl-1-(pyrrol-2'-yl)prop-2-en-1-ones and Their NMR Studies

정은지, 이창규

강원대 화학과

(2E)-3-Aryl-1-(pyrrol-2'-yl)prop-2-en-1-ones having m- and p- substituents on the benzene ring were prepared by the reactions of 2-acetylpyrrole with substituted benzaldehydes and sodium hydroxide in ethanol. The substituents were NO2, Br, Cl, OCH3 and CH3. The yields were 70 ~ 90%. The substituent chemical shifts were examined using the Hammett correlation.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Reduction of N-Phenylmaleimide Derivatives by Triphenylphosphine

이혜선, 이창규

강원대 화학과

A series of N-phenylmaleimide derivatives were reduced to the corresponding N-phenylsuccinimides by the reaction with triphenylphosphine in ethanol. Although the major products were N-phenylsuccinimides, other products such as the amido esters were also formed. Various alcohols such as methanol, isopropyl alcohol, and tert-butyl alcohol were employed to examined the effect. The structural characteristics and possible mechanism for the formation of the products will be presented.

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Preparation of *N*-Arylpropynylamide and Their NMR Studies

최지은, *유지숙, 이창규

*강원대 화학과 *강원대 공동실험실습관*

N-Arylpropynylamides were prepared from the reactions of propiolic acid and substituted anilines with dicyclohexyl carbodiimide in dichloromethane. The substituents were *m*- and *p*-OCH_3, -CH_3, -Cl, -Br, -NO_2. The substituent chemical shifts were examined using the Hammett correlation.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Oxidation of Methylthiophenes to Thiophenecarboxylic Acids

김수진, *유지숙, 이창규

*강원대 화학과 *강원대 공동실험실습관*

Oxidation of methylthiophenes to thiophenecarboxylic acids were carried out by the reaction with sodium dichromate and water in a sealed stainless steel tube. The best results were obtained at 200℃ for 8 h. The thiophenes employed were 2-methyl-, 3-methyl-, 5-bromo-2-methyl-, 2-bromo-5-methyl-, and 2,5-dimethylthiophene. The complete assignments of the ^{1}H and ^{13}C NMR spectra of the thiophenecarboxylic acids were made by COSY and HETCOR spectroscopy.

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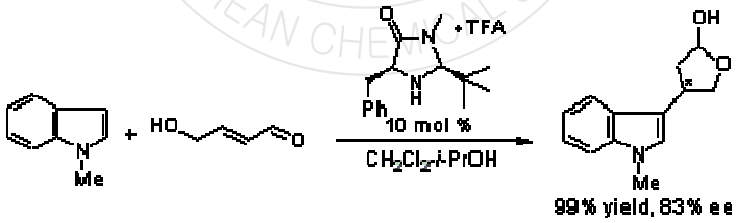
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Organocatalytic Asymmetric Friedel-Crafts Alkylation to γ-Hydroxy α,β-Unsaturated Aldehyde: Facile Synthesis of Chiral 3-Substituted Tetrahydrofurans and β-Substituted γ-Lactones

김성곤

경기대 화학과

we represent the catalytic asymmetric Friedel-Crafts alkylation of appropriate nucleophiles to a γ-hydroxy α,β-unsaturated aldehyde using an imidazolidinone as an organocatalyst which afforded β-substituted γ-lactols. The β-substituted γ-lactols have been obtained in good yields and with up to 87% ee, which lead to chiral 3-substituted tetrahydrofurans, β-substituted γ-lactones and 3-substituted alcohols followed by reduction, oxidation and Wittig reaction respectively.



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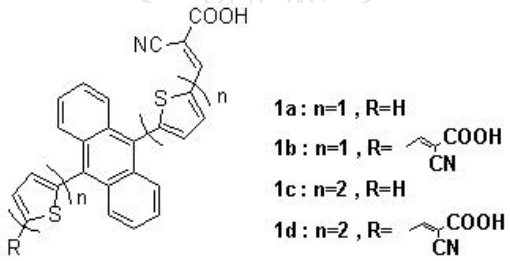
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis of Anthracenyl-oligothiophenes as Candidate Organic Dyes for Solar Cells

류석화, 성남경, 박혜정, 서혜원, 윤웅찬

부산대 화학과

Efforts for development of efficient dye-sensitized solar cells (DSSCs) based on new organic and organometallic complexes have recently attracted increasing attention. We synthesized geminal cyano-carboxy vinyl substituted 9,10-anthranyl centered oligothiophenes (1a~d) as new possible organic dyes for DSSC which can anchor on the surface of semiconductor material such as TiO_2. Newly synthesized anthranyl-oligothiophenes as organic dyes contain variable lengths of conjugation with varying number of thiophene unit (n=1, 2) at 9-and 10-position of the centered anthracene moiety and also carboxy group for anchor at the terminus. Their photophysical, electrochemical properties are characterized.



일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅰ37P293포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

Peptide-Oligonucleotide Conjugates for the Specific Gene Delivery.

박정우, 김병현

포항공과대 화학과

Antisense and siRNA oligonucleotides for the gene therapy show meaningful promise as therapeutic agents. However, oligonucleotide-based gene therapy have some problems which are their low cellular uptake, poor target specificity, and resistance to enzymatic degradation in vivo. For the conquest of their problem, we covalently attached special peptides to oligonucelotides, by using the disulfide bond. In this study, we used the PFVYLIH[1] as a special peptide. PFVYLI is a synthetic peptide which is the C-terminal part of *C105Y*. Because of the six-amino acid sequence,PFVYLI, it is able to enter the cells in an almost same fashion to C105Y. By using this PFVYLI sequence, we synthesize the peptide-oligonucleotide conjugates (POCs). And we check the cellular uptake with FITC labelled POCs and gene down regulation in hepatoma cell line. 1) Melanie Rhee and Pamela Davis, *JBC*. 2006, *281*, 1233-1240.

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Syntheses of Nucleoside-Based Cationic Lipids as siRNA Delivery Agents

양혜원, 김병현

포항공과대 화학과

The clinical success of gene therapy is critically dependent on efficient and safe gene delivery. For this reason, it is necessary to use delivery agents, known as transfection vectors : viral and non-viral vectors. Nucleoside-based cationic lipids are one of the non-viral vectors and have some advantages (1) low cytotoxicity compared to viral vectors (2) similar structure to cell membrane (3) favorable interactions with negatively charged DNA or RNA, and cell membranes (4) interaction with gene through electrostatic, hydrophobic interactions, and moreover hydrogen bonding, π-π stacking, and nucleo-base recognition. The novel uridine-based cationic lipids had been synthesized for the delivery of therapeutic gene, siRNA. The 5' position of uridine was conjugated by triazole ring through click chemistry with basic amino acid, lysine and arginine. To make diverse length and kink on tails, octyl, dodecyl, and oleyl alkyl chain were linked at 2', 3' positions by carbamate group. The lipoplex was prepared by using uridine-based cationic lipids and VEGF siRNAs. From gel-electrophoresis, we confirmed the minimal mol ratio of lipoplex between lipid candidate and siRNA, so this showed nucleoside-based cationic lipids were able to bind siRNA. MTT assay was done for cytotoxicity which indicated the cationic lipids had low cytotoxicity. siRNA knockdown experiment was performed with the cationic lipids and we concluded that uridine-based cationic lipids had positive effect on siRNA delivery.

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Synthesis and Characterization of Dicyanovinyl-Substituted Oligothiophenes as Low-Band-Gap Acceptor Materials

류석화, 유영주, 박별나, 허혜령, 윤웅찬

부산대 화학과

Thiophene-based oligomers are an important and promising class of organic materials for their possible applications in organic photovoltaic (OPV) and organic thin film transistors (OTFT).Further these materials are attractive due to their low density, high flexibility, and processibility for large areas coverage.We designed and synthesized terminal mono- and di-dicyanovinyl-(9, 10-anthranyl) centered oligothiophenes (1a~b and 2a~b). Their photophysical and electrochemical properties are characterized. These materials exhibit dramatic differences in both their electronic and redox properties in comparison the dicyanovinyl group free (9, 10-anthranyl) centered oligothiophenes (3a~b) and display both stable oxidation and reduction processes as expected ones with dicyanovinyl substituents.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthetic Approaches toward Pyridazine Analogue as SGLT2 Inhibitor

강석연, 이준원, 김정민, 이진화

(주)녹십자

With aims at biological improvement over dapagliflizin of BMS, currently the best SGLT2 inhibitor, we designed and synthesized a novel pyridazine analogue efficiently and stereoselectivly. Pyridazine ring was installed by several steps from γ-ketoester, which was prepared from β-C-vinyl glucoside. A stereoselective β-C-vinyl glucoside could be prepared from starting glucolactone with vinylmagnesium bromide and subsequent reduction with triethylsilane and TMSOTf. The overall yield was 5.3% with 13 steps from benzylated-D-glucose. Combination of benzylpyridazinyl and glucose generated a decent SGLT2 inhibitor with IC_{50} = 0.61 μM for human SGLT2. Using the synthetic route disclosed here, further exploration of the in vitro SAR studies as well as in vivo efficacy studies around this compound is ongoing.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Biological Evaluation of Thiazole Analogues as SGLT2 Inhibitors

송광섭, 이석호, 이준원, *김정민, 이진화

*(주)녹십자 종합연구소 의약화학팀 *(주)녹십자 종합연구소 신약개발팀*

Sodium glucose co-transporter 2 (SGLT2) plays a key role in maintaining glucose equilibrium in the human body. The discovery and clinical use of SGLT2 inhibitor, dapagliflozin, has confirmed the clinical utility of inhibiting this target as an antidiabetic agent. Our discovery efforts have led to the identification of novel series of benzylthiazolyl analogues. The key intermediate, thiazolylglucoside, was prepared by the addition of 2-lithiothiazole to gluconolactone. The coupling reaction between the thiazolylglucoside and requisite benzaldehydes was carried out to install the benzyl moiety at the 5-position of the thiazole ring. A halogen atom was introduced into the desired 4-position of the thiazole moiety via the Halogen Dance (HD) reaction using LDA as a base. Biological activities of some of these compounds will be reported.

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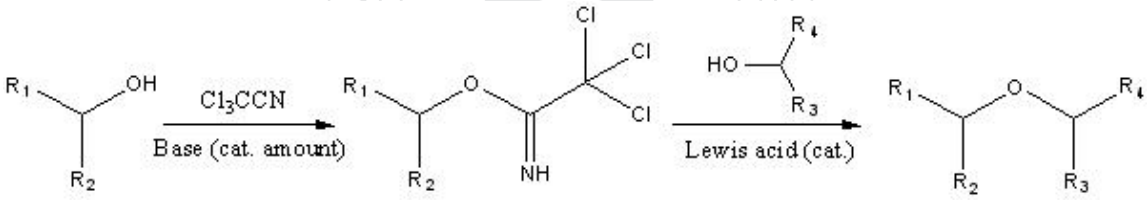
발표종류: 포스터, 발표일시: 목 12:30~14:30

An efficient method for sterically hindered ether formation using trichloroacetimidates

김수정, *박훈규, *김학원

*경희대 화학 및 신소재과학 *경희대 화학과*

Williamson ether synthesis is a usual method to yield an ether compound from two alcohols. However, there are some difficulties for making an ether compound with sterically hindered or base-sensitive alcohols. Therefore, we have studied the mild, efficient acid-catalyzed etherification using trichloroacetimidates.



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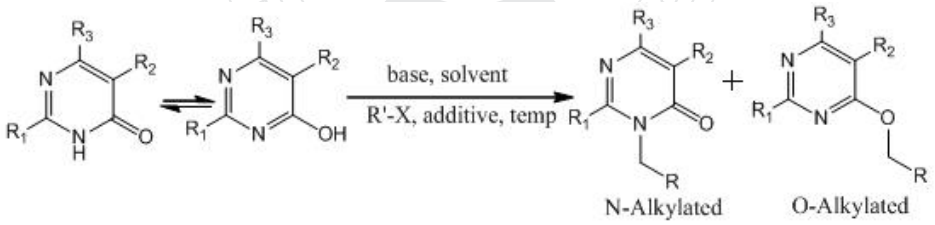
Synthetic studies on the selective N/O-alkylation of 3H-pyrimidin-4-ones

이선화, 김학원

경희대 화학과

Many biologically active compounds containing N-substituted 3H-pyrimidin-4-one moiety have drawn a special interest, recently. However, direct base-mediated alkylation of 4(3H)-pyrimidinones generally gives an O-alkyaltion product as well as an N-alkylation one. In this report, we would describe the effects of some factors (base, solvent, temperature and additives etc) on N/O selectivity.



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Biindole-bridged porphyrin dimer as allosteric molecular tweezers

이치화, 장우동

연세대 화학과

Allosteric guest binding is one of the fundamental regulation mechanisms in biological events, such as molecular recognition and catalytic activity. Many proteins having multiple-guest binding sites show allosteric guest binding phenomena, in which the occurrence of guest binding can influence other binding sites through conformational changes to regulate additional guest-binding affinity. Though various types of molecular tweezers have been reported,very few examples have controlled their guest binding affinity by external stimuli. Therefore, the allosterism of molecular tweezers is particularly interesting, from the viewpoint of binding affinity control by external stimuli. Very recently, by combining zinc porphyrins and biindole, we designed a new type of molecular tweezers for the simultaneous binding of DABCO as well as anionic guests. In this work, we report a multiple-guest-binding molecular tweezers that exhibits notably strong positive allosteric guest binding phenomena.

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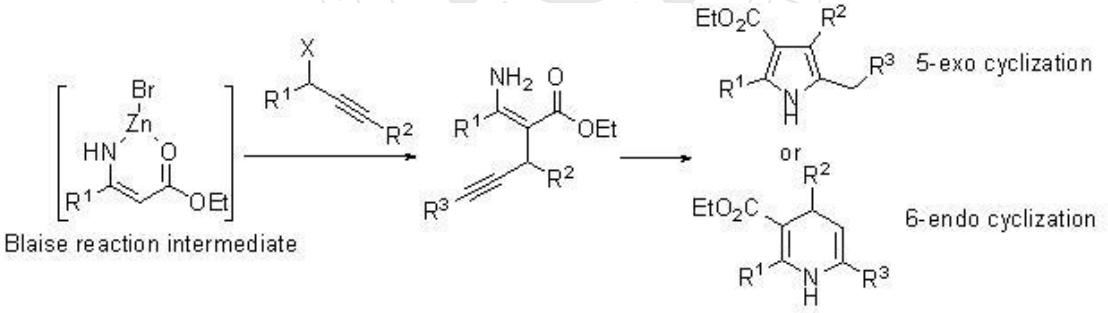
The Regioselective Tandem Synthesis of N-Heterocyclic Compounds by using the Blaise reaction intermediate

박보영, 이상기

이화여대 화학/나노과학과

Reaction of the Blaise reaction intermediate with terminal propargylic compounds proceeded via an S_N2 mechanism to afford α-propagylated β-enaminoester, which can be cyclized in 5-exo manner to afford polysubstituted pyrroles. The reaction profiles of the Blaise reaction intermediate toward internal propargylic compounds have also been investigated, which will lead to the formation of dihydropyridines.



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발표코드: **Ⅰ37P302포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 12:30~14:30

A perfect method for preparation of aldehydes from esters

유민, 안덕근

강원대 화학과

Partial reduction of ester to aldehyde is one of the most important and highly desirable methods in organic synthesis, and a large number of reducing agents for this purpose have been reported. However, most developed reducing agents until now have some handicaps that these reagents cannot achieve general reduction of both aliphatic and aromatic esters and not satisfied yield. Accordingly, we have tried to make the new reducing agents to solve these problems in the partial reduction of esters for several years. And, we could solve many problems thought an efficient new reducing agents that making our laboratory. However, we cannot satisfy the around 90% yield.Recently, we carried out a lot of experience to find excellent method of partial reduction, as the result, we have found the perfect synthetic method of aldehydes from esters in quantitative yields (>99%) for 10min although we have to confirm reliable mechanism and reaction condition.

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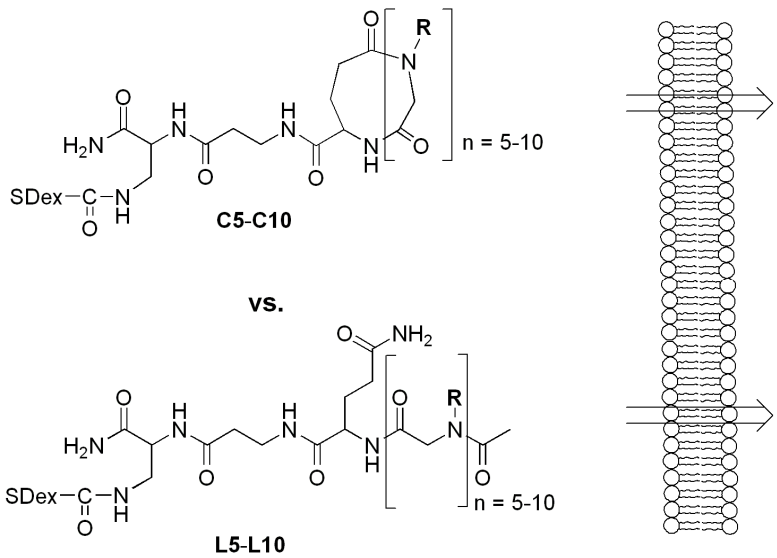
발표종류: 포스터, 발표일시: 목 12:30~14:30

Efficient Solid-Phase Synthesis of a Series of Cyclic and Linear Peptoids for the Cell Permeability Studies

조수경, 권용억

이화여대 화학.나노과학과

Cyclic peptides and depsipeptides are of considerable interests as drug candidates and potential chemical modulators of proteins, due to their numerous interesting biological activities. It has also been speculated that they might have improved cell permeability relative to linear molecules by providing internal hydrogen bond and generally decreasing the conformational flexibility. Herein we report the rational design and efficient solid-phase synthesis of a series of cyclic and linear peptoid-dexamethasone conjugates for their systematic cell permeability studies by using reporter gene-based assays. These model compounds may reveal how cell permeability of cyclic molecules is affected by several physicochemical properties, especially, intramolecular or internal hydrogen bond potential, reduced conformational flexibility and ring size.



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Glucosylation of 2-Phenylimino-1,3-thiazoline Derivatives

남기달, 한호규, 신동윤, *마혜덕, **한민수, ***허정회

*KIST 생체과학연구부 *경기대 화학과 **KIST 케모인포메틱스연구단 ***고려대 화학과*

2-Phenylimino-1,3-thiazoline derivatives were known to agrochemical fungi toxic with selectivity against rice blast. As a lead optimization process glucose moiety was introduced to the molecule. Starting 4-aminomethyl-1,3-thiazoline was synthesized from chloroacetone through 4 steps in 80% yield. α-D-Glucopyranosyl isothiocyanate and β-D-glucopyranosyl isocyanate were obtained by a dehydrochlorination of α- or β-D-glucosamine hydrogen chloride salt followed by the reaction of either thiophosgen or triphosgen respectively. 2-Phenylimino-1,3-thiazoline derivatives were synthesized from a reaction of isothiocyanato-α-D-glucopyranose and isocyanato-β-D-glucopyranose with 4-aminomethyl-2-phenylimino-1,3-thiazoline derivatives. The structures were confirmed by their 1H NMR spectra. The biological properties of the synthesized compounds will be discussed.

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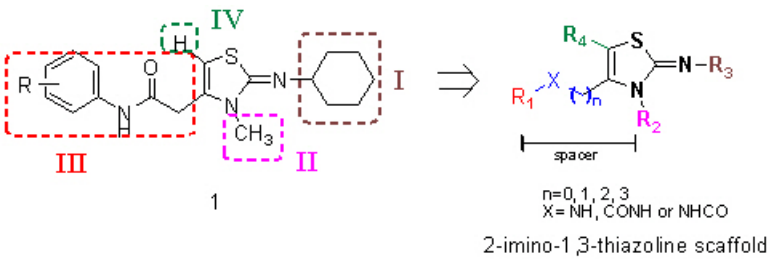
발표종류: 포스터, 발표일시: 목 12:30~14:30

Combinatorial Library of Novel 2-Alkylimino-1,3-thiazolines and Their Biological Activity of T-type Calcium Channel Inhibition

한민수, *한호규, *남기달, *신동윤

*KIST 케모인포메틱스연구단 *KIST 생체과학연구부*

Combinatorial chemistry serves as a powerful tool in lead discovery and lead optimization by allowing a rapid generation of potential candidates for screening. Heterocyclic scaffolds represent the most promising molecules as leading structures for the discovery of novel synthetic drugs. To develop T-type Ca2+ channel blocker, our in-house small molecule chemical library were biologically evaluated against T-type Ca2+ channel to degree of inhibition of T-type Ca2+ current. The structure of hit compound 1 was modified systematically including the 4 variable diversity points (I~IV) in the scaffold based on the structure-activity relationship using the combinatorial chemistry technology. Hundreds of the compounds were constructed by the parallel synthetic fashion from building blocks, thioureas, α-haloketones, amines, acyl chlorides, and aldehydes.



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발표종류: 포스터, 발표일시: 목 12:30~14:30

Synthesis and Biological Activity of 2-Guanyl-1,3-thiazole Derivatives as Novel T-type Calcium Channel Blocker

허정회, *한호규, *신동윤, *남기달

*고려대 화학과 *KIST 생체과학연구부*

Ca^{2+} plays a unique role among ions by acting as an intracellular messenger. Its binding proteins sense increase in Ca^{2+}concentration to trigger cellular processes. T-type Ca^{2+}channel belongs to low voltage gated transmembrane ion channel superfamily and is known to relation with hypertension, angina pectoris, epilepsy, cancer and neuropathic pain. For a purpose of exploration of new T-type Ca^{2+} channel inhibitor 2-guanyl-1,3-thiazole derivatives were synthesized by the combinatorial synthetic fashion. The 2-guanyl-1,3-thiazole molecule comprises guanidyl and 1,3-thiazole moieties which is known to privileged structure are present in a molecule. The synthesis of the 2-guanyl-1,3-thiazole derivatives and their inhibitory screening results will be presented.

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Synthesis of New quinone Derivatives for KAPAS Inhibition as Herbicide Target

이정석, *한호규, *신동윤, *남기달

*KAIST *KIST 생체과학연구부*

Biotin biosynthetic pathway may provide new targets for herbicide design because biotin plays a key role in carboxylation reactions which are critical to plants. We found quinone derivatives showed inhibitory biological activity (in vitro) against 2-keto-8-aminopelargonic acid synthase (KAPAS) in the biotin synthetic pathway. As a lead optimization process, the quinone analogues were designed by the molecular modification and synthesized starting from phenol derivatives. We will introduced the KAPAS as the herbicide target and the synthetic scheme will be presented.

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Variation of photochemical behaviors of phenyl alkyl ketones upon minor changes in their structures

류혁준, 박봉서

동국대 화학과

Sterically demanding phenyl alkyl ketones containing a leaving group at alpha position to carbonyls have been prepared and their photochemical behaviors have been investigated. Product distribution was heavily dependent upon reaction solvents, temperature, irradiation wavelength, size of substituents, and leaving groups. A mechanism explaining the observed product selectivities has been proposed and compared with that of the less sterically demanding analogues.

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Photochemistry of α,α-dichloro-o-methylacetophenone

정성진, 박봉서

동국대 화학과

Photochemistry of acetophenones containing a leaving group at alpha position to carbonyls has received much attentions mainly due to their interesting application into photocages or photoinduced removable protecting groups. The product distribution is known to change depending upon various reaction conditions such as solvents and leaving groups. In our continuing efforts to elucidate the relationship of structure and photochemical reactivities, the title compound was prepared and its photochemical behaviors were investigated. Experimental results together with a proposed mechanism will be presented and the origin of different reactivity from its mono substituted analogue will be discussed.

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Chromene derived organic–dye sensitizers for dye-sensitized solar cells

김다정, 장정인, 박용선

건국대 화학과

We have developed novel organic–dye sensitizers for dye-sensitized solar cells (DSSCs) and investigated solar cell performance of the DSSCs. We have designed various organic sensitizers that contain a chromene molecular frame. The chromene derivatives were well-known for their electron-transfer ability of the conjugated molecular structure. Possibility of low cost production, high efficiency, and high long-term stability were shown by the solar cell.

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(S)-Mandelate-mediated asymmetric nucleophilic substitution of α-bromo esters

이윤민, 박용선

건국대 화학과

(S)-Mandelate-mediated dynamic kinetic resolution of α-bromo esters in asymmetric nucleophilic substitution has been investigated. Reactions with various aryl and alkyl amine nucleophiles in the presence of TBAI and DIEA can provide various amine substituted products up to 97:3 dr. The simple procedure with spontaneous removal of the chiral auxiliary provides an efficient synthetic method for the enantioenriched dihydroquinoxalinones, dihydrobenzoxazinones and morpholinones.

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발표종류: 포스터, 발표일시: 목 12:30~14:30

박달나무(Betula schmidtii) 수피로부터 미백화합물의 분리 및 구조 규명

왕다혜

덕성여대 화학과

박달나무(*Betula schmidtii*)는 자작나무과(Betulaceae)에 속하는 낙엽교목으로 일본, 중국, 시베리아등지에 분포하며 우리나라에서는 지리산, 오대산, 속리산 등지에 널리 퍼져있다. 본 연구진은 천연수목으로부터 부작용이 없고 안정성이 뛰어나며 미백효과를 함유하는 기능성소재 탐색을 목적으로, 박달나무 수피의 80% ethyl alcohol 추출물을 n-hexane, chloroform, ethylacetate 및 butanol 로 분획하여 얻은 분획물에 대한 생리활성을 검색하였다. 연구결과, 세포독성, 항산화 및 미백효능이 우수한 chloroform 과 ethylacetate 분획물에 대해 silica gel open column chromatography 와 vacuum liquid column chromatography 를 반복적으로 실시하여 순수물질을 분리한 후, EI-MS, FAB-MS, ^{1}H-NMR, ^{13}C-NMR, DEPT, ^{1}H-^{1}H COSY, HMBC, HMQC 등의 분광학적 분석기법을 활용하여 화학구조를 규명하였다.

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Synthesis and Properties of New 3-alkylthiophene Containing Non-linear-optical Active Group

박영진, 김인태, 정연준

광운대 화학과

For the purpose of preparing materials for nonlinear optics applications, a 3-hexylthiophene bearing an NLO-active chromophoric group was designed and synthesized. The structure of the new material was characterized by ^{1}H NMR, ^{13}C NMR and FT-IR. The optical properties of the material was investigated by UV-Vis spectroscopy and PL spectroscopy. Oxidation and reduction potential were measured by cyclicvoltammetry. The new material will be polymerized by oxidative coupling method using $FeCl_3$ and electrochemical method.

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Cyclo-dipeptides Dervatives as Low-Molecular-Weight Gellator for protic solvents

김정아, *장우동

*연세대 이과대학 화학과 *연세대 화학과*

Nowadays, one of the fascinating areas in modern supramolecular chemistry is the organogelater via self-assembly of low molecular weight compounds.Coupling Cyclo(L-Tyr-L-Ala) and penta,tert(ethylene glycol) were synthesized and investigated as organo-and hydrogelators. They enabled the gelation of not only a number of organic solvents such as Dichloromethane, Chloroform, Tetrahydrofuran, Acetonitrile and alcohols but also water. They are of great interest due to its secondary structures in self-assembled nanofiber. Intermolecular hydrogen bonding was essential driving forces of organo-and hydrogel formations. Organogelation occurs when its concentration reaches 0.3 ~ 1 wt% under the assist of sonication. Hydrogel is created coupling cyclo-dipeptide and penta(ethylene glycol) at 6 wt%. The self-assembled fibrillar networks in the gels were distinctly evidenced by SEM observation.

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pH & Temperature responsive dendritic linear block copolymer

이은영

연세대 화학과

최근에 외부자극에 응답하는 stimuli-responsive polymer 에 관한 많은 연구가 이루어지고 있다. 이러한 연구들을 바탕으로 본 연구에서는 pH-sensitive pendent 를 갖는 dendron 과 thermo-sensitive linear polymer 를 결합하여 pH 와 온도에 민감성을 보이는 dendritic linear polymer 를 합성하였고, 이를 1H NMR 을 통해 확인하였다. 합성된 copolymer 의 분자거동을 알아보기 위하여 low critica solution temperature(LCST)를 측정하였고 그 결과 LCST 가 pH 와 농도변화에 의존함을 알 수 있었다. DLS 측정을 하였는데, 이를 통해 온도와 pH 변화에 따라 micelle structure 를 형성할 것으로 기대된다.

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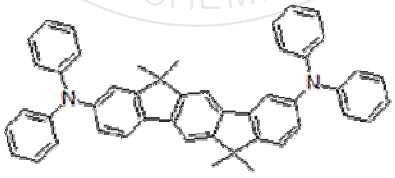
New Synthetic Method of Indenofluoreneamine as Blue Light Emitting Material

팜반충, 주동준, 이재열

경희대 화학과

One of the major concerns in the fabrication of full color OLEDs is the equal performance of the three primary colors of red, green and blue. Due to the large band gap energy, blue light emitting materials have a low affinity for the electron from the cathode in OLED devices. Therefore, the performance of blue emitters is usually inferior to that of green or red emitters and it is not satisfactory. Especially, the color purity and stability require improvement for blue OLEDs. In this respect, indenofluoreneamine (1) as new blue light emitting dopant was recently reported. Herein, we describe the improved synthetic process of indenofluoreneamine for high purity and high yield.



indenofluoreneamine (1)

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Ammouinm salt-supported precursors via click linkage for simple purification of F-18 labeled compounds

임송이, *이병세, **이상주, ***오승준, **지대윤

*인하대 화학과 *(주)퓨처켐 표지화학연구소 **서강대 화학과 ***서울아산병원 핵의학과*

we prepared two sulfonate precursors 1 and 2. Azide-condaining sulfonate precursor 1 was synthesized by the reaction of alcohol compound and 3-azidopropanesulfonyl chloride. The [18F]fluorinated compounds were prepared using 3 mg of precursor 1 by two-step synthesis i.e., [18F]fluorination and click reaction. [18F]Fluorination of 1 was performed in t-amyl alcohol solvent at 120 oC for 15 min, and then propargyl triethylammonium mesylate (6 mg), 0.2 M aq. CuSO4, and 0.2 M aq. Na-ascorbate were added to the reaction mixture for the next click reaction. After 15 min at room temperature, the mixture was filtered with a short silica column and washed with ethyl acetate. Compared to direct HPLC analysis, additional click reaction offered the great clearance of byproducts based on HPLC-UV profile. We also synthesized ammonium salt precursor 2 using precursor 1 and click reaction. Through one-step synthesis, [18F]fluorinated compounds was also obtained in excellent radiochemical yield (RCY) and in shorter time after filtration with a short silica column. With the successful result from naphthalene model compound, we applied this method to the synthesis of [18F]FLT and [18F]FMISO.

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Novel prothetic group F-18 labeling of biomolecules

이보람, *이병세, 이상주, **오승준, 지대윤

*서강대 화학과 *(주)퓨처켐 표지화학연구소 **서울아산병원 핵의학과*

We designed a novel N-succinimidyl ester to avoid interim base and acid treatment, which is thought to make the manual preparation of [18F]SFB tedious and difficult. By using click chemistry in the second step, such laborious handling would would be eliminated. As shown in Scheme 1, 18F-labeld azido compound can react with N-succinimidly propiolic ester to give the desired 18F-labeled active ester. Noteworthy, we also found that electron-deficient terminal alkyne can make 1,2,3,-triazole with azido compound under slight heating and copper-free condition (not published result). It also provides regioslective 1,4-regioisomer almost exclusively. Typical click condition using Cu(Ⅰ) was found to break N-succinimidyl ester bond to be carboxylic acid due to slightly basic environment. Therefore, copper-free 1,2,3-triazole formation is essential factor for study. [18F]Fluorination of azido tosylate (1) under typical F-18 labeling condition yielded F-18 labeled azido intermediate (2) in 95% radio TLC conversion. The reaction mixture was filtered with a short silica column to remove inorganic base and salts. Copper-free click reaction of 18F-labeled azido compound was performed with N-succinimidyl propiolate in small volume of t-amyl alcohol and THF at 80 oC to give excellent radio-TLC conversion. The resulting novel 18F-labeled prosthetic group was purified by HPLC in 70% RCY (n = 3) and then reacted with several simple amines to validate amide formation.

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Formation of Polymer Brush grafted from Graphene oxide (GO) by Surface-Initiated, microwave irradiation supported Polymerization

박민수, 윤국로

한남대 화학과

Due to the unique mechanical, electrical, thermal, and optical properties graphene oxide (GO) platelets have been investigated for quantum electronic transport, a tunable band gap, extremely high mobility, high elasticity and electromechanical modulation. We investigated surface-initiated, microwave irradiation supported Polymerization of benzyl chloride carrying vinylates from the surface of graphene oxide (GO) platelets for tailoring surface properties of GO platelets. The resulting graphene oxide (GO) platelets/polymer Nanocomposites were characterized by infrared spectroscopy, scanning electron microscopy, atomic force microscopy, and thermogravimetric analysis.

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Fluorescent Chemodosimeter for Cyanide Anion

김건중, 김해조

경기대 이과대학 화학과

A new coumarin-based fluorescent sensor (1) was developed for the selective detection of cyanide anion. The chemodosimeter has shown a selective and sensitive response to cyanide anion over other various anions through Michael addition reaction of cyanide to (1). When cyanide anion was added, the fluorescent intensity of (1) was remarkably increased and the color of (1) was changed from yellow to pink enough to detect cyanide by the naked eye.

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Highly Sensitive and Fluorescence Turn-On Probe for Gold(Ⅲ) Ion

도정호, 김해조

경기대 이과대학 화학과

We have shown a highly sensitive fluorescence turn-on probe for gold(Ⅲ) ion using a latent fluorophore, which is operating in alcoholic solvents and shows a fluorescence turn-on property by overcoming the competing coordinating solvents. This latent fluorophore can be applied to monitoring a reaction in a highly dilute condition by fluorescence and to screening an effective catalyst, which are on the way of further research.

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Platinum-Based Self-Assembly with Functionalized Linear Linkers

vajpayee vaishali, 문미은, *P. J. Stang, 지기환

*울산대 화학과 *Department of Chemistry, University of Utah, SLC 84112, USA*

The coordinative-bond approach has been extensively used for the building of rings, polymers and networks. In addition to this, a great variety of self-assembly processes are possible if the aromatic N-heterocyclic ligands carry structural moieties that allow conformational rearrangements and directional hydrogen bonding to control the self-assembly of supramolecular systems. To exploit the functionality of the linear linkers we intended to synthesize new platinum-based self-assembled motifs which are characterized by UV, IR, NMR studies and efforts are doing to grow the single crystal for x-ray structural analysis.

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Eco-Friendly Bromination and Chlorination of Aryl Amines viaArenediazonium Tosylates in a Solvent-Free Condition

최영화, 문미은, 이영민, 지기환

울산대 화학과

Aromatic diazonium salts have been used as an important building block in modern as well as classical organic synthesis. Recently we have developed very stable diazonium tosylate salts which are useful for diazotization-iodination of aromatic amines. To broaden the applicability of aryl diazonium tosylates in various fields of organic synthesis, solvent-free reaction conditions for bromination and chlorination of aryl amines via arenediazonium tosylates have been scrutinized. Environment-friendly solvent-free synthetic methods are finally developed for the bromination by using tetrabutylammonium bromide as a brominating agent, and the chlorination by using benzyltriethylammonium chloride as a chlorination agent. Moderate to good yields of the desired products are obtained by using the new methodologies.

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The Reaction of Diethyl Phosphonate with Grignard Reagents and The preparation of diphenyl aryl(hydroxy)methylphosphonates

권대길, 김경만

한국화학연구원 에너지소재센터

The reaction of diethyl phosphonate with methyl and ethyl Grignard reagents has been investigated. Chemical and physical evidence suggest that the intermediate is not a diethyoxyphophinylmagnesium halide [$(RO)_2P(\rightarrow O)MgX$] but is a trivalent phosphorus species [$(RO)_2POMgX$]. The latter undergoes rapid substitution with methyl Griganard reagent at 25° to give the halomagnesium dimethyl- and diethylphosphinites (R_2POMgX).

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Binding Affinity of Dopamine Functionalized Poly(p-phenylenevinylene)(PPV) for Metal Nanopaticles

최원석, 윤국로

한남대 화학과

Poly(p-phenylenevinylene)(PPV) derivative polymers are widely used in various end-use devices , organic LEDs, photovoltaic cells, and thin film transistors, etc. The properties of the resulting polymers depend on the molecular weight and structure of the substituted side groups. The polymerization was achieved by a mixture of potassium tert-butoxide, 2-(2,5-bis(bromomethyl)-4-methoxyphenoxy) propanoic acid in anhydrous tetrahydrofuran at room temperature for 16 h.We demonstrated that novel functionalized Poly(phenylenevinylene)(PPV) was decoration with inorganic nanoparticles by sonication. The resulting inorganic/F-PPV hybrids particles were characterized by infrared spectroscopy, scanning electron microscopy, atomic force microscopy, and transmission electron microscopy. Considering the importance of nano-materials, this method could be beneficial in many areas, such as devices, medicines, sensors and functional materials.

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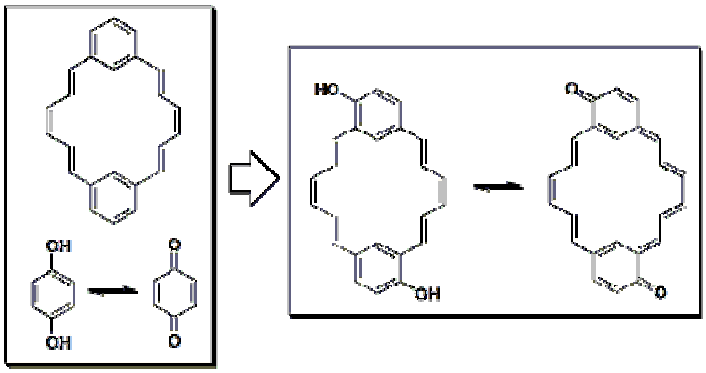
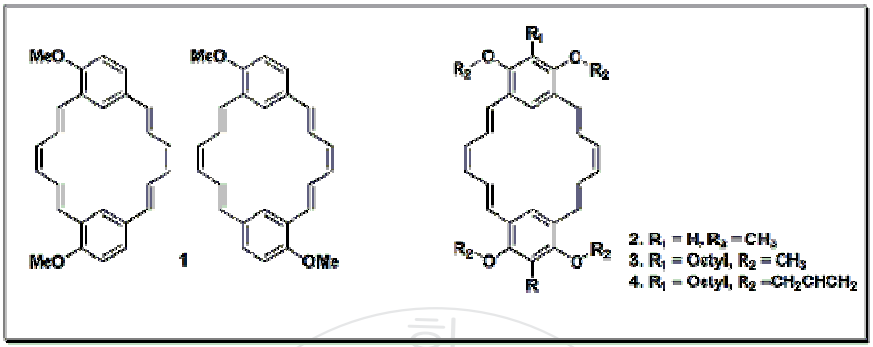
Synthesis of Conjugated Macrocycle: An Attempt to an Extended Diquinone SystemSoulgie Hong, Juhee Kim and Bongjin Moon*Department of Chemistry, Sogang University, Seoul 121-742, Koreabjmoon@sogang.ac.kr

홍슬기, 문봉진

서강대 화학과

Areno-condensed annulenes tend to have weak or no macrocyclic aromaticity due to electron localization on benzene fragments or cross-conjugation. In this study, we have tried to circumvent these problems by using the redox reaction between dihydroquinone and quinone. An extended dihydroquinone was applied in the areno-condensed annulenes. They were expected to show macrocyclic aromaticity after oxidation where they lose their local benzenoid form. We have first synthesized macrocycles 1 and 2. Demethylation and oxidation experiments were attempted. However, we were not able to observe the macrocyclic aromaticity of compound 1 and 2 due to their poor solubilities. In order to increase the solubility we also synthesized macrocycle 3 with octyl groups on both aromatic rings. Solubility of macrocycle 3 was enhanced enough and it could be fully characterized by conventional analytical techniques. However conjugation system was not stable under acidic condition. To circumvent this problem, allyl groups, which can be removed under mild condition with Pd catalyst, were introduced instead of methyl group.





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Reversible Colorimetric Changes of Nanoporous Conducting Polyaniline Particles with Metallic Ions.

차은혜, 송영호, 지기환

울산대 화학과

Among conducting polymers, polyaniline is known to exist in various oxidation states, such as emeraldine base (EB), leucoemeraldine base (LB), and pernigraniline base (PB). And polyaniline has been very attractive and interesting material due to its high conductivity, good redox reversibility and high stability even in an aqueous solution for its applications in electrochromic displays, electrocatalysis, rechargeable batteries, and various sensors. Thus, we have been interested in the reversible colorimetric changes of two structurally similar PANI systems, EB and LB, bearing amine or imine groups. Reversible colorimetric changes of PANI are finally identified with metallic ions, such as Ag^{+}, Cu^{2+}, and Cr^{3+}. The results will be discussed in detail in the poster session.

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Reversible Photochromic Switch Ensemble and Photoimaging Using the Spiropyran and Fluorescein molecules in Polymer Bound

송영호, 이영일, 류광선, 지기환

울산대 화학과

Photochromism of molecules has recently been the subject of much attention due to its potential applications in the development of optical waveguides, light modulators, logic gates, and optical storage media. The spiropyrans are defined as a group of light-switchable organic molecules. The photochromism of spiropyran (SP) involves interconversion among the three different states (a spiro form, a zwitter ionic form, and a cationic form). Fluorescein (FL) is also known as a fluorophore under basic condition and a proton source for proton transfer reactions. Thus, photochromic and photoimaging behaviors of a mixed SP-FL system in a liquid solution and in a PMMA polymer film have been studied and will be discussed in the post session. Intermolecular interactions such as ionic and hydrogen bonds seem to be a key factor for these phenomena.

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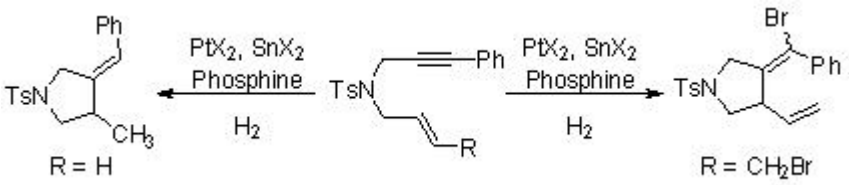
Pt(II)/SnX_2 (X = Cl, Br)-Catalyzed Cyclization: Completely Different Reactivity of the Pt Complex toward 1,6-Haloenynes and 1,6-Enynes

장민수, Wang Xi, 장우영, 장혜영

아주대 에너지시스템학부

Transition metal complex-catalyzed enyne cyclizations have recieved considerable attention due to the application to the synthetically and biologically important carbo- and heterocyclic building block synthesis.In the present study, using a Pt catalyst generated from PtX_2, SnX_2, phosphines, and H_2, the cyclizations of haloenynes and enynes without a halide substituent were investigated. Under the similar Pt catalyst conditions, the reaction routes were partitioned into the cycloisomerization of the haloenynes and the cycloreduction of the enynes without a halogen substituent. Through the optimization of the reaction conditions and control experiments, catalytic cycles to account for the bifurcation of the reaction mechanisms was identified.



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Rhodamine-Based Fluorescent Probes for the Detection of Gold Ions

이선호, 양영근, 태진성

연세대 화학과

Gold and its compounds are widely used in nanomaterial, biotechnology, electrical, pharmacil, and cosmetics industries etc. Application of gold nanoparticle production is broadly a part of biological systems as in the form of drug, gene delivery, biosensing, and bioimaging. Au^0 can be oxidized to Au^+ and Au^{3+} as a result of slow oxidation by H_2O_2 and oxygen in the biological environment. Although Au^0 is nontoxic, Au^{3+} ions are especially toxic because they bind very strongly to DNA and nervous systems, can also cause DNA, protein and peptide cleavage in the biological systems. Therefore, in addition to the convenient methods, simpler detection tools such as fluorogenic and chromogenic probes are in demands for the detection of Au^{3+} in various situations. However, despite widespread interest and recent advances in this area, there is no fluorescent probe for detection of Au^{3+} ions yet. Thus, it is imperative to develop the necessary analytical methods for detection and monitoring of gold ions in vitro and in vivo. We will present our recent results on selective fluorogenic probes for the detection of Au^{3+} ions in aqueous media.

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Fluorescent Chemosensor from Courmarin Derivatives for Lead Ion

이아름, 류병주, 남계춘

전남대 화학과

Sensors based on the ion-induced changes in fluorescence appear to be particularly attractive due to the simplicity and high detection limit of the fluorescence. Especially, coumarin-based fluorescent chemosensors have received increasing interest in recent years by virtue of their less toxicity and easy to be modified. Advantages of fluorescence-based chemosensors are high detection limit and simplicity. Coumarins generally show good spectral features such as large Stokes shifts and high quantum yields. We will synthesize coumarin-based sensor with crown ether site. Coumarin-based sensor can be used for the detection of lead ion. The sensing capability will be investigate with ^{1}H-NMR and fluorescence methods.

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Self-Assembling Rotaxane from Bipyridyl Salts and Crown Ethers

전남중, 여형민, 남계춘

전남대 화학과

The rotaxanes are an important class of interlocked compounds, and various synthetic methods have been developed. Among them, the template method has been widely utilized. Interactions such as metal-ligand bonds, hydrogen bonds, and ionic interactions and hydrophobic interactions have been extensively utilized for this synthetic method. These template-directed syntheses rely on the formation self-assemble in solution from functionalized bipyridyl salts thread and macrocyclic polyether rings. The rotaxane formation process investigated with ^{1}H-NMR and fluorescence methods.

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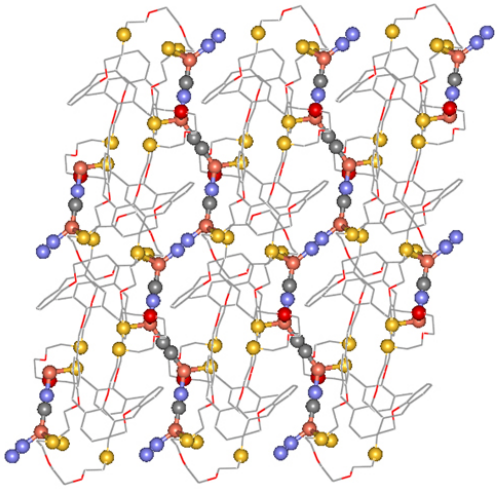
Calix[4]thiacrowns: 1D-3D and Endo/Exocyclic Complexations

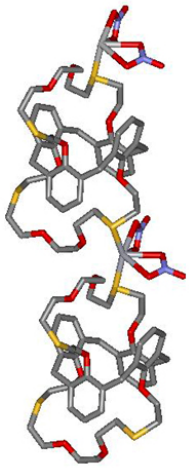
이재영, 심원보, 김다정, 구보람

건양대 나노바이오화학과

A series of calix[4]arene derivatives containing a thiacrown ring in the fixed 1,3-alternate conformation were designed and synthesized from calix[4]arene in moderate yield. Single crystal of the complex of the calixthiacrown with Ag(I), K(I), Cu(I) and Hg(II) ions were obtained and the solid state structure of the complex was determined by the X-ray crystallography.



2D-(**L**)CuCN



1D-(**L**)$HgNO_3$

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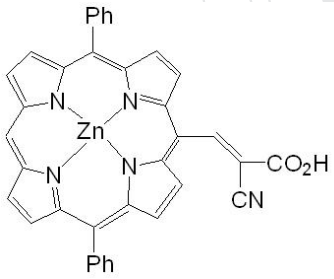
meso-conjugated Porphyrin Dyes for Dye-sensitized Solar Cell

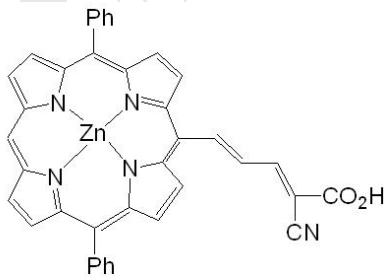
이상희, 김동희, 양병선, 유수창, *박형순

*군산대 화학과 *프로바이온 연구개발*

For development of dye-sensitized solar cell, porpyrin dyes 1 and 2 were synthesized. The *meso*-position of porphyrin was formylated using Vilsmeier reagent and the resulting aldehyde was condensed with cyanoacetic acid which is anchor group to TiO_2 in dye-sensitized solar cell. Photoelectric properties of 1 and 2 were compared with their *beta* conjugated porphyrin derivatives.



1



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Novel Indenofluorene alternating copolymers for Light-Emitting Diodes and Solar cell

V. Tamilavan, 현명호

부산대 화학과

A series of new indenofluorene - based copolymers, P1 (INTPT-1) and P2 (INTPT-2), have been synthesized and studied in PPVCs and PLEDs. The new polymers were characterized by thermal, structural, photophysical and electrochemical properties. The molecular weights (Mw) of the polymers were determined to be 5.66 x 104 g/mol and 2.13 x 104 g/mol, respectively. The PPVCs studies of these polymers show a reasonable open circuit voltage (Voc) of 0.75V and 0.70V with conversion efficiency (PCE) of 0.234% and 0.113%, respectively. The luminance property examination showed these are highly conjugated green emitting polymers; the effect of PEG addition in luminance layer was also studied. The best performance PLEDs have a very low turn on voltage 3 V and 4.5 V, the maximum brightness and luminance efficiency was 2103 cd/m2 at 10 V and 0.37 cd/A , 702.3 cd/m2 at 12 V and 0.16 cd/A, respectively.

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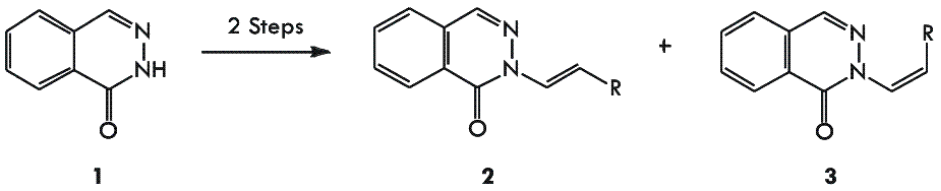
Synthesis of *N*-(arylvinyl)-1(2*H*)-phthalazinone

김보람, 이형근, 박송은, 김은정, 윤용진

경상대 화학과

The development of luminescent molecules is an active field of research in supramolecular chemistry. The chemosensors also have the advantages of possessing high sensitivity and selectivity, as well as providing on-line and real time analysis. However, the development of a useful fluorescent probes is difficult because of the lack of flexible design strategies. The design also is largely empirical at present. Thus, the tuning of the photophysical properties introducing the substituent is very useful in this field.Therefore, we desired organic molecules that contain 1-(2*H*)-phthalazinone moiety. In this poster, we synthesized diethyl (1-oxophthalazin-2(1*H*)-yl)methylphosphonate from 1-(2*H*)-phthalazinone. And then aldehyde derivatives and potassium tert-buthoxide with diethyl (1-oxophthalazin-2(1*H*)-yl)methylphosphonate reacted and synthesized *N*-Styrylazinones.



R= substitued-(C_6H_5), styryl, heterocycle etc.

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New Synthetic Method of Coumarin Derivatives

김선대, 이필호

강원대 화학과

Coumarin derivatives exist widely in nature, especially in plants and many of them show a wide range of biological activities. Also, they are used as anticoagulants, additives in food and cosmetics and in the preparation of insecticides, optical brighteners and dispersed fluorescent and laser dyes. These properties have made coumarins into interesting targets for organic chemists. Coumarin have been synthesized by several routes including Pechmann, Perkin, Knoevenagel, Reformatsky and Wittig reactions and by flash vacuum pyrolysis. The Pechmann reaction is the most widely used method, as the reaction involves the condensation of phenols and β-ketoesters in the presence of a variety of acidic condensing agents. The use of various reagents such as H2SO4, FeCl3, ZnCl2, AlCl3 and HCl are all well documented in the literature. In this poster, we report new synthetic strategy of coumarin derivatives.

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Synthesis of Naphthalene Derivatives with Platinum Catalyst

강동진, 이필호

강원대 화학과

The study of transition metal catalysts for the cyclization reactions is very important in organic synthesis. In particular, cyclometalation of dienes, enynes, diynes, allenenes, and allenynes have been demonstrated to be highly efficient for the synthesis of cyclic compounds. We developed an efficient synthetic method of naphthalene derivatives using platinum catalyst. Naphthalene is used in the synthesis of a precursor for various dye stuffs, pigments, rubber processing chemicals and other miscellaneous chemicals and pharmaceuticals.

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Efficient Synthesis of Multi-Substituted Pyrroles

엄다한, 이필호

강원대 화학과

Transition metal-catalyzed cross-coupling reaction is one of the most important ways to construction of carbon-heteroatom bond. Among these, formation of carbon-sulfur bond has received much attention since sulfur-containing compounds play important function in synthetic, biological, pharmaceutical, and material interest. With this regard, various transition metal catalysts (Cu, Pd, Ni, and Co) applied to carbon-sulfur bond forming reactions. In this poster, we reported efficient synthetic method of multi-substituted pyrrole derivatives containing sulfur.

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Copper Catalyzed Cyclization of 2-azetidinone Derivatives to Their Carbapenem Skeletons

박애리, 이필호

강원대 화학과

Carbapenem antibiotics are often the last resort in the treatment of infections caused by bacteria resistant to penicillins and cephalosporins. Although many carbapenems are natural products, they are produced by multistep total synthesis for medicinal use. Studies of carbapenem biosynthesis are of significant interest as they may enable the development of more efficient biochemical production methods. There are several notable reports on the construction of carbapenem skeletons with palladium, silver, and gold catalyzed intramolecular cyclization. We describe that treatment of 2-azetidinone derivatives with catalytic copper produced the bicyclic -lactam products, carbapenem skeletons, in good yields.

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Preparation of Bicyclic Compounds Using Intramolecular Cyclization Catalyzed by Platium

모준태, 이필호

강원대 화학과

During the studies on the addition of activated 2,3-allenoate to aryl substrates, we found an interesting intramolecular cyclization reaction. Development of an efficient cyclization method is very important for the biological and pharmaceutical applications, so we have prepared various 2,3-allenoates and their cyclization was achieved with platinum catalyst and silver triflate. Various type of 2,3-allenoates applied to the preparation of new bicyclic products with this catalytic system. These processes are not only efficiency but also many advantages such as direct synthesis of complex molecules under mild conditions and high atom economy. We will also study about application of this reaction. All of these results will be discussed in this poster.

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Synthesis of Furan Derivatives from Propargyl Acetate with Indium Tri(organothiolate)

신두섭, 이필호

강원대 화학과

Transition metal-catalyzed cross-coupling reaction is one of the most important ways to construction of carbon-heteroatom bond. Among these, formation of carbon-sulfur bond has received much attention since sulfur-containing compounds play important function in synthetic, biological, pharmaceutical, and material interest. With this regard, various transition metal catalysts (Cu, Pd, Ni, and Co) applied to carbon-sulfur bond forming reactions. In this poster, we report efficient synthetic method of furans having four substituents from the reaction of propargyl acetate with indium tri(organothiolate) in the presence of Pd-catalyst.

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Efficient Synthesis of Indolizine Derivatives

이광무, 이필호

강원대 화학과

Development of synthetic method of Indolizine, which exhibit intriguing molecular structures featured by an N-bridgehead bicyclic ring system, has received much attention in recent years. Many of the synthetic and natural indolizines have displayed important biological activities which can find a variety of applications in pharmaceutical use. They are also useful in the field of material science owing to their unique photophysical properties. Although a number of methods are available for the synthesis of indolizine, the development of general and efficient synthesis of functionalized indolizines is still highly attractive. In this poster, we describe an efficient synthetic method of indolizines from pyridine having electrophile moiety an 2-position and organoindium reagent.

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Synthesis and Properties of bis-Crown ethers containing Perylene and Naphthalene.

장승현, 류웅태

대구대 화학과

New two host bis-crown ethers containing perylene and naphtalene compounds. Fluorophore containing crown compound was synthesized from 2-(aminomethyl)-15-crown-5, 2-(aminomethyl)-18-crown-6 and 3,4,9,10-perylene tetracarboxylic dianhydride. The other fluorophore Crown ether was prepared 2-(aminomethyl)-15-crown-5, 2-(aminomethyl)-18-crown-6 and 1,4,5,8-naphthalene tetracarboxylic dianhydride. We will also present some of recent recognition results. Binding interaction of the new bis-crown ethers with metal cations was studied through absorption spectroscopy and emission spectroscopy.

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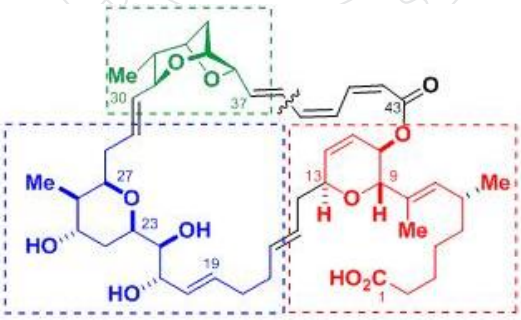
Synthetic Study on (+)-Sorangicin A: Construction of the C1-C15, C16-C29, and C30-C37 Fragments

이성로, 박수호, 이효원

충북대 화학과

Sorangicin A is a new type of macrolide polyether antibiotic isolated from the gliding bacterium Sorangium cellulosum. The dihydropyran ring of C1-C15 was constructed using RCM reaction. Fragment of C16-C29 was synthesized using key reactions such as the Evans aldol reaction and the Horner–Wadsworth–Emmons reaction. The C30-C37 fragment was prepared the Sharpless asymmetric epoxidation and the ring opening of epoxide under acidic condition. The details of our synthetic work will be disclosed.



(+)-Sorangicin A

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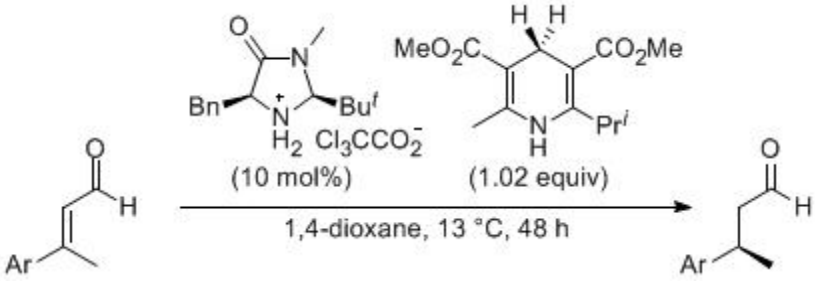
Metal-Free, Organocatalytic Asymmetric Transfer Hydrogenation of α,β-Unsaturated Aldehydes

양정운, *Maria T. Hechavarria Fonseca, *Nicola Vignola, *Benjamin List

*성균관대 에너지과학과 *Max-Planck-Institut für Kohlenforschung*

Metal-free based imidazolidinone salt as a chiral organocatalyst was used to promote biomimetic transfer hydrogenation of α,β-unsaturated aldehydes using Hantzsch ester as the hydrogen source. This transformation led to the formation of the corresponding saturated aldehydes in high yields as well as high chemoselectivities and enantioselectivities (90-96% ee).



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Direct, Site-specific Immobilization of natural sugar on Hydrazide coated glass slide

박성진

연세대 화학과

The understanding of glycan-protein interactions at the molecular level provides deep insight into glycan-mediated biological processes and enables the development of more effective therapeutic agents and diagnostic tools in the post-genomics era. Carbohydrate microarrays, which are composed of diverse glycans orderly and densely attached to a single chip substrate, have been extensively developed as reliable and efficient tools for the rapid analysis of carbohydrate-based biomolecular interactions.The most general method for construction of these microarrays involves site-specific and covalent immobilization of chemically modified carbohydrates to properly derivatized surfaces. This immobilization strategy requires the availability of modified glycans whose syntheses in many cases are time-consuming and difficult. In recent investigations directed at this goal, we have developed a novel, direct, site-specific technique for immobilization of unmodified carbohydrates, including simple carbohydrates, oligosaccharides and polysaccharides, on hydrazide-derivatized surfaces. This method eliminates the need for laborious and tedious glycan derivatization. To demonstrate the scope and applicability of this approach, carbohydrate microarrays containing a variety of glycans (fifty eight glycans) have been constructed by using one-step, direct attachment of free carbohydrates to a hydrazide-coated surface. These microarrays have been employed for analysis of sugar binding specifities of lectins, antibodies and bacterial cells. In addition, this microarray format has been applied to the determinination of binding affinities between proteins and glycans.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Pd-Catalyzed Allenyl Cross-Coupling Reactions Using Organoindium Reagent

이상규, 이필호

강원대 화학과

Since allenes are versatile building blocks both for organic synthesis and transition metal-promoted carbon-carbon bond-forming reactions, development of practical methods for their preparation is of great interest. Allene moieties can be prepared by alkylation of allenylmethyl halides with an appropriate carbanionic species, by SN2'-type selective displacement of propargyl alcohol derivatives with organocopper reagent, and by intramolecular regio- and stereoselective reduction of alkynes. The synthesis of allenes by metal-catalyzed cross-coupling reaction is an alternative method. In this poster, we describe new synthetic method of allenes using Pd-catalyst and organo-indium reagents through cross-coupling reaction.

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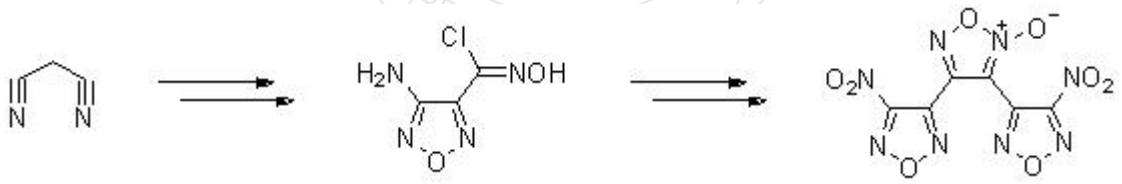
발표종류: 포스터, 발표일시: 금 10:30~12:30

Studies on the Synthesis and Characterization of 3,4-Bis(nitrofurazano)furoxan

김경호, 임충환, 정규현

인하대 화학과

The furoxan ring is a highly energetic heterocycle whose introduction into organic compounds is a known strategy for increasing crystal density and improving explosive performance. 3,4-Bis(nitrofurazano)-furoxan was recently synthesized and comparable with HMX as a novel energetic material. The compound was prepared from commercially available malononitrile by multistep process, including dimerization of nitrile oxides and oxidation. We will discuss its thermoanalytical data and some important reactions.



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Synthesis of Dihydrofyran Derivatives with Copper Catalyst

김상혁, 이필호

강원대 화학과

Dihydrofuran derivatives widely occur as important structural units in a variety of natural products that can be applied as pharmaceuticals and flavor and fragrance compounds. Because they are useful and versatile synthetic intermediates for heterocyclic compounds, the development of methodologies for the synthesis of dihydrofuran is of significant interest. To date various transition metal-, acid-, and base-catalyzed synthetic methods for dihydrofurans have been reported. Recently, we have developed efficient synthetic method of dihydrofuran derivatives using copper catalyst.

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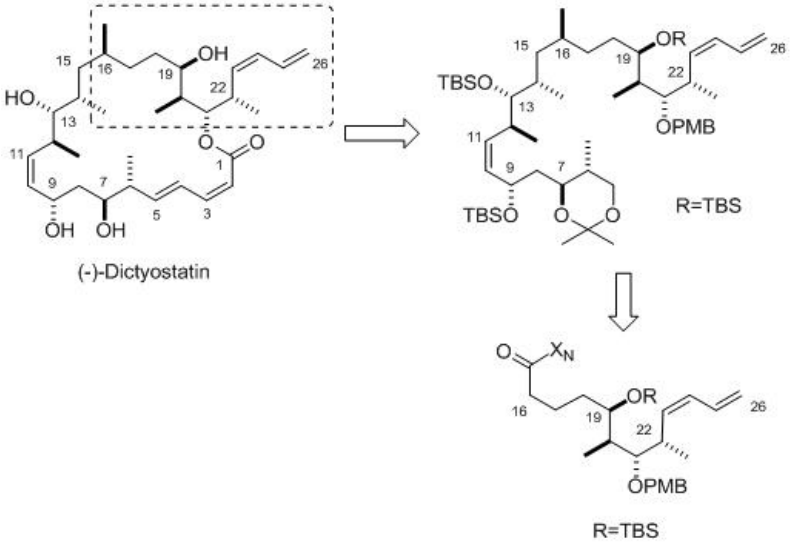
Synthesis of the Northern Part Comprising C16-C26 of (-)-Dictyostatin

우대구, 박수호, 이효원

충북대 화학과

The 22-membered macrolide (-)-dictyostatin was first isolated from the marine sponge Spongin sp. by Pettit in 1994 and is structurally related to discodermolide. Dictyostatin inhibits the growth of human cancer cells by stabilizing tubulins like taxol but it is active against taxol® resistant tumors. We achieved the asymmetric synthesis of C16-C26 fragment the northern part of (-)-dictyostatin. This structural unit was prepared using chemical manipulations such as ring-closing metathesis (RCM) employing the Grubbs' catalyst, a reaction upon lactol intermediate to introduce C22-C26 cis-diene unit, and the Evans aldol reaction for the syn product. The details will be disclosed.



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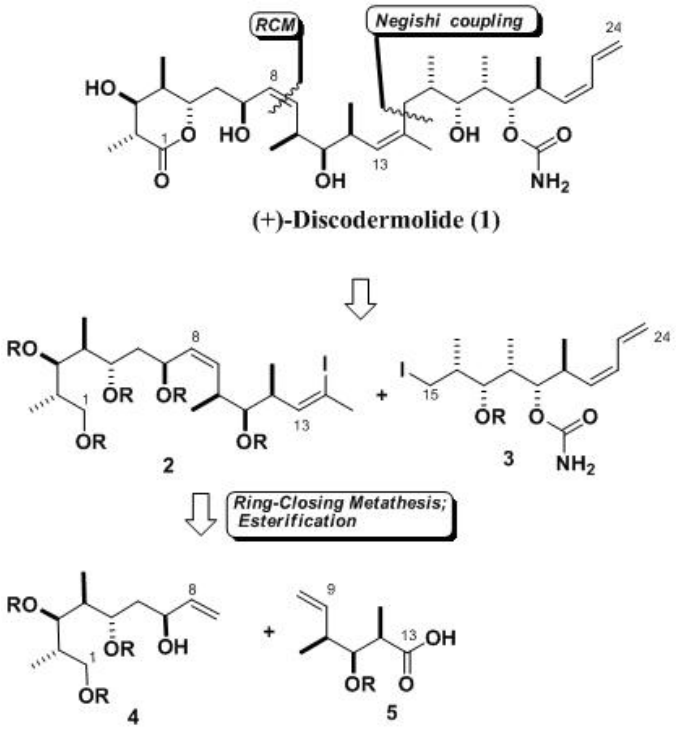
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of C1-C13 Fragment of Discodermolide

양준하, 박수호, 이효원

충북대 화학과

Discodermolide (1) is a linear 24-membered polyketide isolated from the Caribbean sponge Discodermia dissolute in 1990. It promotes tubulin assembly. The resulting stabilization of microtubules leads to apoptosis of cancer cells. This biological activity is known to be similar to that of paclitaxel (taxol) or epothilones. Herein, we report synthesis of key fragments of discodermolide by utilization of several key reactions such as ring-closing metathesis (RCM) for the preparation of (Z)-double bond (C8-C9), Cope elimination for the terminal (Z)-diene (C21-C24), and the Evans aldol reaction.



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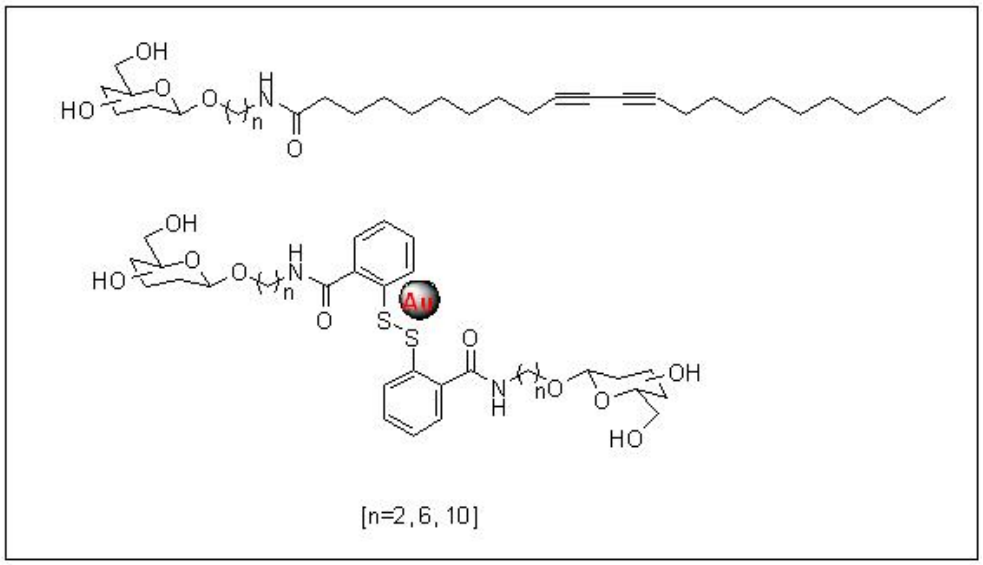
Functionalization of Anomeric Center in Carbohydrate Derivatives: Application to Bio-Sensor Technologies

최진선, 장은희, 안철진

창원대 화학과

Carbohydrates and functionalization of carbohydrates as a biosensor is important to recognize the specific cell surface. The role of carbohydrate is recognition of cell, and functionality of carbohydrate is sensing material. The length of carbon chain between carbohydrate and sensing functional group make flexibilty of these compounds. In this paper, we will describe the preparation method of connecting carbohydrate and sensing functional group(PCDA and GNP) with carbon tether.



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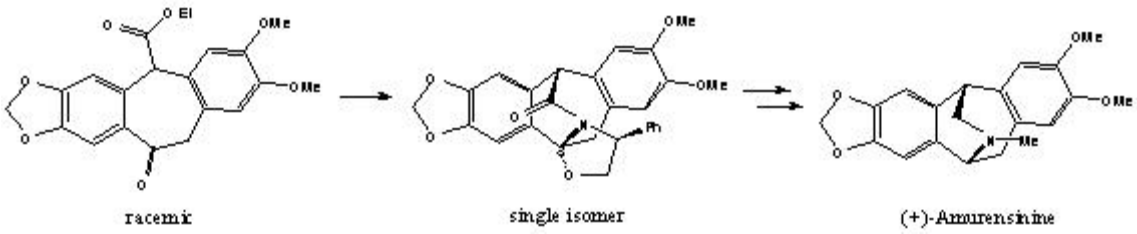
Asymmetric synthesis of (+)-amurensinine using chiral cyclic lactam

표성완, 김건철

충남대 화학과

(-)-Amurensinine belongs to a family of alkaloids, the isopavines, originally isolated from Papaveraceae plants. The isopavines display biological activity relevant to neurological disorders such as Parkinson's disease, Down's syndrome, Alzheimer's disease, amyotropic lateral sclerosis, and Huntington's chorea. Despite of the potential medicinal applications of the isopavines and their analogues, relatively few total syntheses of these natural products have been reported. A key feature of our synthesis of (+)-amurensinine is the simultaneous establishment of two contiguous stereogenic centers via the deracemization of an achiral keto-ester. We felt that condensation of racemic keto-ester with (S)-(+)-phenylglycinol would produce a pair of diasteremeric N-acyliminium ion intermediates. We speculated that if equilibration was a facile process, then intramolecular cyclization might proceed under thermodynamic control with selecivity for the desired tetracyclic lactam.References1. J. Am. Chem. Soc. 2008, 130, 137452. J. Org. Chem. 1996, 61, 58133. Angew. Chem. int. Ed. 2004, 43, 24364. J. Org. Chem. 1982, 47, 4808



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One-pot synthesis of indoles from 1-nitro-2-(2-nitroaryl)ethenes *via* indium-mediated reductive heterocyclization reaction

최재환, 김재호, 전영무, *이병민, 김병효

*광운대 화학과 *한국화학연구원 신화학연구단*

Indoles have been known as pharmacologically and biologically active compounds. Even though there are the many reports on indole ring synthesis, one-pot reduction-triggered heterocyclizations of 1-nitro-2-(2-nitroaryl)ethenes to indoles have not been reported yet, which will be a valuable method for various indole derivative synthesis. In addition, indium metal has recently drawn increasing attention owing to its unique properties such as low toxicity and stability in water and air compared with other transition metals. Thus, the synthesis of indole using indium and proper additives was attempted in this study. By applying the reaction condition such as indium/AcOH in benzene, 1-nitro-2-(2-nitroaryl)ethenes cyclized toward indoles by intramolecule reductive cyclization reactions. Herein, we report the indole derivative synthesis *via* indium-mediated intramolecular reductive heterocyclization reactions.

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Efficient Synthesis of Vinyl allene and Its Application to Carbocycles

최수빈, 이필호

강원대 화학과

Because allene is a very interesting compound having a hybrid character of C-C double and triple bond, vinyl allenes have been recognized as versatile building blocks in organic synthesis. In particular, vinyl allenes take part in not only the Diels-Alder reaction as the 1,3-diene moiety but also transition metal-catalyzed organic reactions, affording efficient synthetic methods for complex ring compounds. However, because it is not easy to effectively prepare a variety of vinyl allenes, its application to organic reactions has been limited despite the potential of vinyl allenes in organic synthesis. Although vinyl allenes were used in the Diels-Alder reactions, development of synthetic method of cyclic compounds having exo-methylene group is still required due to its utility in synthesis of natural products with biological activities. Recently, we have demonstrated that cyclic compounds having exo-methylene group were selectively produced through the Diels-Alder reaction of vinyl allene with various dienophile in good to excellent yields.

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N-(2-hydroxyaryl)benzamide synthesis *via* indium-mediated reductive migration of 2-nitroaryl benzoates

이혜정, 전영무, 김병효

광운대 화학과

Bioactive natural products contain amide moiety frequently and amide derivatives were reported to possess anticonvulsant, anticancer, and antiepileptic activities. Therefore, a number of methods have been reported for the synthesis of amide derivatives. Pure indium in metal form is considered non-toxic by most sources. Thus, it has been used as a utility synthetic tool. We examined various reactions *via* indium-mediated reductive reactions and reported the cyclizations, the ring opening of epoxides, and 1,4-addition reactions etc.. Recently, we found some interesting results when 2-nitroaryloxy benzoates were reacted in the reductive condition; i.e. in the presence of indium/AcOH, it was migrated into *N*-(2-hydroxyphenyl)benzamide derivatives in good yield. Herein, we report the novel one-pot synthesis of *N*-(2-hydroxyphenyl)benzamide synthesis using indium metal.

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Synthesis of various of Ir(III) complexes and study of photophysical and electrochemical properties

김연영

광운대 화학과

Electrogenerated chemiluminescence (ECL) is a well-known method for emitting the light and organometallic electrophosphoresent materials become important for ECL. Recently, iridium(III) complexes have been explored as ECL materials. In this report, we have studied ligand effect by introducing various base and auxiliary ligands to the iridium. For the detailed studies, various cyclometalated Ir(III) complexes were synthesized; 1) ionic Ir(III) complexes having cyclometalated (C^N) ligands including electrondonating methoxy group at different positions of phenyl moiety, such as $[Ir(C^N)_2(N^N)]PF_6$ ((C^N) = o-, m-, p-methoxyppy, (N^N)=4-4'-dimethyl-2-2'-dipyridyl (dmbpy), 1,10-phenanthroline (o-phen)), 2) non-ionic Ir(III) complexes having β-diketone moiety as an auxiliary ligand, such as $Ir(C^N)_2(acac)$ ((C^N) = o-, m-, p-methoxyppy, (acac) = DBM-OH). As a result, the synthesized Ir(III) complexes showed much stronger MLCT absorption at 380-430 nm and emission at 530-620 nm than $[Ru(o\text{-}phen)_3]^{2+}PF_6$. In particular, the ECL intensities of $[Ir(p\text{-}methoxyppy)_2(dmbpy)]^+PF_6$ and $[Ir(o\text{-}methoxyppy)_2(dmbpy)]^+PF_6$ were observed to be as high as 10- and 8-fold greater than that of $[Ru(o\text{-}phen)_3]^{2+}PF_6$.

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Synthesis and photophysical study of electrochemiluminescent ruthenium(II) and iridium(III) complexes containing bithiophene moiety

함선미, *강창훈, *이원용, 김병효

*광운대 화학과 *연세대 화학과*

In organometallic complexes, charged transition heavy metal complexes using ruthenium or iridium core are useful for application of light-emitting electrochemical cell (LEC) and organic light emitting device (OLED). Also electrochemiluminescence (ECL) based on transition metal complexes has been used as a sensitive detection method for analysis of a wide range of compound. Recently, as a continuous effort for the development of efficient ECL materials, new ionic iridium complexes, such as $[Ir(C^\wedge N)_2(N^\wedge N)]PF_6$ ($C^\wedge N$) = dfppy, ($N^\wedge N$) = 5,5-dibromo-2,2'-bipyridine, 5-(2,2'-bipyridine-5-yl)-2,2'-bithiophene, and 5-(5-bromo-2,2'-bipyridin-5'-yl)-2,2'-bithiophene), were synthesized and their photophysical and electrochemical properties were studied. Auxiliary ligands ($N^\wedge N$) having bithiophenyl group on bipyridine ring moiety were synthesized through Stille coupling. For a comparative study of electrochemiluminescent Ru(II) complexes, several Ru(II) complexes that are similar to Ir(III) complexes, such as $[Ru(bpy)_2L](PF_6)_2$ (L = 5-bromo-2,2'-bipyridine, 5,5-dibromo-2,2'-bipyridine, 5-(2,2'-bipyridine-5-yl)-2,2'-bithiophene, and 5-(5-bromo-2,2'-bipyridin-5'-yl)-2,2'-bithiophene), were synthesized. Herein, synthesis of ruthenium(II) and iridium(III) complexes and their photophysical and electrochemical studies will be discussed..

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Synthesis and application of iridium(III) complexes asymmetrically ligated with silyl or silylacetylenic bipyridyl ligands

강태경, 한해리, 김신한, 전영무, 김병효

광운대 화학과

Organic light emitting devices (OLEDs) prepared with heavy-metal complexes, such as iridium(III) or platinum(II) complexes, are suitable host materials with theoretical internal quantum efficiencies of 100%. It has been studied variously to disclose the characteristics of homoleptic iridium complexes and silicon-containing complexes. However, studies on the characteristics of heteroleptic iridium complexes that have ancillary ligands have not been well developed yet. Therefore, silyl or silylacetylenic group containing asymmetric bipyridine (bpy) ligands were designed and synthesized in this study expecting higher phosphorescence as well as their structural effects caused by the differences of the conjugated substituents. Ionic type iridium complexes $[Ir(III)(C^N)_2(L)]PF_6$6 (C^N ; dfppy = (2,4-difluorophenyl)pyridine, L = H, CCH, bpy-SiR_3, and bpy-CC-SiR_3) were synthesized and their physical properties were studied to develop the highly efficient devices.

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Total Synthesis of Narbomycin and Pikromycin

강한영, 오홍세

충북대 자연과학대학 화학과

We have been involved in the synthesis of the macrolide antibiotics which appear in the pikromycin biosynthesis. As results, we have successfully developed synthetic routes to prepare methymycin family of macrolide antibiotics. Total syntheses of methymycin, neomethymycin, and novamethymycin have been successfully achieved. The pikromycin family of macrolide antibiotics, however, has not been reported to be synthesized. We naturally have investigated the synthesis of narbomycin and pikromycin which have 14-membered macrolactones as aglycones. We have found that similar strategies and reactions have been successfully applied to the synthesis of pikronolide and narbonolide, although there have existed some differences in reactivity during the synthesis of the corresponding macrolides. Glycosylation of the corresponding sugar portion to the aglycones required some experimentation to achieve the total synthesis of pikromycin and narbomycin, which will be presented as the culmination of our effort to synthesize the polyketide marolide antibiotics from the pikromycin biosynthetic pathway.

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An Efficient One-Pot Synthesis of Diastereomerically Pure 1,4-Dideoxy-1,4-Imino-D-Arabinitol from a chiral aziridine

박동식, *최환근, *이원구, 심태보

*KIST 생체과학연구본부 *서강대 화학과*

1,4-Dideoxy-1,4-imino-D-arabinitol first isolated from the fruits of Angylocalyx boutiqueanus in 1985 turned out to possesses -glucosidase inhibitory activity. The -glucosidase inhibitors have proved to block carbohydrate metabolism and been successfully launched on the drug market for diabetes treatment. Moreover, it has also been reported -glucosidase inhibitors exhibit antitumor, antiviral and apoptosis-inducing activities. The broad spectrum of biological activity of -glucosidase inhibitors led us to be interested in synthesizing 1,4-dideoxy-1,4-imino-D-arabinitol, a -glucosidase inhibitor in highly efficient and stereoselective fashion. We would like to present a chiral aziridine could be readily transformed into 1,4-dideoxy-1,4-imino-D-arabinitol in one-pot and chirospecific manner via ring opening of chiral aziridine, followed by ring formation of five-membered imino sugar.

1,4-Dideoxy-1,4-Imino-D-Arabinitol, α-Glucosidase Inhibitor

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Synthesis of Natural and Unnatural Theopederin Derivatives

심진희, 안홍열, *김동수, *조영애, 함정엽

*KIST 천연물소재연구센터 *강릉대 화학과*

Theopederin and its derivatives such as Mycalamides, onnamides, isolated from marine sponge, have been reported to exhibit potent antiviral and antitumor properties due to their ability to arrest protein synthesis. The unique chemical structures of them have provided motivation for the development of synthetic strategies toward these marine natural products. As a part of an ongoing anti-cancer drug discovery program, we are developing a facile synthetic method for preparation of theopederin E and its derivatives which are substituted with various aryl moieties. Herein, we describe the synthetic method for the preparation of natural and unnatural theopederin derivatives.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Preparation of Azide containing Potassium Organotrifluoroborates

조영애, 김동수, *심진희, *안홍열, 경영수, *함정엽

*강릉대 화학과 *KIST 천연물소재연구센터*

Azide functional group 은 유기화학 및 의약화학 amine group 의 전구체로 이용되어왔다. 특히 이러한 azide 화합물과 terminal alkyne 에 의한 click reaction 화합물의 중요성이 대두되면서 다양한 organoazide 화합물을 손쉽게 얻을 수 있는 방법에 대한 필요성이 증가하고 있다. 최근 유기화학분야에서는 Suzuki-Miyaura cross-coupling reaction 에 potassium organotrifluoroborate 류가 coupling partner 로써 많이 사용되고 있다. 하지만 아직도 boron 과 azide 기가 같이 존재하는 화합물은 제조된바 없다. 따라서 본 연구진은 azide 기를 포함한 다양한 형태의 azidoaryltrifluoroborate 화합물을 제조하고, Suzuki-Miyaura cross-coupling reaction 을 통해 손쉽게 azidoaryl compound 를 합성하는 새로운 방법을 성공적으로 개발하였다.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Formation of poly(L-lysine) graft on the magnetic nanoparticles by surface-initiated ring opening polymerization

장혜미, 윤국로

한남대 화학과

Magnetic nanoparticles were used for developing target specific magnetic resonance imaging (MRI) contrasts agents and bioseparation applications. We demonstrated a simple method for surface modified nano-materials, where magnetic iron oxide nanoparticles were functionalize with poly(L-lysine) by Surface-Initiated Polymerization. Considering the material importance of nano- materials, the method described herein would be beneficial in many areas, such as devices and sensors. The resulting organic/inorganic hybrid magnetic nanoparticles were characterized by scanning electron microscopy (SEM), atomic force microscopy (AFM), Transmission electron microscopy (TEM), Dynamic light scattering (DLS), X-ray diffraction (XRD), Fourier transform infrared (FT-IR).

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Formation of hybrid Carbon Nanotube/Quantum dot (CdTe) composites by "grafting to" technique

한송이, 윤국로

한남대 화학과

The unique mechanical, optical, and electrical properties of carbon nanotubes (CNTs) make them very attractive building blocks for the fabrication of advanced materials with improved performance or even with new properties. Pristine multi-walled carbon nanotubes (P-MWNTs) were functionalized with 4-Aminobenzoic acid via ''direct'' Friedel-Crafts acylation in polyphosphoric acid (PPA)/phosphorous pentoxide (P2O5) condition. We have demonstrated the deposition of Quantum dot (CdTe) onto shorted multi-walled carbon nanotubes (MWNTs) by covalent bonds. The resulting hybrid CdTe/MWNT composites were characterized by SEM(scanning electron microscope), FT-IR spectroscopy, TGA(Thermogravimetric Analysis), OM(Optical Microscopy), TEM(Transmission electron microscopy), EDX(Energy Dispersive X-ray Spectroscopy).

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Formation of functionalized patterned polymer brushes by soft lithography

이동현, 윤국로

한남대 화학과

Polymeric thin films have attracted a great deal of attention because of their applications to biocompatible medical implants, sensors, and microfabrication. Among the methods for forming polymeric thin films, surface-initiated polymerization (SIP) has been a great success in grafting polymers onto solid substrates. SIP, in which a polymerization initiator is directly bound onto a surface and a polymer chain is grown from the surface, has been investigated to improve the stability of grafted polymers and to increase grafting density of polymers on substrate surfaces. The method consists of two simple steps: (1) formation of patterned self-assembled monolayers (SAMs) terminating by PDMS stamp and (2) SIP of MMA, initiated from the surface-bound hydroxyl group. The PEGMA films were further characterized by X-ray photoelectron spectroscopy (XPS), contact angle measurement, Scanning Electron Microscopy (SEM) and atomic force microscopy (AFM).

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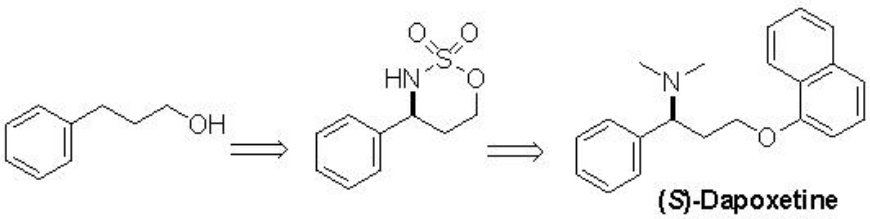
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Highly efficient and enantioselective synthesis of (S)-(+)-dapoxetine and (R)-(-)-dapoxetine from 3-phenyl-propanol

강소영, *이현규

*과학기술연합대학원대 의약 및 약품화학 *한국화학연구원 신약연구단*

Selective serotonin reuptake inhibitors (SSRIs) are a class of compounds typically used as antidepressants in the treatment of depression and anxiety disorders. Recently, it has been proposed that premature ejaculation (PE) might be associated with perturbation in serotonergic 5-hydroxytryptamine (5-HT) neurotransmission. (S)-(+)-Dapoxetine hydrochloride [1: (S)-(+)-N,N-dimethyl-[3-(naphthalen-1-yloxy)-1-phenyl-propyl]-amine] (Priligy®) is a potent SSRI with a short half-life developed specifically for the treatment of PE and was first launched in 2009 in Finland and Sweden for the oral on-demand treatment of PE in men. We report herein a highly efficient and enantioselective synthesis of (S)-(+)-dapoxetine and (R)-(-)-dapoxetine from easily available 3-phenyl-propanol through 6-membered ring sulfamate esters as key intermediates which were prepared from the Du Bois asymmetric C-H amination reaction of prochiral sulfamate catalyzed by chiral dirhodium(II) complexes.



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Unprecedented Reactivity of *N*-Heterocyclic Carbenes Toward2-Alkynylbenzaldehydes Leading to Novel Synthesis of Isochromene Dimers

윤소원, Sachin V Bhilare

부경대 화학과

The appealing properties of *N*-heterocyclic carbenes (NHCs) as ancillary ligands and nucleophilic reagents have attracted much attention in modern organic chemistry. However, their application as an catalyst is still in its infancy and growing rapidly. Transesterifications, nucleophilic substitution reactions, and umpolung reactions are examples in which NHCs can play an important role as an organocatalyst.In the present study we have uncovered an interesting reactivity profile of the *N*-heterocyclic carbenes and thus demonstrated a novel reaction that offers a simple and efficient route to the synthesis of isochromene dimer derivatives in high yields. It should be noted that a wide range of biologically active molecules contain isochromene moieties.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Calix[4]pyrrole bearing a chromogenic 1,3-indanedione at beta-pyrrolic position: synthesis and cyanide-selective ratiometric chemosensors

이창희, 홍성진, 김숙희

강원대 화학과

Calix[4]pyrrole-based, dual functional, chemodosimeteric sensor models were synthesized and studied as a cyanide selective ratiometric indicator. The receptor bearing dicyanovinyl group at beta-position exhibited fast color bleaching upon cyanide addition only. Complete bleaching was observed even in the co-presence of excess other anions. The binding affinities for a variety of other anions were calculated from the absorption changes produced in the presence of various anions and found to be similar to those of normal calix[4]pyrroles. The receptor bearing nitrovinyl group at beta pyrrolic position, on the other hand, showed slow color bleaching upon cyanide addition. The calixpyrrole-based anion binding sites present in the current system, combined with an electrophilic carbon site, are thought to reduce substantially the inhibitory effect other anions might be otherwise expected to play. Secondary, benzene-strapped calix[4]pyrroles bearing chromogenic, 1,3-indane-dione at beta-pyrrole positions have been synthesized and characterized. Since the enhanced anion affinity of the system has been well estabilshed, the receptors reported here would be ideal colorimetric sensor model. The chromogenic responses with various anions were studied using proton NMR, UV-vis spectroscopy and ITC measurement. The synthesized receptors displayed exceptionally high affinity toward fluoride and pyrrophosphate anion. Also, the system exhibited ratiometric response with cyanide anion. The systems reported here, possess anion-binding cavity as well as nucleophilic carbon site, which can be utilized depending on the analyte anions.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Expanded meso-alkylidene porphyrinoids: meso-Akylidenyl-(benzi)-pentaphyrins and their anion binding and protonation selectivity

이창희, 정승두, 김현진

강원대 화학과

meso-Alkylidenyl-(m-benzi)pentapphyrin (A) bearing two exocyclic double bonds at meso-position and meso-alkylidenyl-(p-benzi)pentapphyrin (B) bearing one exocyclic double bonds at meso-positions were synthesized and characterized. The one-pot condensation of meta-substituted, dipyrryl methyl benzene, pyrrole and pentafluorobenzaldehyde in acidic condition afforded corresponding porphyrin (A) in 4% yield. On the other hand, when para-substituted, dipyrryl methyl benzene, pyrrole and pentafluorobenzaldehyde were condensed under the same conditions, a tautomeric product bearing single exocyclic double bond at meso-position. Among the possible tautomeric forms, porphyirn (B) possesses single exocyclic double bond and one enol function. Protonation studies carried out with proton NMR spectroscopy, indicates that the protonation occurs at inner pyrrole nitrogen in both porphyrin (A) and (B). The anion binding studies carried out in organic solvent indicates that the compounds could be excellent chromogenic anion receptors for fluoride and cyanide anion.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Oligoether-strapped calix[4]pyrroles as novel ion-pair receptor and ion transport motif

이창희, 박인원

강원대 화학과

Calix[4]pyrroles bearing diametrically crossing polyether strap have been synthesized and fully characterized. The combined functions of anion binding properties of calix[4]pyrrole and cation binding properties of crown ether could be ideal models for size-dependent ion-pair recognition. The synthesized receptors contain both cation- and anion-recognition moiety and expected to bind with ion-pair. The synthesis is accomplished by condensation of polyether-linked bis-dipyrromethanes with acetone in the presence of acid catalyst. 1H NMR spectroscopic analyses confirm that the receptor forms a strong 1:1 complex with fluoride anion in acetonitrile solvent. The measured affinity constants for various anions are much smaller than those of other strapped calix[4]pyrroles. The fact that the bound fluoride anion to the host was easily decomplexed upon treatment with Na+ or Li+ cation, also support this conclusion. These findings indicate that the titled hosts have superior reversibility and thus could be applied in the fluoride anion transport.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Polymer-supported Precursors Via Click Linkage for Simple Purification of F-18 Labeled Compounds

이병세, *이상주, *이자영, **오승준, *지대윤

*(주)퓨처켐 표지화학연구소 *서강대 화학과 **서울아산병원 핵의학과*

we developed a new sulfonyl chloride reagent to attach precursor (naphthalene model compound) to styrene-based monomer via click reaction. Generally, it is not ease to make chemical bond between precursors and polymeric supports. Styrene-based monomers could be readily synthesized by using 3-azidopropanesulfonyl chloride and click reaction. Subsequently, radical polymerization of precursor monomers and divinylbenezene produced the corresponding precursor-containing polymers in excellent yield. After checking cold fluorination with polymer precursors, [^{18}F]fluorination was confirmed using 50 mg of polymer precursor in t-amyl alcohol at 120 ^{o}C. After 30 min, the reaction solution was filtered to remove polymer residue and washed with ethyl acetate. Although 20% of radioactivity remained on polymer residue, radio-TLC analysis of filtrate solution showed 85% [^{18}F]fluorination. More importantly, the HPLC-UV showed not only simpler mass pattern, but also very small amount (calculated by internal standard) of total mass compounds. With the successful result from naphthalene model compound, we applied this method to the synthesis of [^{18}F]BAY94-9172 and [^{18}F]FLT.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of novel perylenequinone derivatives through an efficient construction of its core from 1-indanones

김범태, *신영민, *송춘호, *김혜진, **김보승, *오광중, *황기준

*전북대 생리활성물질연구소,헬스케어기술개발사업 *전북대 화학과*
***전북대 생리활성소재과학과*

The multisubstituted naphthoquinones have attracted much attention because of their potential as key intermediates in the synthesis of the naturally occurring and biologically important perylenequinoid compounds such as hypocrellin B and chalphostins. In our program to develop novel bioactive perylenequinones, we have developed efficient synthetic route to construct 3-substituted-1,2-naphthoquinones by the ring expansion of 2-substituted-1-indanone-2-ethylcarboxylates with SmI2. Specifically, the required 1-indanone was prepared by modified Hoesch acylation in satisfied yield. Now, the intensive endeavor to dimerize some of 1,2-naphthoquinones for perylenequinone derivatives is under progress.

일시: 2009년 10월 28~30일(수~금) 3일간
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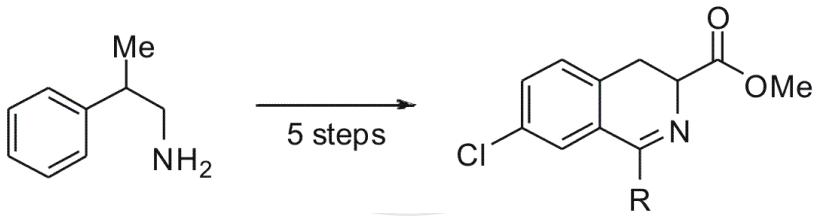
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of New Isoquinoline Derivatives

이형근, 김보람, 박송은, 김은정

경상대 화학과

The isoquinoline, which is key structural units in many natural products, drugs and chiral ligands are play an important role in organic chemistry, and supra molecular chemistry. For these reasons, the efficient synthesis of isoquinoline ring system continues to attract the interest of synthetic chemists. In order to evaluate the biological activity, we attempted to synthesize some new Isoquinoline Derivatives.



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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Kinetics and Mechanism of Solvolyses of Alkyl Fluoroformate Esters Under Solvolitic Conditions

성미혜, 최송희, 경진범

한양대 응용화학과

The specific rates of solvolysis of *tert*-butyl fluoroformate have been measured at 40.0°C in pure and binary solvents. These give a satisfactory correlation over the full range of solvents when the extended Grunwald-Winstein equation is applied. The sensitivities to changes in solvent nucleophilicity and solvent ionizing power, and a solvent deuterium isotope effet of MeOH/MeOD are very similar to those for solvolyses of ethyl chloroformate in aqueous fluoroalcohol solvents, consistent with an ionization pathway being rate-determining. For four representative solvents, studies were made at several temperatures and activation parameters determined. The results are also compared with those reported ealier for other alkyl fluoroformate esters.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and characterization of naphtopyrans containing novel photochromic compound

조우형

한남대 화학과

Photochromic compounds are widely used in information storage, holograms, optical filters and plastic lenses. Naphthopyrans are one of the most studied classes of photochromic compounds due to their use in plastic lenses. we report the synthesis and photochromic behavior of these novel compounds.In the study, The synthesis of new bis-5-hydroxy-7H-benzo[c] fluoren-7-one-1,1'-(4,4'- (phenylazanediyl) bis(4,1-phenylene)) bis (1-phenylprop -2-yn-1-ol) is described. The resulting polymers were characterized by 1H and 13C NMR spectroscopy, Fourier-transform infrared spectroscopy, thermogravimetric analysis, mass spectrum analysis and GC analysis.

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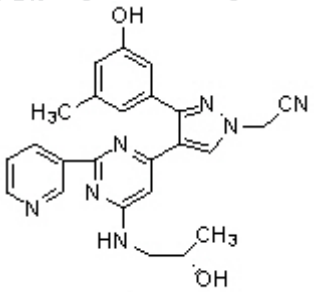
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Design, synthesis and biological evaluation of new potent and highly selective Ros1-tyrosine kinase inhibitor

박병선, *El-Deeb Ibrahim, **정수진, 이재열, **이소하

*경희대 화학과 *과학기술연합대학원대 생체분자과학 **KIST 바이오소재연구센터*

Ros1 protein is a receptor tyrosine kinase that has been reported mainly in meningiomas and astrocytomas, and until now, there is no selective inhibitor for this kinase. In this study, we illustrate for the synthesis of a highly potent selective inhibitor for ROS1 kinase. The synthesized compound 1 was tested initially at a single dose concentration of 10 μM over 45 different kinases. At this concentration, a 94% inhibition of the enzymatic activity of ROS1 kinase was observed, while the inhibition in activity was below 30% in all of the other kinases. 1,2-Pyrazole compound 1 showed an IC_{50} value of 199 nM for ROS1 kinase.



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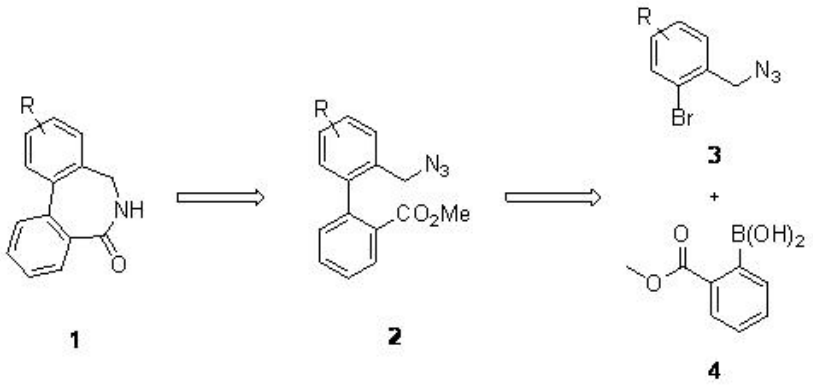
장소: 대전컨벤션센터
발표코드: **Ⅲ37P129포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 6,7-Dihydro-*5H*-dibenz[*c,e*]azepin-5-ones via Suzuki-Miyaura Coupling and Lactam Formation

고영형, 김건철, *김범태, *허정녕

*충남대 화학과 *한국화학연구원 신약연구단*

A concise and efficient strategy for the synthesis of 6,7-dihydro-*5H*-dibenz[*c,e*]azepin-5-ones 1 has been developed. The approach relies on a key transformation involving Suzuki-Miyaura coupling of 2-bromobenzyl azides 3 with 2-(methoxycarbonyl)phenylboronic acid (4), followed by either one-pot hydrogenation/base-mediated lactam formation or a stepwise sequence involving Staudinger reaction and lactam formation.



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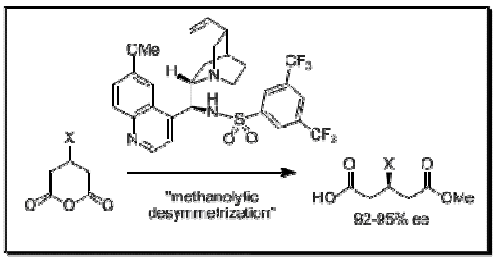
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

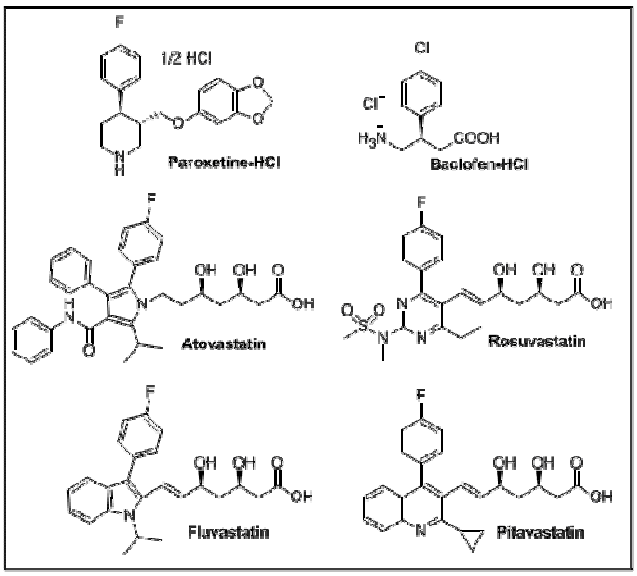
Highly Enantioselective, Self-Association Free, Sulfonamide-based Bifunctional Organocatalysts for Methanolytic Desymmetrization of meso-Glutaric Anhydrides

박상은, *남은혜, Surajit Some, 장형빈, 송충의

*성균관대 화학과 *성균관대 물리협동융합과정*

Alcoholytic desymmetrization of meso-glutaric anhydrides produce the corresponding chiral hemiesters 2 which are the essential building blocks for the synthesis of a numerous pharmaceutically important compounds. For examples, 3-aryl glutaric acid monoesters are key intermediates for the synthesis of Paroxetin•HCl, a selective serotonine receptor antagonist, and, Baclofen•HCl, a selective GABAB receptor agonist. 3-Hydroxyglutaric hemiester can also be used for the synthesis of HMG-CoA reductase inhibitors called “Statin” which have an inhibiting activity to suppressing the biosynthesis of cholesterol. We achieved unprecedentedly highly enantioselective methanolytic desymmetrization of meso-glutaric anhydrides using self-association free sulfonamide-based bifunctional organocatalysts. DFT computation shows detailed insight into the observed sense of enantioselectivity.





대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

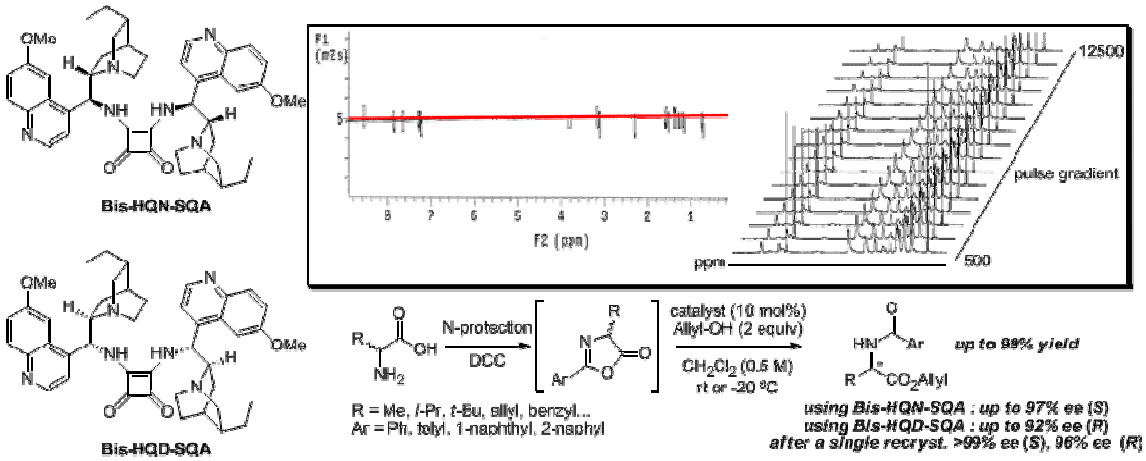
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅲ37P131포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Self-Association-Free, Bifunctional, Squaramide-based Dimeric Cinchona Alkaloid Organocatalysts for Dynamic Kinetic Resolution of Racemic Azlactones: Unprecedented Catalytic Activity, Enantioselectivity

오중석, 배한용, 송충의

성균관대 화학과

We developed self-association-free, bifunctional, squaramide-based dimeric cinchona alkaloid organocatalysts that showed unprecedented catalytic activity and the highest levels of enantioselectivity reported to date in the dynamic kinetic resolution (DKR) reaction of a broad range of racemic azlactones. Moreover, the robust nature of these catalysts toward chemicals allowed for a convenient "one-pot" process starting from the N-protected racemic -amino acids. Moreover, the poor solubility of the catalysts in organic solvents enabled their easy recovery after the reaction by a simple precipitation method, allowing their repeated recycling without any loss of turnover time or enantioselectivity. Experimental and DOSY NMR spectroscopic evidence showing that the dimeric alkaloid catalysts do not self-aggregate is also provided.



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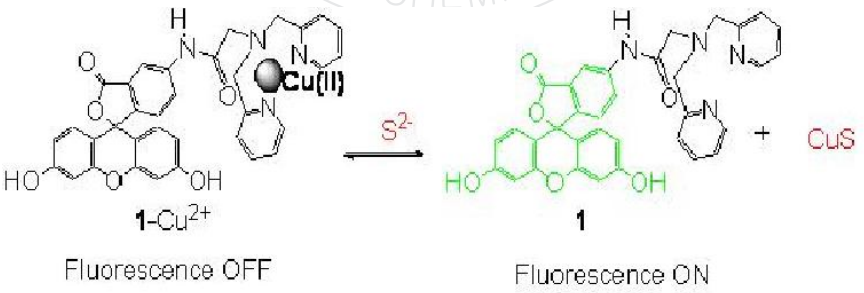
발표종류: 포스터, 발표일시: 금 10:30~12:30

Sulfide-selective Chemosensor Based on a Cu(II) Complex of Dipicolylamine Appended Fluorescein.

최명길, 차선영, 이해경, 전혜림, 장석규

중앙대 화학과

The detection of sulfide has gained significant importance as a consequence of the toxicity of hydrogen sulfide and the corresponding risks associated with exposure in a number of workplaces. We have prepared a new sulfide-selective chemosignaling system based on a Cu^{2+} complex of fluorescein fluorophore which is conjugated with a dipicolylamine (DPA) binding site. Fluorescein-DPA conjugate 1 exhibited a prominent on-off type fluorescence response toward Cu^{2+} ion in aqueous media. Compound 1 in the presence of Cu^{2+} ion (1-Cu^{2+}, quenched state) revealed a selective turn-on type signaling behavior in response to the sulfide ion with a detection limit of 800 nM in 100% aqueous media.



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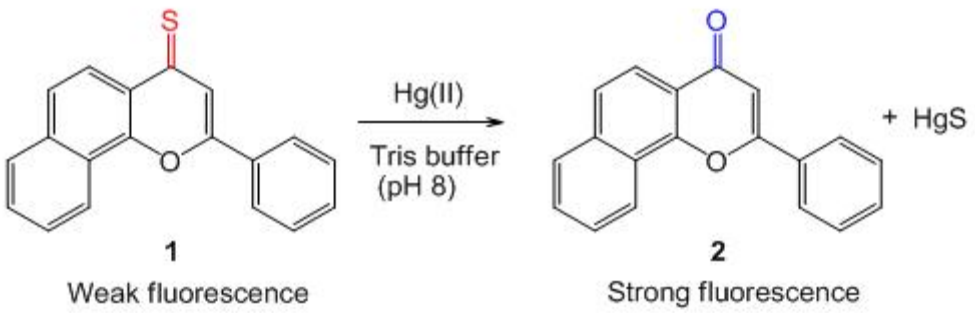
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Hg^{2+}-selective Fluorogenic Chemodosimeter Based on Naphthoflavone

남궁지은, 전혜림, 김윤환, 최명길, 장석규

중앙대 화학과

Conversion of thiocarbonyl compounds into their carbonyl analogues has attracted the interest of synthetic organic chemists. We have prepared a simple chemodosimeter system for selective Hg^{2+} signaling that is based on the Hg^{2+}-induced transformation of flavothione into its oxygen analogue flavone. α-Naphthoflavothione showed a sensitive, Hg^{2+}-selective off-on type signaling behavior in an aqueous environment. Upon interaction with various metal ions, the fluorescence intensity at 438 nm was markedly enhanced (45-fold) with Hg^{2+} ions, while other metal ions did not cause any noticeable responses. The proposed transformation was confirmed by 1H NMR, UV-vis absorption, and fluorescence measurements.



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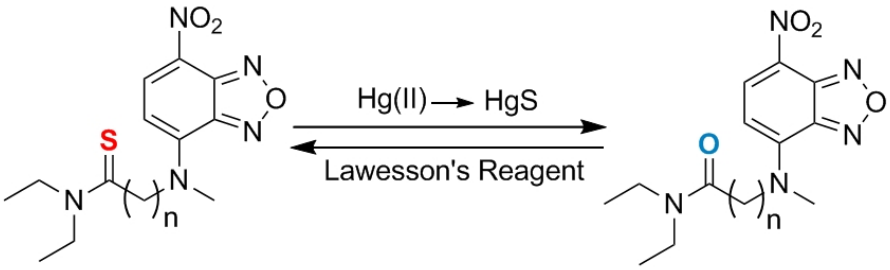
발표종류: 포스터, 발표일시: 금 10:30~12:30

Hg(II)-Selective Chemodosimetric Behavior shows Fluorescence Enhancement Based on NBD-Aminothioamdies Derivatives

노재현, 류대훈, 김희정, 어수영, 장석규

중앙대 화학과

We have prepared a series of simple NBD-Thioamide derivatives and investigated their transition metal selective chemodosimetric behaviors. Prepared compounds exhibited pronounced fluorescence turn-on type Hg^{2+}-selectivity by the Hg^{2+}-promoted desulfurization transformation from thioamide to amide in aqueous environment. Chemodosimeter having methylene spacer (n=1) was found to be relatively optimized and exhibited selective and sensitive signaling behaviors toward Hg^{2+} ions over other common interfering metal ions in aqueous media.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Platinum-Catalyzed Hydrogenative Cyclization of Yne-enones and Yne-aldehydes

Shinde Mahadev, 장혜영

아주대 에너지시스템학부

Pt complexes were used in the presence of phosphine ligands, $SnCl_2$, and H_2 for coupling reactions of alkynes with electrophiles under environmentally benign hydrogenation conditions, providing 5- and 6-membered cycloreduction products in moderate to good yield. Deuterium labeling studies suggested the occurrence of a catalytic cycle including the platinacyclic intermediate derived from the oxidative addition of a platinum complex to substrates possessing alkyne and carbonyl functional groups.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Organocatalytic Regioselective Allylic Substitutions of Morita-Baylis-Hillman Acetates: Synthesis of α-Methylene-β-Pyrrole Esters

권수현, 조창우

경북대 화학과

The Morita-Baylis-Hillman (MBH) reaction is one of the most efficient methods for the synthesis of α-methylene-β-hydroxy carbonyl compounds as versatile intermediates for pharmaceuticalsand biologically active natural products. Considerable efforts have been devoted to the development of MBH reactions and their application to the synthesis of biologically potent compounds. Recently, stoichiometric and organocatalytic variants of allylic substitutions of MBH acetates *via* an S_N2'-S_N2' tandem mechanism have come to light. Different types of nucleophiles such as $TsNH_2$, phthalimides (*N*-based nucleophiles), dialkyl malonates, 2-silyloxyfuran (*C*-based nucleophiles), and phenols (*O*-based nucleophiles) have been reported in the organocatalytic allylic substitutions of MBH acetates. However, to the best of our knowledge, there are no examples stating the use of pyrroles as *N*-based heterocyclic nucleophiles in the organocatalytic allylic substitutions of MBH acetates, even though pyrroles are important moieties in many natural products, pharmaceuticals, and materials. Here, the first examples of organocatalytic allylic substitutions using pyrroles as *N*-based heterocyclic nucleophiles for the synthesis of various α-methylene-β-pyrrole esters will be discussed.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Microwave-Assisted Aminolysis of Epoxides

이상길, Meng Lijuan, 안철진, 원태진, 신동수

창원대 화학과

3, 4-Dihydro-2H-l-benzopyran derivatives have been synthesized and demonstrated to possess potent relaxant activity on blood vessels, cardiac muscle, and other smooth muscles. They may find use in the treatment of a variety of diseases such as hypertension, asthma, ischemia, and urinary incontinence. Herein a novel series of 3, 4-dihydro-2H-1-benzopyran derivatives synthesized by alumina-catalysed aminolysis of epoxides with a variety of amines in butanol under microwave irradiation was firstly reported. This protocol is superior to the existing methods in light of its operational simplicity, short reaction time, simple purification procedure, excellent yields, low-cost catalyst and environmentally friendly conditions. The determination of biological activities of these compounds is underway.

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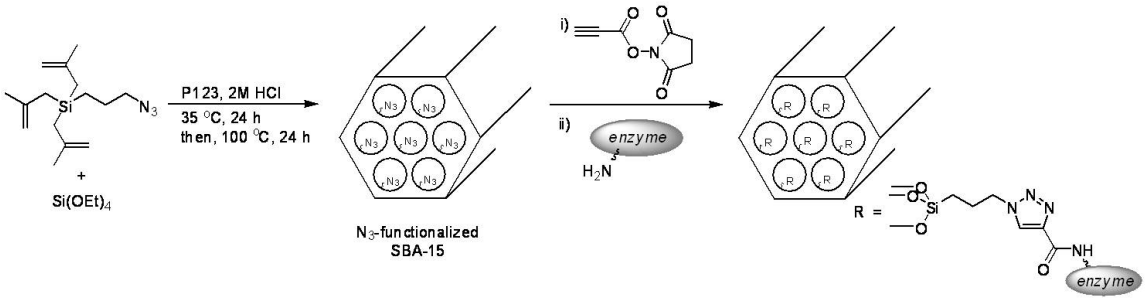
Efficient method for Immobilizing Enzyme by Co-condensation method of Methallylsilane derivatives

임수현, 전철호

연세대 화학과

There is currently considerable interest in mesoporous silicas for enzyme support. Immobilized enzyme inside the mesoporous materials can enhance the stability of the enzyme. However, it is likely to leach out from mesoporous support because the noncovalent interactions between mesoporous materials and enzyme are too weak. We develop covalent enzyme immobilization in mesoporous support by co-condensation method of methallylsilane derivatives. We synthesize azido group functionalized SBA-15 by co-condensation method and introduce N-hydroxysuccinimide ester (NHS) group through further transformation. NHS-ester group reacts with enzyme, and enzyme is covalently bonded onto surface of SBA-15.



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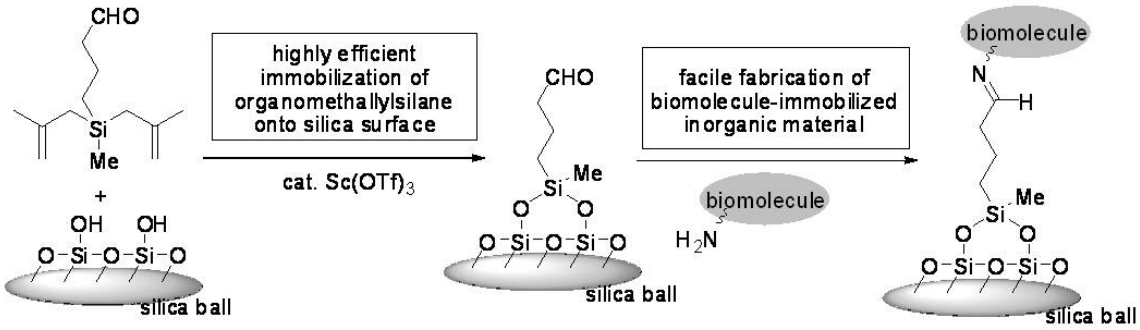
발표종류: 포스터, 발표일시: 금 10:30~12:30

Catalytic Grafting with Aldehyde group-functionalized Methallylsilane onto Silica Surfaceand Its Comparison with Traditional Grafting Method

김선아, 전철호

연세대 화학과

Immobilization of biomolecule has important advantages such as enhanced stability, repeated use, easy separation from reaction mixtures. For the highly efficient immobilization of biomolecules, the catalytic grafting method using aldehyde-functionalized methallylsilane was used because of mild reaction condition, high loading rate, and facile introduction of reactive functional group. Aldehyde-functionalized silica can be prepared easily from purely isolated aldehyde-functionalized methallylsilane through catalytic grafting with $Sc(OTf)_3$ catalyst. The resulting aldehyde-functionalized silica simply reacted with biomolecules to afford biomolecule-immobilized silica with high loading efficiency.



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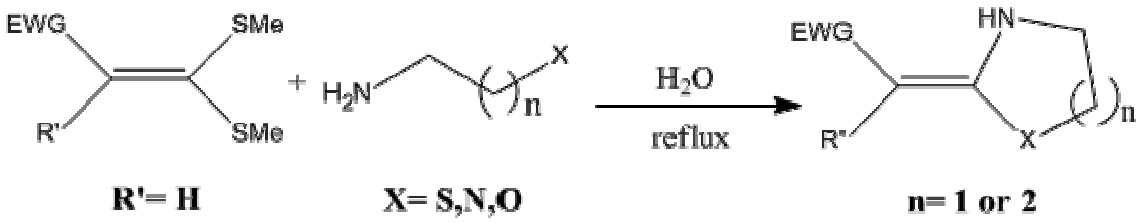
발표종류: 포스터, 발표일시: 금 10:30~12:30

Regioselective Synthesis of Heterocyclic Ketene N,N-, N,O- and N,S-Acetals in Aqueous Medium

천은정, 박지희, 정희정, 안진영, 장상훈, 이상경

경상대 화학과

Organic reactions in aqueous media have increasingly attracted the attention of synthetic chemists, because water is one of the most abundant, cheapest, non toxic and environmentally friendly solvent. Keeping in our mind this theme of green chemistry, we examined the potential for using alternative benign reaction media for the synthesis of heterocyclic ketene N,N-, N,O-, N,S-acetals. Ketene N,N- and N,S-acetals are versatile ambident synthetic intermediates, which combine the nucleophilicity of enamines and the electrophilicity of enones. The reactions of ketene dithioacetals with ethane-1,2-diamine, propane-1,3-diamine, 2-aminoethanol, 3-aminopropanol, 2-aminoethanethiol in ordinary water in the absence of any acid/base catalyst afforded the heterocyclic ketene N,N-, N,S-, N,O-acetals in good yields.



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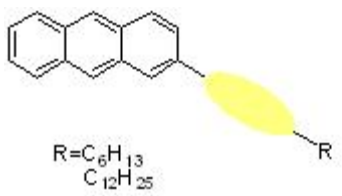
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of Solution-Processable Asymmetric Anthracene Derivatives for OTFTs

박지희, 정희정, 천은정, 장상훈, 안진영, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Recently, many organic conjugated materials have been developed for electronic devices. Organic field-effect transistors (OFETs) offer promise for use in applications such as low cost devices, smart cards, and the driving circuits for large-area electronic devices. But the OFETs have lower mobility and switching speeds compared to silicon semiconductors.In the recent, several strategies have been explored to improve the stability of organic semiconductors through the design of large band gap semiconductor materials, such as anthracene derivatives. Therefore we designed a series of asymmetric anthracene derivative. In this poster, we report synthesis and characterization of anthracene derivative with ethynyl group.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Properties of New Oligothiophene for OTFTs

정희정, 박지희, 천은정, 안진영, 장상훈, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Organic field-effect transistors(OFETs) have attracted much attention because of their potential applications to low-cost electronic devices and their integrated circuits. Conjugated oligomers are highly interesting for the fabrication of plastic electronic devices such as OFETs. In particular, oligothiophenes are good for such applications because of their excellent electronic properties, stability under ambient conditions, and ease of chemical modification. In this poster, we report synthesis and characterization of new oligothiophene for OTFTs.

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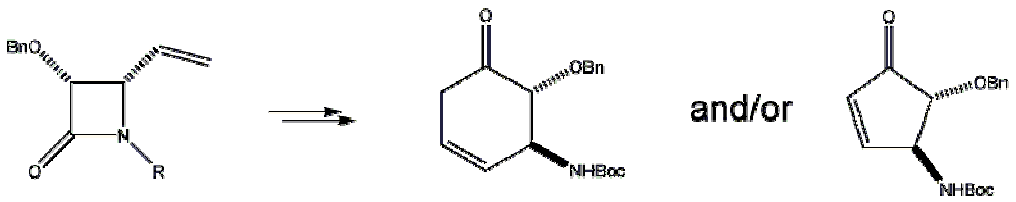
A Stereoselective synthesis of highly functionalized cyclohexenone and cyclopetenone as chiral intermediates for polyhydroxylated aminocyclitols from 2-azetidinone

한주애, *이현규

*과학기술연합대학원대 의약및 약품화학 *한국화학연구원 신약연구단*

The cyclic polyhydroxylated amines, also known as aminocyclitols, possess a wide variety of biological activities. These sugar-mimetic compounds have attracted much interest because they are not only considered as glycosidase inhibitors but also constitute a key segment of aminoglycoside antibiotics. As part of our ongoing investigations on the application of readily accessible 2-azetidinones as chiral synthon to other classes of molecules, we report herein a convenient and stereoselective synthesis of the unsaturated cyclohexanone and unsaturated cyclopentanone derivatives as valuable chiral intermediates for various polyhydroxylated aminocyclitols. By carbon ring rearrangement of 2-azetidinone with four-membered ring as a starting material could provide six or five-membered ring including variety chiral centers.



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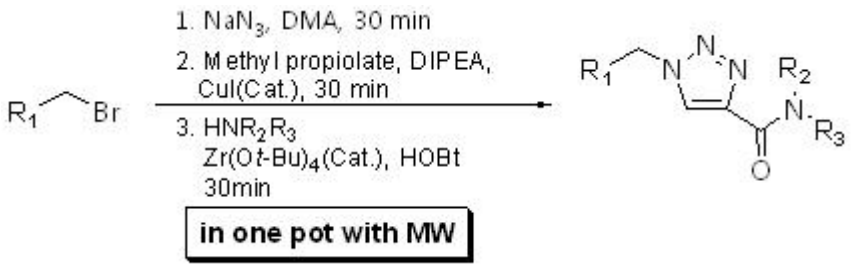
An Efficient Synthesis of C-carbamoyl-1,2,3-triazole from Alkyl bromide by One-pot Sequential Addition: Conversion Ester to Amide using Zr(Ot-Bu)4

권미현, 양동식, 장유진, 전홍배

광운대 화학과

The synthesis of biologically active 1,2,3-triazoles with an amide substituent have been achieved generally by 1,3-dipolar cycloaddition of organic azides to acetylenic amides. Herein we present the economic and efficient synthesis of C-carbamoyl-1,2,3-triazoles by sequential addition of NaN3, methyl propiolate, and amines to alkyl bromides in one-pot without any isolation of intermediates under microwave irradiation. The one-pot sequential reaction with microwave irradiation for short reaction time and the use of Zr(Ot-Bu)4 and HOBt as catalysts to 1,2,3-triazole ester, which is the intermediate after reaction with methyl propiolate, afforded the desired C-carbamoyl-1,2,3-triazoles in excellent yields.



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Efficient Synthesis of Diglycerol and Triglycerol

송정한, Meng Lijuan, 이상길, 신동수

창원대 화학과

Linear di- and triglycerols are known compounds that have previously been prepared either by direct syntheses involving bis(hydroxylation) of diallyl ether and 1,3-di-O-allylglycerol or by coupling of solketal with either its tosylate or with glycidyl solketal ether, furnishing either diglycerol or triglycerol after the removalof acetonide groups. We therefore focused our attention on the synthesis of diglycerol and triglycerol from readily available solketal and epichlorohydrin. Depending on the equivalent of epichlorohydrin, we prepared diglycerol and triglycerol sucessfully with phase transfer catalyst (PTC) in good yield. The corresponding polyglycerol esters were obtained to study the application of the polycerols.

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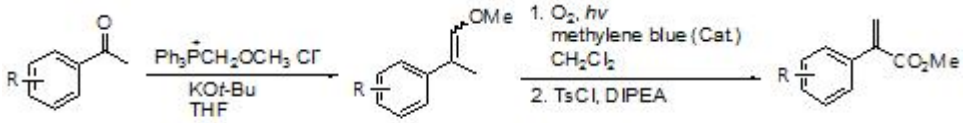
Synthesis of α-aryl-α,β unsaturated esters via singlet oxygen ene reaction

양동식, 박상준, 전홍배

광운대 화학과

α-Aryl α,β-unsaturated esters have been very important precusors in organic synthesis due to their high reactivities. We present herein the synthesis of α-aryl α,β-unsaturated esters from aryl methyl ketone via Wittig reaction and singlet oxygen ene reaction. The reaction of aryl methyl ketone with (methoxymethyl)triphenylphosphonium chloride gave the corresponding methyl enol ether as E and Z mixture in good yield. Treating of the methyl enol ether with singlet oxygen, which was generated from molecular oxygen and methylene blue under IR lamp, followed by tosyl chloride and diisopropylethylamine afforded α-aryl α,β-unsaturated ester in moderate yield.



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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of functionalized donor-fluorene-donor type organic dyes and their nonlinear absorption properties

이현명, 윤국로

한남대 화학과

There is still a growing interest in organic chromophores with large two-photon absorption (TPA) cross-section and high up conversion emission properties due to its potential for application in a wide range of areas such as frequency-up converted lasing, optical power limiting, 3-D optical data storage, 3-D lithographic micro-fabrication, and photondynamic therapy.We have synthesized novel donor-fluorene-donor type organic dyes which contain an alkyl fluorene unit bridging two fuctionalized donor groups. In order to enhance the two photon absorption efficiency it is important to increase the electron donating ability as well as the coplanarity of the molecule. Optical power limiting was measured to investigate the two-photon absorption efficiency of these dyes.

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Organocatalytic Asymmetric Intramolecular Allylic Substitutions of Morita-Baylis-Hillman Acetates: Synthesis of Chiral 2-(α-Methylene)-Pyrrolidines

배주연, 조창우

경북대 화학과

Recently, various organocatalytic allylic substitutions of Morita-Baylis-Hillman (MBH) acetates, *via* an S_N2'-S_N2' tandem mechanism, with different types of nucleophiles have been reported. However, to the best of our knowledge, there are no examples stating an intramolecular version of the organocatalytic allylic substitutions of MBH acetates, even though the intramolecular reactions provide versatile heterocyclic intermediates for pharmaceuticals and natural products. Here, the first examples of the intramolecular variant of the organocatalytic asymmetric allylic substitutions with MBH acetates containing protected amine moiety as a nucleophile in order to provide various chiral 2-(α-methylene)-pyrrolidine derivatives as important moieties of a large number of pharmaceuticals and biologically active natural products will be discussed.

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A Study on the Synthesis of Mollugin and Derivatives

최다혜, 전종갑

한림대 화학과

The natural product Mollugin was isolated from the rhizome of Galium mollugo (Rubiaceae). It has been shown to possess antitumor activity, antimutagenic activity and antiviral activity against the hepatitis B virus. Mollugin was prepared in 3 steps from 1,4-naphthoquinone, including oxidation using sodium hydrosulfite, methoxycarbonylation and phenylboronic acid mediated condensation. Mollugin derivatives also has been prepared by change the functional groups.

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Organocatalyzed α-oxyamination of aldehydes using anodic oxidation

xuanhuongho, 모선일, 장혜영

아주대 에너지시스템학부

Recently, electrochemistry has gained attention for complicated organic synthesis due to it's powerful and clean conditions. In the anodic oxidation process, the radicals are formed by electrochemical oxidation and generated for further chemical reactions. By using the anodic oxidation, stoichiometric amount of oxidants can be avoided, leading to green chemical processes. For developing green catalytic reactions using electrolysis, the anodic oxidation of enamine used for asymmetric bond forming reaction has been tried. In this research, the chiral amine catalyzed enantioselective coupling of aldehyde to TEMPO using electrochemical oxidation has been studied. The enamine formation from the sec-amine catalysts and aldehydes as an intermediate of the reaction was also verified via cyclic voltammetry (CV).

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Preparation of Several Benzo[b]furan Natural Products and Derivatives

황정운, 최다혜, 전종갑

한림대 화학과

An efficient and practical total synthesis of benzo[b]furan natural product XH-14, Egonol, Ailanthoidol is demonstrated. Introduction of iodine into the structure and optimization of the synthetic sequence were essential for the successful synthesis of benzo[b]furan natural products. Wittig reaction, Sonogashira coupling with iodobenzene, iodine induced cyclization, formylation, and Colvin rearrangement are critical in the high yield total synthesis of benzo[b]furan derivatives. New benzofuran derivatives including indole and benzo[b]thiophene derivatives were prepared not only to develop new class of biologically active substances but also to evaluate their antioxidant effects.

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Synthesis of Stilbene Derivatives and Comparison of their Antioxidant Effects

이현석, 전종갑

한림대 화학과

Stilbene 유도체는 발정(發情), 항(抗)말라리아, 제암(制癌) 등의 생리작용을 하는 것이 알려져 있다. 특히 폴리페놀 구조를 갖는 Stilbene 의 강력한 항산화효과를 통해 다양한 생리활성을 나타내는데 치환그룹의 종류, 위치 및 개수에 따라 효과적 특이성을 나타낸다. Stilbene 화합물들의 구조 활성관계를 조사 하기 위해 Stilbene 유도체를 Wittig-Horner reaction 반응을 통해 Piceatannol, Resveratrol 을 포함한 치환체의 위치에 따른 다양한 유도체들을 합성하였고, Piceatannol 화합물의 trans-olefin 작용기를 amide 또는 imine 작용기로 교체한 유도체 화합물들을 합성하였다. 이 유도체들을 DPPH, ABTS, 그리고 L-Tyrosine 과 L-Dopa 를 이용한 Tyrosinase Enzyme 기법을 통하여 각 유도체들의 항산화효과를 비교하였다.

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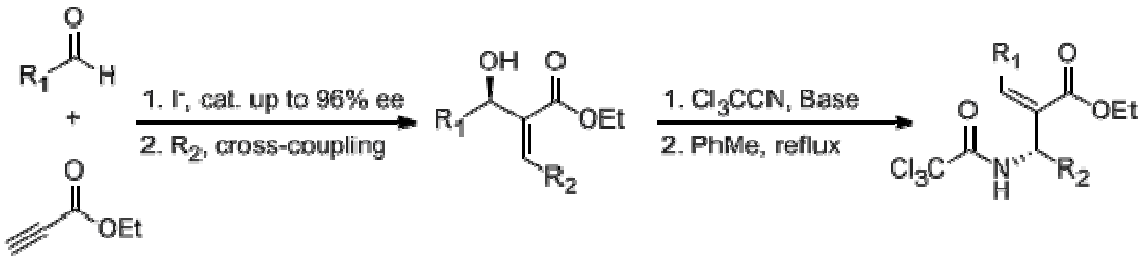
Facile Approach to Optically Pure α-alkylidene-β-amino esters by Thermal Overman Rearrangement

이성일, 류도현, 문순영

성균관대 화학과

Organic chemists always desired about artificial synthesis of unnatural amino acid long years ago. Especially, β-amino acid can be adopted to preparation of various natural products or drug candidates. For these reasons, methods for synthesis of β-amino acid was enormously reported by many organic chemists since several decades ago. There are few methods for synthesis of β-amino acids which has α-alkylidene substituted among these various methodologies. We found that α-alkylidene-β-amino esters can be synthesized from (Z)-β-Iodo Morita–Baylis–Hillman Esters without loss of chirality. We report herein facile method for preparation of optically pure α-alkylidene-β-amino esters by thermal Overman rearrangement.



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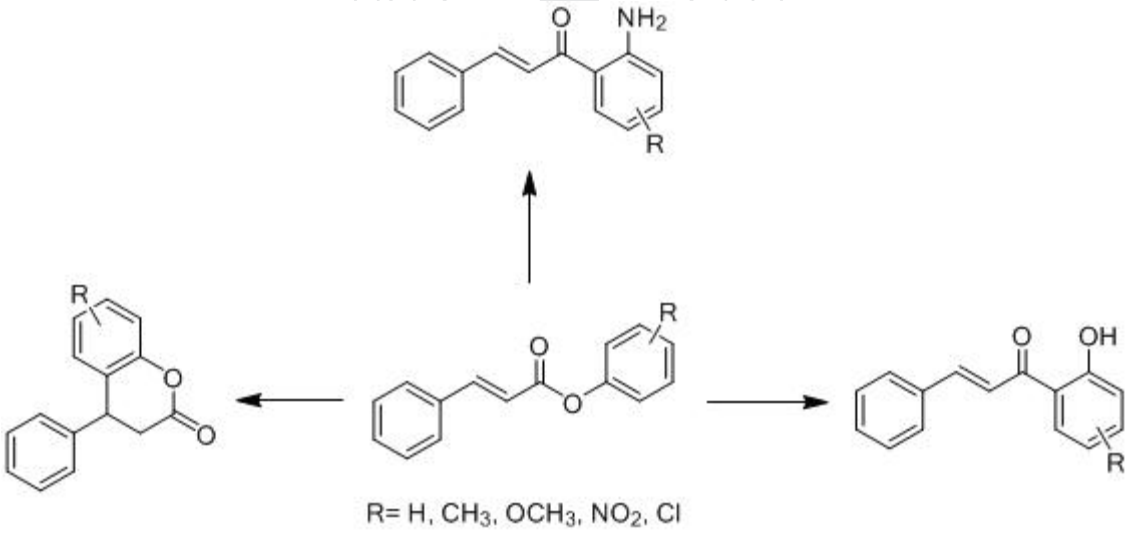
Study on the selective synthesis of dihydrocoumarins and chalcones from conjugated ester

양덕모, 전종갑

한림대 화학과

Coumarin has clinical medical value as the precursor for several anticoagulants, notably warfarin, and is used as a gain medium in some dye lasers. Chalcones show antibacterial, antifungal, antitumor and anti-inflammatory properties. Some chalcones demonstrated the ability to block voltage-dependent potassium channels. In this study, dihydrocoumarins and chalcones were selectively prepared by using cyclization or Fries rearrangement from conjugated ester respectively.



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Synthesis of Quinone Methide Derivatives and Comparison of their Antioxidant Effects

김미란, 전종갑

한림대 화학과

Flavonoid 계통의 화합물인 Chalcone 은 혈압강하, 혈당조절, 항염증 작용과 최근 주목받고있는 항산화효과등의 생리활성을 갖는다고 알려져 있다. Chalcone 화합물은 A ring 의 Catechol 구조와 B ring 의 Resosinol 구조를 갖는 화합물이 뛰어난 항산화 효과를 나타낸다. 이러한 구조적인 특징을 확인하기 위하여 치환기의 위치를 바꾸어 보았다. Base 조건과 Acid 조건에서 Aldol Condensation 으로 Chalcone 화합물을 합성하였고, 합성된 화합물을 Quinone Methide 형태로 oxidation 하여 Chalcone 화합물과 Quinone Methide 의 항산화력을 DPPH 와 ABTS 를 이용하여 radical scavenging 효과를 비교하였다.

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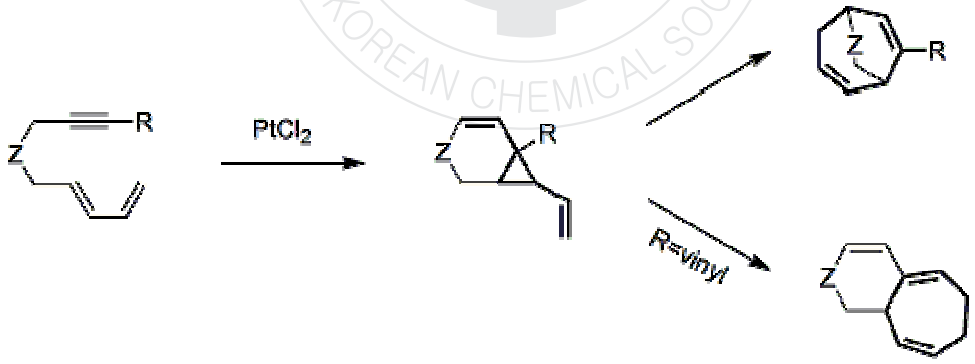
Sequential Platinum Dichloride-Catalyzed Cycloisomerization and Thermal Rearrangement of Dienynes

박유정, 정영근

서울대 화학부

A tandem PtCl2-catalyzed cycloisomerization and thermal rearrangement of dienyne provides bicycle[3.2.2]nonadienes, and 1,6,7,9a-tetrahydrocyclohepta[c]-pyrans and –pyridines in good to excellent yields. 7-vinylbicyclo[4.1.0]hept-4-ene bearing divinylcyclopropane is obtained as a product in the cycloisomerization of dienyne, and a subsequent thermal rearrangement of the divinylcyclopropane entity present in 7-vinylbicyclo[4.1.0] hept-4-ene lead to the isolation of seven-membered compounds.



Scheme 1. Sequential Pt^{II}-Catalyzed Cycloisomerization and Thermal Rearrangement of Dienynes.

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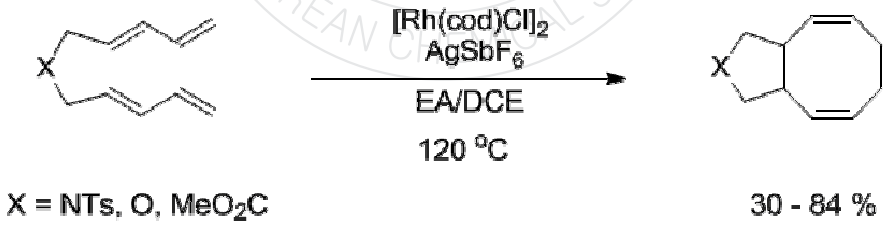
Rhodium-Catalyzed Intramolecular [4+4] Cycloaddition of Bisdienes to Eight-memberd Rings

홍미라, 정영근

서울대 화학부

The rhodium(I)-catalyzed cycloaddition has been developed. This is the first example of a rhodium-catalyzed intramolecular [4+4] cycloaddition of bis-dienes to eight-membered ring compounds. The reaction was highly sensitive to the counteranion, the reaction medium, and the reaction temperature. The best yields were obtained when the reaction was carried out in EA/DCE with the SbF_6^- anion. Various bisdienes, including nitrogen, carbon, oxygen tethered bis-dienes, were transformed into 1,5-cyclooctadienes in reasonable to high yields.



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Synthesis and characterization of Electrolytes Containing Ionic Liquid

유주영

명지대 화학

전도성 고분자 단량체인 Pyrrole 과 1-methyl imidazole 을 이용하여 이온성 액체인 1-[4-(N-Pyrrolyl)butyl]-3-methylimidazolium bromide(PyC4MIM+Br-)를 제조하였다. 또한, 다양한 기능성 도판트(DBSA, DEHSA 등) 용액내에서 이온성 액체인 PyC4MIM+Br-를 산화 중화시켜 이온성 액체 고분자 전해질을 제조하였다. 이온성 액체 고분자 전해질은 다양한 용매에 용해성을 갖을 뿐 아니라, 고분자화에 의한 내열성 및 전자와 이온 이동경로에 의한 우수한 전도도를 갖는 것을 확인할 수 있었다.

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Naked eye anion chemosensors based on 2-Amino-6-nitrobenzothiazole

강성옥, *김택현

*전남대 신화학소재공학부 *전남대 응용화학공학부,기능성나노신화학소재사업단*

Development of chemosensors for the recognition and detection of anions is gaining attention as an important research area in modern superamolecular chemistry. Colorimetric anion chemosensors based on 2-Amino-6-nitrobenzothiazole were synthesized. The addition of tetrabutylammonium salts of F-, OAc-, H2PO4- to the solution of this receptor caused dramatic color changes which was clearly observed by naked eye. The anion binding properties will investigate by different methods - UV-vis, NMR titration, ITC.

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A Fluorescence discrimination of γ-amino carboxylates with (*o*-carboxamido)trifluoroacetophenones and the other aminocarboxylates

전미은, 안교한

포항공과대 화학과

The molecular recognition and sensing of anions have attracted much research interest with multiple disciplines,1 because anions play significant roles in biological and chemical processes,2 and have implications in medicine, catalysis and environment.3 For the development of recognition and sensing probes for such anions, the insightful design of recognition motifs and corresponding fluorescence sensors has been pursued.Recently, we have demostrated a novel anion binding motif based on *o*-CATFA((*o*-carboxamido)trifluoroacetophenone) that recognizes anions particularly α-amino carbnoxylates. Its *o*-carboxamido group forms H-bonding with anionic adducts at ortho position to the trifluoroacetyl group. This H-bonding stabilization through intramolecular H-bonding, which seems to suppress otherwise possible quenching processes by anionic species as well as increases the conformational rigidity of the adducts, thereby resulting in the fluorescence enhancement.4 In this presentation, we wish to develop the previous fluorescence turn-on sensor through modification of anthracene fluorophore. This modificated Fluorescence sensor is expected to recognize the other type of amino carboxylates particularly GABA(γ-aminobutanoic acid) or other aminocarboxylates.

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Synthesis and characterization of ionic liquids with High thermal stability

조용우

명지대 화학과

Amine 계 cyclic compound, alkyl carboxylic acid 및 epoxy 구조를 이용하여 높은 열안정성을 갖는 Benzimidazole, glycidyl alkylimidazole 계 화합물을 합성하였다. 합성된 화합물에 다양한 alkylation 과 counter ion 을 사용하여 내열성과 이온전도성이 우수한 이온성 액체를 제조하였으며, 또한 polymerization 을 통해 낮은 휘발성과, 비가연성의 특성을 나타내는 고분자형 이온성 액체 화합물을 합성하였다. 합성된 이온성 액체는 1H-NMR, GC-MSD 등으로 확인할 수 있었고 TGA, UV-vis 등을 통해 우수한 전기적, 물리적 특성을 확인할 수 있었다.

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A Wide-range Optical pH Sensor Based on A Fluorescent 2-[2-Styrylpyridin-4(1H)-yildene]malononitrile Derivative

허준, *임현섭, *박새별, **김형진

*전남대 신화학소재공학과 *전남대 신화학소재공학과, 기능성나노신화학소재 사업단*
***전남대 응용화학공학부*

With the aim of preparing a new fluorescent sensor covering a broad pH sensing range, we designed a 2-[2-Styrylpyridin-4(1H)-ylidene]malononitrile derivative consisting of two different styryl groups, each possessing different protonation-deprotonation functionalities : -OH and –NR2. This organic dye displayed a strong fluorescence emission at 550 nm with excitation wavelength of 470 nm, and its emissive intensities increased in the direction of protonation within pH 3 – 11 ranges. Its synthesis, spectral properties and pH sensing properties will be presented.

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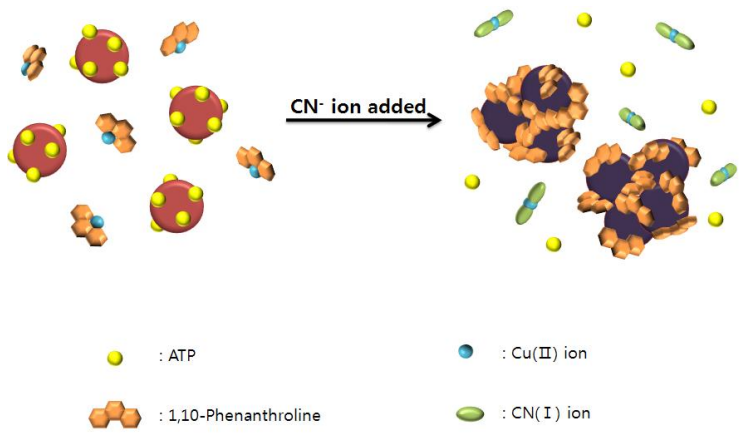
Colorimetric sensor for cyanide anions using ATP-stabilized gold nanoparticle and phenanthroline-Cu^{2+}

김미희, 장현혜, 이수정, 김수덕, 이나희, 한민수

중앙대 화학과

Cyanide is extremely toxic and even small amount of this species is lethal to humans. The Toxicity results from its bind to the cytochrom-c in mitochondria and prevents respiration. Nonetheliss, cyanide is produced in large quantities and used in various industrial processes, which induceds the contamination of environment. Therefore, routine detection of cyanide is central to the environmental monitoring of rivers and larger bodies of water and for evaluating the safety of foods. Many colorimetric sensor based upon AuNPs was reported. However, limited examples in these sensing systems were working in pure aqueous solution, and moreover, anion sensing ensemble based on AuNPs has not been developed. In this presentation, a new simple colorimetric sensing ensemble for selective and sensitive detecting cyanide anion in aqueous solution was prepared by combing ATP stabilized AuNPs, as reporter unit and penathroline-Cu^{2+} complex as receptor unit. A detail result of the ensemble will be presented.



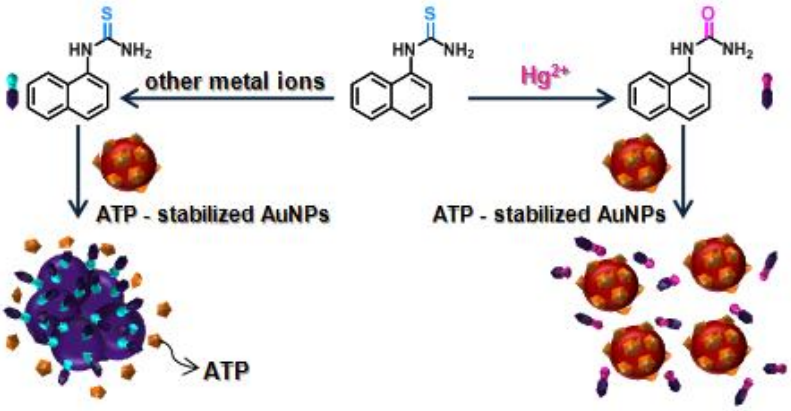
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅲ37P164포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Colorimetric sensing of mercury(Ⅱ) ion using ATP-stabilized Gold nanoparticles and thiourea compound.

이나희, 김미희, 장현혜, 이수정, 김수덕, 안상두, 한민수

중앙대 화학과

Au nanoparticles (AuNPs) are simply mixed with adenosine triphosphate. The AuNPs thus stabilized are stable over a wide range of buffer pH even in the presence of high concentrations of salt and protein. However, these stabilized AuNPs aggregate immediately when exposed to thiourea; this in turn results in a visible colour change in the AuNP solution from red to blue. However, in the presence with Hg^{2+} ions, the thiourea is easily converted to urea and the product (urea) can't induce a colour change of the AuNPs. With these properties of AuNPs and thiourea, we developed the colorimetric sensing method for Hg^{2+}. This method has high selectivity for Hg2+ over other cations and, moreover, detects less than 5 μM of Hg^{2+} with naked eyes.



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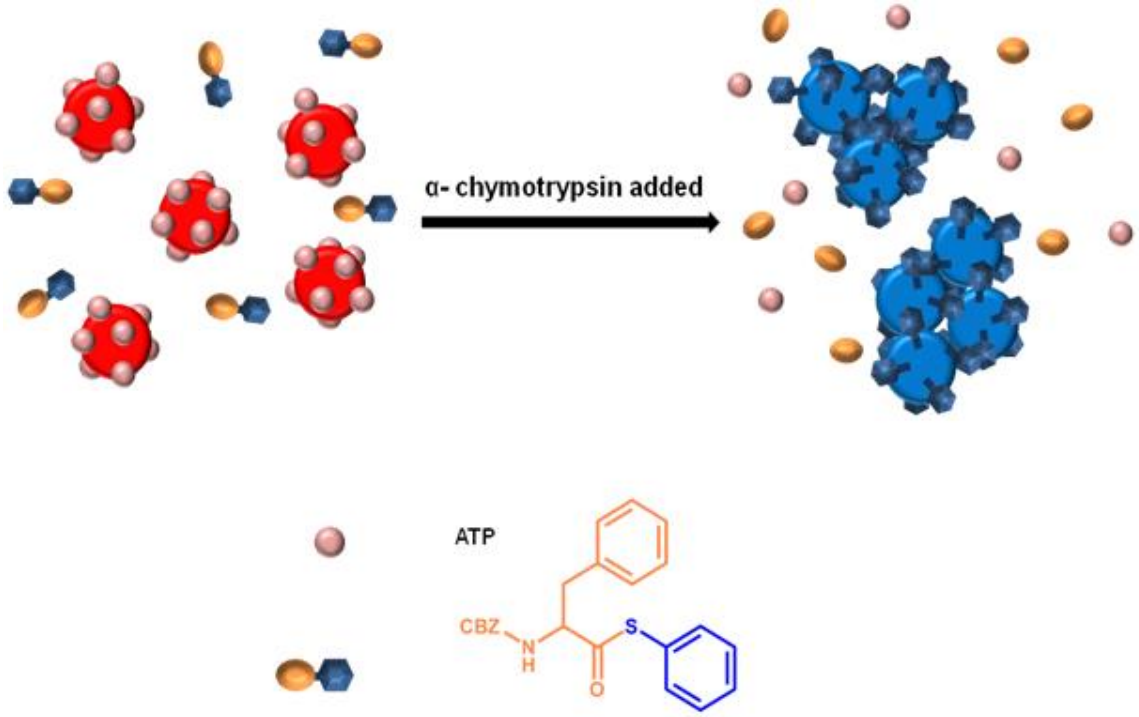
Real-Time Colorimetric Screening of Endopeptidase Inhibitors Using Unmodified Gold Nanoparticles

김미희, 장현혜, 이수정, 김수덕, 이나희, 한민수

중앙대 화학과

A new method for the real-time colorimetric assay method using ATP-stabilized unmodified gold nanoparticles (AuNPs) and thioester-bearing endopeptidase substrate enables real-time monitoring of the inhibition potencies of various endopeptidase inhibitors and activity of endoprotease. This assay can discriminate the inhibition activities of various protease inhibitors for endoprotease on the basis of the colour change of the assay solution.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Isomerism in bis-isothiouronium salt based on anthracene and application of this salt for anion sensing

정송이, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부,기능성나노신화학소재사업단*

The design and synthesis of anion receptors have gained much attention in molecular recognition chemistry since anions play significant roles in biology. Recently, the ability of thioureas to complex anions has been thoroughly exploited in the field of molecular sensors due to the binding anions through hydrogen bonding. The use of thiouronium groups has not been explored very much in the area of anion binding. Such groups would enhance the acidicity of the NH moieties and therefore can function as a better binder compared to the thiourea group. In this study, a novel fluorescent anion chemosensor based on bis-isothiouronium was synthesized. This sensor contained two isomers in equilibrium and showed significant fluorescence enhancement upon the addition of fluoride, acetate and dihydrogen phosphate anions.

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Synthesis of a novel Wang resin supported 2-amino-2-oxazoline chiral auxiliary for asymmetric alkylation reactions in the solid phase

N.P.B.Quynh, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부,기능성나노신화학소재사업단*

Polymer bound chiral auxiliaries, which enable the asymmetric synthesis of libraries of homochiral compounds, have received increasing interest within the last few years. Such solid supported chiral auxiliaries offer some advantages as compared to their application in the solution phase, including a simple 'filtration' procedure for the isolation of the desired compounds or the recovery of the expensive chiral auxiliaries, and their possible extension to a continuous flow system. In addition, the microenvironment of the polymeric backbone could lead to an improvement in the stereoselectivity for a given transformation. In this study, a novel Wang resin supported 2-amino-2-oxazoline chiral auxiliary was synthesized via 6 steps. Its efficiency in asymmetric alkylation reactions will be discussed

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Highly sensitive and selective near-infrared fluorescent Chemosensors for ions

정소영, *Chen Xiaoqiang, **신인재, ***윤주영

*이화여대 화학.나노과학과 *이화여대 나노과학부 **연세대 화학과 ***이화여대 화학과*

The fluorescence imaging method has revolutionized the process of quantifying trace ions within biological samples owing to their sensitivity, selectivity and ease of use. Many fluorescent probes imaging have been developed recently, some of which are well suited for biological applications.However, they still have several limitations when applied to detect ions in biological samples. First, most of them need to be excited by UV light, which can cause damage to living cells. Second, their fluorescence lies in the visible region, which cannot penetrate deep enough into human tissue. Compared to visible light, near-infrared (NIR) region at around 650–900 nm is less absorbed by biomolecules and exhibits the least autofluorescence background. Several NIR fluorescence probes have been developed and used in imaging in biological systems. So we report here the design, synthesis, and application of a novel NIR fluorescent probe, which is sensitive and selective for imaging specific ions.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Cu^{2+} and Fe^{3+} Selective Ratiometric and "Off-On" Sensor Based on the Rhodamone Derivative Bearing Pyrene and Nitrile Group

Wang Fang, Zhou Ying, *김영미, **김성진, **윤주영

*이화여대 화학.나노과학부 *이화여대 화학-나노과학과 **이화여대 화학과*

Rhodamine derivatives are nonfluorescent and colorless, whereas ring-opening of the corresponding spirolactam gives rise to strong fluorescence emission and a pink color. Recently, spirolactam(nonfluorescent) to ring opened amide (fluorescent) process was utilized for the detection of metal ions. A new rhodamine-pyrene derivative (PRC) synthesized as a ratiometric and "Off-On" sensor for the detection of copper ion in aqueous solution. PRC displayed a highly selective and ratiometric fluorescence change and a colorimetric change upon the addition of Cu^{2+}, in which the spirolactam (nonfluorescent) to ring opened amide (fluorescent) process was utilized. Furthermore, pyrene moiety served successfully as a source of ratiometric changes of PRC with Cu^{2+}.

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Au^{3+} Selective Fluorescent and Colorimetric Sensor

조민정, **Chen Xiaoqiang,** 김하나, *이상기, **김해조, ***윤주영

*이화여대 나노과학부 *이화여대 화학/나노과학과 **경기대 이과대학 화학과 ***이화여대 화학과*

Sensors based on the metal ion induced changes in fluorescence appear to be particularly attractive due to the simplicity and high detection limit of the fluorescence. In this regard, metal-selective fluorescent chemosensors serve as useful tools for detection of metal ions and thus have been widely exploited to detect biologically or environmentally relevant metal ions. Rhodamine derivatives are nonfluorescent and colorless, whereas ring-opening of the corresponding spirolactam gives rise to strong fluorescence emission and a pink color. Inspired by this strategy, spirolactam (nonfluorescent) to ring opened amide (fluorescent) process was utilized for the detection of metal ions. Herein, we introduced rhodamine derivative as a selective fluorescent and colorimetric sensor for Au^{3+}. Among the various metal ions, new rhodamine derivative displayed a highly selective fluorescent enhancement as well as colorimetric change upon the addition of Au^{3+}

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Pyrophosphate Selective Fluorescent Chemosensors Based on Coumarin-DPA-Cu(II) Complexes

김민정, *김영미, **김성진, **윤주영

*이화여대 화학.나노과학부 *이화여대 화학-나노과학과 **이화여대 화학과*

Pyrophosphate (PPi) is a biologically important target because it is the product of ATP hydrolysis under cellular conditions, and the detection of pyrophosphate is being investigated as a real-time DNA sequencing method. Recently, the detection of PPi has become an important issue in cancer research. Finally, patients with calcium pyrophosphate dehydrate (CPPD) crystals and chondrocalcinosis have also been shown to have a high synovial fluid PPi level. In this regard, sensing PPi has been the main focus of several studies over the last 10 years with particular attention being paid to fluorescent chemosensors for PPi. However, two important points should be considered for designing PPi sensors; sensing in aqueous solution and selectivity for PPi over related analogues, such as ATP, ADP, AMP and inorganic phosphate (Pi). Two new coumarin derivatives displayed highly selective “Off-On” fluorescence changes with pyrophosphate among various anions including ATP, ADP, AMP and inorganic phosphate in 100% aqueous solution.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

The detection of surfactants using conjugated polydiacetylene supramolecules

Chen Xiaoqiang, 조민정, *김민정, **윤주영

*이화여대 나노과학부 *이화여대 화학.나노과학부 **이화여대 화학과*

Surfactants have been reported as pollutants environmentally since they are heavily used as surface cleaning agents. Accordingly, it is necessary to develop convenient method for the detection of cationic or anionic surfactants. Polydiacetylenes (PDAs), a family of conjugated polymers, can display an apparent color shift from blue to red and fluorescence enhancement upon environmental stimulation. In this report, we report firstly cationic or anionic surfactants selective PDA sensors, which can display fluorescent enhancement as well as colorimetric change in the presence of cationic and anionic surfactants, respectively. Owing to the structural differences, the hydroxybenzaldehyde (HBA)-containing two DA monomers are expected to adopt different headgroup interactions (intramolecular hydrogen bondings or intermolecular hydrogen bondings) when they are transformed to PDA molecules. The assays results show the colorimetrically and fluorometrically changes come from the disruption of the intermolecular-type hydrogen bondings rather than intramolecular hydrogen bondings with the addition of cationic surfactants, in which both ammonium group and long alkyl chain play necessary roles.

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A Serial of Boron Complexes: Novel Emission and Electron-Transporting Materials in OLED

Zhou Ying, 김민정, *윤주영

*이화여대 화학.나노과학부 *이화여대 화학과*

During the development of novel organic semiconductor materials, more and more consideration has been given to boron-containing organic compounds due to their excellent electron-accepting abilities and good chemical stabilities. In present paper, the synthesis and property studies of a serial of novel Boron-complexes showed that these well-designed Boron complexes exhibited strong solid state photoluminescence, advantageous thermal stability and electrochemical properties, which enabled these compounds as efficient emitters as well as suitable electron-transport materials. The OLED devices with these compounds worked in EML (emission layer) or in ETL (electron-transporting layer) proved the boron-containing complexes are newly arisen type of organic emitters and semiconductors.

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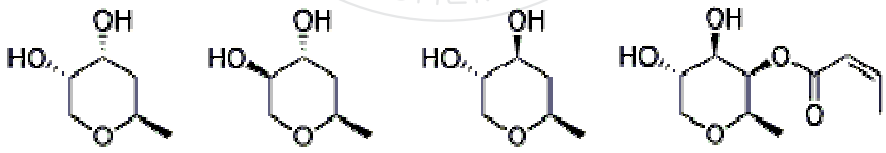
Synthesis of Ophiocerins from Non-carbohydrate Sources

강한영, 홍희정, 이동민

충북대 화학과

Ophiocerins are a series of natural products isolated from the cultures of fresh water fungi and have an interesting array of stereochemical centers along the tetrahydropyran core. We have been interested in the synthesis of ophiocerins and consequently, we have reported ophiocerins based on the carbohydrates as starting materials. Although these carbohydrate-based approaches were successful, it occured to us that a more efficient synthesis of ophiocerins would be achieved with starting materials that are not carbohydrates. Because developing more efficient synthetic routes for the tetrhydropyrans with diverse sterocenters is of value, we have been involved in searching for simpler and more direct synthetic routes for ophiocerins. Our efforts and results for the synthesis of ophiocerins will be presented.



Ophiocerin A (1) Ophiocerin B (2) Ophiocerin C (3) Ophiocerin D (4)

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Synthesis and Characterization of Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylene vinylene-co-Oxadiazole Poly(*p*-phenylenevinylene) Copolymer compared with Homopolymer

장희현, 이수민, 윤국로

한남대 화학과

Poly(*p*-phenylenevinylene)s (PPVs) have received a great deal of interest due to their unique physical properties such as conductivity, electroluminescence, and solubility of selected derivatives, which allows for facile processing in the manufacture of microelectronic devices. Polymer-based conjugated materials offer the advantage of being directly processible from solution, permitting deposition through spin and blade coating under atmospheric conditions.We attempted synthesis of stable polymers possessing oxadiazole, alkylfluorene and phenylenevinylene linkage in the main chain and investigated its properties. The resulting MEH-co-Oxadiazole PPV copolymer was characterized by infrared spectroscopy, scanning electron microscopy, atomic force microscopy, and transmission electron microscopy, photoluminescence spectra(PL) and compared with the homopolymer.

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Fluorescence "Turn-on" Sensing of Amino Carboxylates by Anthracene-bis(CATFA) Systems

류도욱, 안교한

포항공과대 화학과

Fluorescence sensing of anions has attracted continuing interest given that a variety of anion molecules are involved in chemical and biological systems. A number of fluorescence anion sensors have been developed based on different disciplines in the sensor design. However, the development of fluorescence turn–on type sensing systems for anions of biological importance remains as a challenging issue, because in many cases fluorescence quenching rather than enhancement results.Recently, we have demonstrated that introduction of a H-bonding donor such as carboxamide or sulfonamide group at ortho position to the trifluoroacetyl group stabilizes the anionic adducts and thus enhances the association constant toward anions such as carboxylates to a useful level. This H-bonding stabilization approach enabled us to introduce novel fluorescent, colorimetric, and electrochemical probes for cyanide, carboxylates, and dicarboxylates.Herein, we wish to disclose some of our recent results obtained from the recognition and sensing of amino carboxylates.

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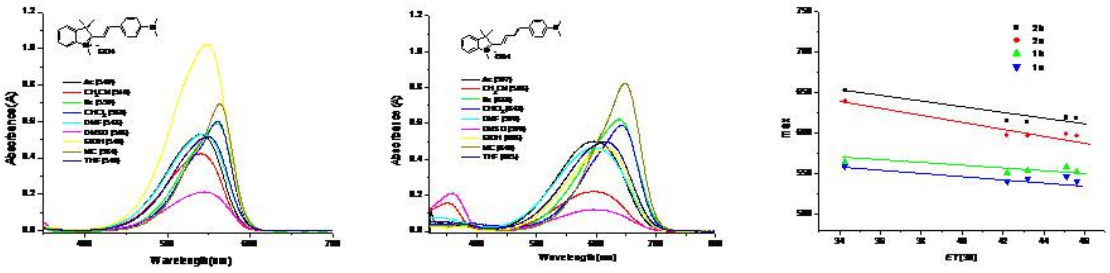
Solvatochromic Study of Hemicyanine Dyes; 1,3,3-Trimethyl-2-styrylindolium perchlorates and Its Analogous

노세정, 금삼록

고려대 소재화학과

Hemicyanine dyes, 1,3,3-trimethyl-2-styrylindolium perchlorate 1a-1b and more extended analogous 2a-2b were synthesized from the reaction of substituted benzaldehyde or cinnamaldehyde with 1,2,3,3-tetramethylindolium perchlorate. These cyanine dyes showed a pair of absorption bands in UV-Vis region: a shorter around 300-350nm and a longer band in the region of 550-650nm. The longer absorption band of those dyes showed a remarkable hypsochromic shift as the solvent polarity increased. Namely, UV-Vis spectral behaviors of the prepared cyanine dyes showed a remarkable negative solvatochromism in the whole region of solvent polarity examined. Excellent linear relationships were observed between λmax and the solvent polarity parameter, ET(30) for the all cyanine dyes examined.



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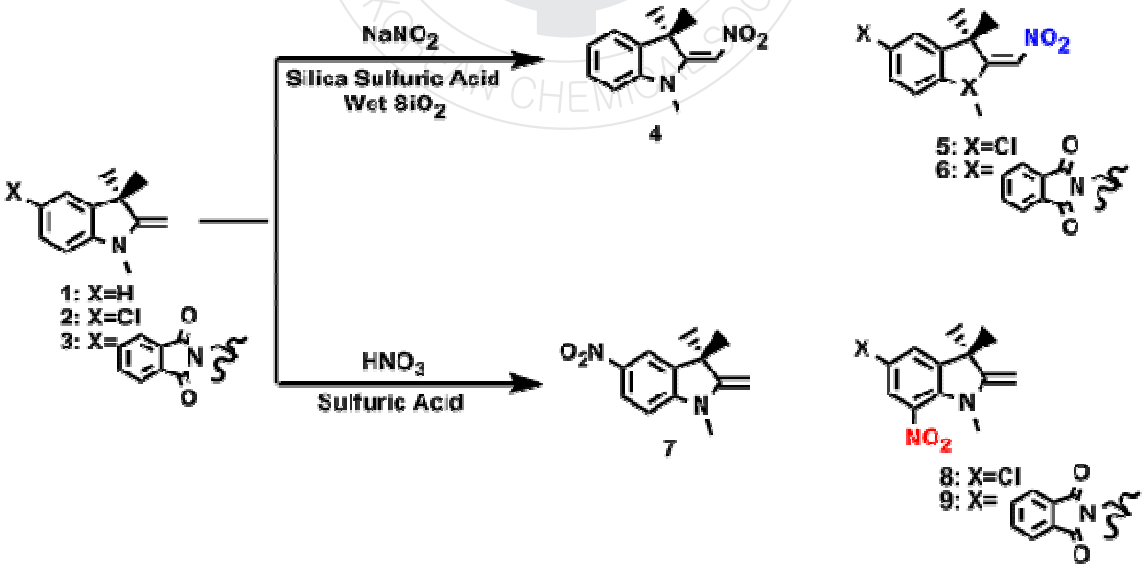
Regioselective Nitration of Fischer Base Derivatives with Silica Sulfuric Acid/Sodium Nitrite in the Presence of Wet SiO_2

마소영, *금삼록

*고려대 소재화학과 *고려대 소재화학과*

From the reaction of Fischer base derivatives with silica sulfuric acid, $NaNO_2$ and wet SiO_2 at room temperature, 2'-nitro Fischer base derivatives were obtained as a sole product, whereas with the conventional nitrating reagent, a mixed solution of HNO_3/H_2SO_4, 5-nitro Fischer base derivatives were obtained. The geometry of the products has been determined by means of DIFNOE experiments. The prepared molecules 4-9 were characterized by ^{1}H and IR spectroscopy.



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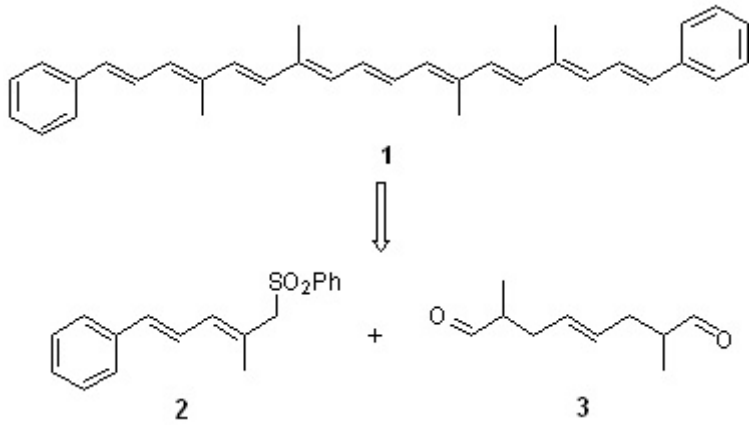
Convenient Synthesis of Allylic sulfone unit for the unnatural Carotenoids

임보람, *구상호

*명지대 나노공학과 *명지대 화학과*

The unnatural carotenoids 1 have polyene chains with aromatic substituents to provide extra stability. The unnatural carotenoids can be efficiently synthesized through systematic construction of two part; allylic sulfone 2 containing various substituents and dialdehyde unit 3. For the construction of allylic sulfone, the homoallylic alcohol can be prepared by the Indium-mediated addition of haloallylic sulfone to aldehyde. The reaction provides high stereoselectivity as well as an absolute regioselectivity. The selectivity is originated from the substituents; A Me group to *anti* selectivity and a Ph group to *syn* selectivity. By the oxonia-cope rearrangement to homoallylic alcohol, the allylic sulfone containing conjugated polyenes can be efficiency constructed applied to the stereoselective formation,



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Free Radical Cyclization of Isoprenoid Chain Molecules

LIZHILONG, *구상호

*명지대 나노공학과 *명지대 화학과*

It is utmost important to develop biochemical and chemical methods of synthesizing cyclic structuresdue to their prevalence in the biologically important natural products. The controlled cyclization strategy can be diversely applied to the syntheses of cyclic natural products. We progressed the research to efficiently control the mode of cascade cyclization of isoprenoid chain molecules, which can be used in the synthesis of various natural products. The research used radical cyclization condition to control the mode of cyclization of isoprenoid chain molecules. This method utilizes oxidative free radical cyclization of β-keto ester with Mn(OAc)3•2H2O to form the bicyclic products. β-Keto esters can be used for Mn(III)-based oxidative cyclizations at room temperature or slightly above.We found a novel cyclization reaction, in which oxygen radical was involved to give a bicyclic compound in a highly stereoselective manner. The mechanism was proposed based on the isolated reaction intermediates with different substrates under various reaction conditions.We expect that the new radical cyclization can be more efficiently used in the synthesis of various kinds of natural products.

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Synthetic Route of Various Carotenoid as the Nano Wire

맹주완, *구상호

*명지대 나노공학과 *명지대 화학과*

The carotenoids are an important class of organic molecules with delocalized π-electrons. A typical carotene molecular wire consists of a polyene backbone of alternating single–double bonds terminated by phenyl rings at the end. We have successfully demonstrated the efficient syntheses of natural carotenoids, which can be extended to the synthesis of unnatural carotenoid wires. The unnatural carotenoids can be disconnected into two parts for the systematic construction: the allylic sulfone containing aromatic substituents and dialdehyde. These two subunits can be assembled for the synthesis of unnatural carotenoids by the process of the following reactions: coupling, protection of the resulting alcohols, and the double elimination reactions. The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would provide an extra stability and excellent electronic characteristics compared with those of the natural carotenoids.

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Synthesis and morphology of Self-assembled Retinyl Ethers

박선영

명지대 나노공학과

Retinol is valuable nutrient for cell growth and differentiation. Some of its ether derivatives show prophylaxis effect on diverse cancers. We developed a synthetic method of retinyl ethers from various alcohols. Especially, the retinyl ether of amino acid tyrosine were self-assembled and showed an interesting morphology depending on the solvent used for extraction presumably due to the strong hydrogen bonding and the extensive π-stacking interaction between molecules. The morphology and structure of the retinyl ether were analyzed by transmission electron microscopy.

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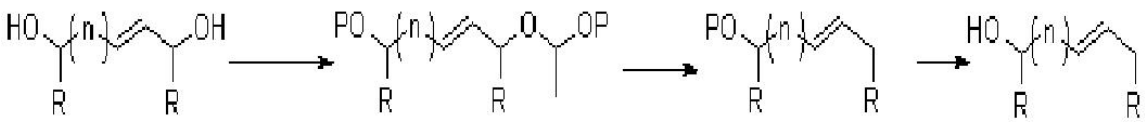
Pd-catalyzed Reduction of Allylic Alcohols:An Efficient and Selective Removal Process for Alcohols

Liang Su

명지대 화학과

It has beea a tough job to activate the compounds that have more than one alcohol groups, namelyto selectively activate one alcohol group over the others. We have developed a method for selectiveremoval of the allylic alcohol in the presence of non-activated alcohol. Our selective reduction method of allylic alcohols was done by the formation of 1-alkoxyallyl ethersand Pd-catalyzed, Super Hydride reduction sequence. This unique selective reduction method has already been applied to the synthesis of Lavandulol, which is an important additive in the perfume industry. More applications and details will be shown during the presentation.



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Synthesis of Resveratrol derivatives for Cerebral & Cardiovascular Diseases

임은영, 이용남, 정만길

연세대 화학과

Naturally occurring resveratrol (*trans*-3,4,5-trihydroxystilbene), isolated from grapes is the most representative compound of stilbene analogues, and it exhibits a wide range of intriguing biological activities. A convenient synthesis and biological properties of new amides, esters and other derivatives of resveratrol are described. The key synthetic strategies involve the well-known Wadsworth-Horner-Emmons reaction to generate (*E*)- or (*Z*)-olefins and coupling reaction of an acid and various amines to give *trans*-stilbene derivatives in high yields. All analogues were evaluated for free radical-scavenging activity, suppression of LPS-induced NO generation, and anti-excitotoxicity in vitro. Most of the *trans*-stilbene derivatives showed 2–3 times more radical-scavenging activity than resveratrol. They were also potent inhibitors of nitrite accumulation in LPS-stimulated microglia BV-2 cells. Some compound showed the most potent neuroprotective activity in the glutamate–induced primary cortical neuron cells.

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Convenient Synthesis of ProDOT Derivatives via Cross-olefin Metathesis

정규관

전북대 과학교육학부

The purpose of this study is develop new synthetic methodology to synthesize the monomers for conducting polymers having various functional groups. The procedures known for monomers mainly rely on individual synthetic route for each monomer. The idea of the study lies on that the intermediate is first synthesized and then a variety of monomers can be efficiently derived from the intermediate via a simple synthetic method. In this study, both MProDOT and ProDOT-allyl was synthesized as the intermediates. Olefin cross-metathesis of MProDOT and various terminal alkenes afforded MProDOT derivatives equipped with various functional groups and the subsequent hydrogenation upon them gave various alkyl substituted ProDOT derivatives. In addition, olefin cross-metathesis of ProDOT-allyl and terminal alkenes also yielded various alkyl substituted ProDOT-allyl derivatives. The procedure was also extended over the alkenes with functional groups such as halides, nitrile, and others. In conclusion, olefin cross-metathesis of MProDOT and ProDOT-allyl with various alkenes provided an efficient route for ProDOP derived monomers in moderate to good yields.

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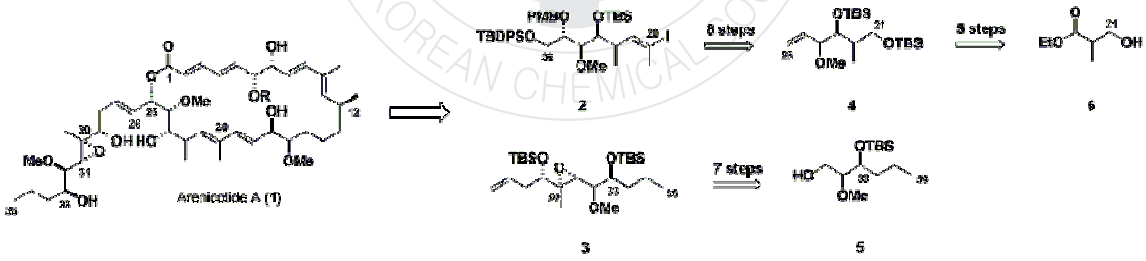
A Stereoselective Synthesis of C20-C26 and C27-C36 Fragments of Arenicolide A

이정열, 이덕형

서강대 화학과

Arenicolide A (1), an 26-membered macrolide with anti-cancer activity, was isolated from the large-scale fermentation of the *S. arenicola* in 2007. The C20 ~ C26 fragment 2 of arenicolide A (1) was prepared in 13 steps and the C27~ C-36 side chain 3 was prepared concisely and efficiently in 10 steps. Key steps were the diastereoselective epoxidation of α–methoxy allylic alcohol, sharpless asymmetric dihydroxylation and construction of vinyl iodide.



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Synthesis of New Iridium Complexes Containing Trimethylsilyl Group for OLEDs

소기호, 강현희, 오대환, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Organic light-emitting diodes (OLEDs) have attracted great attention in the past decades because of their potential advantages in full-color displays. In particular, phosphorescent metal complexes have been considered to be promising materials because of their ability to achieve maximum internal quantum efficiency, nearly 100%, as well as high external quantum efficiency in OLEDs. In this research, we report the synthesis of iridium complex uniting trimethylsilyl group. Trimethylsilyl units is known for good solubility, thermal stability and steric bulk via higher volume. Therefore, the combination of ppy and bulky trimethylsilyl units would be expected to be the best way to achieve an efficient phosphorescent emitter.

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New P-type Organic Semiconductors Based on Poly(thiophene) Derivative

이민정, 박현태, *박종원, **권순기, 김윤희

*경상대 화학과 *경상대 고분자공학과 **경상대 나노신소재공학부*

Organic thin-film transistors (OTFTs) have advantages over traditional thin-film thransistors (TFTs) based on inorganic materials for applications in flexible, large area electronics devices such as bendable displays, electronic paper, ID tags, and sensors.Especially, easy solution-processable polymeric semiconductors can be deposited using low-cost solution processing methods such as spin-coating, ink-jet printing, and gravure printingWe designed and synthesized novel conjugated polythiophene derivatives for solution processed OTFT. The obtained polymers were characterized by various spectroscopic methods such as IR and NMR. The thermal, optical and electrical properties of polymers were also investigated.

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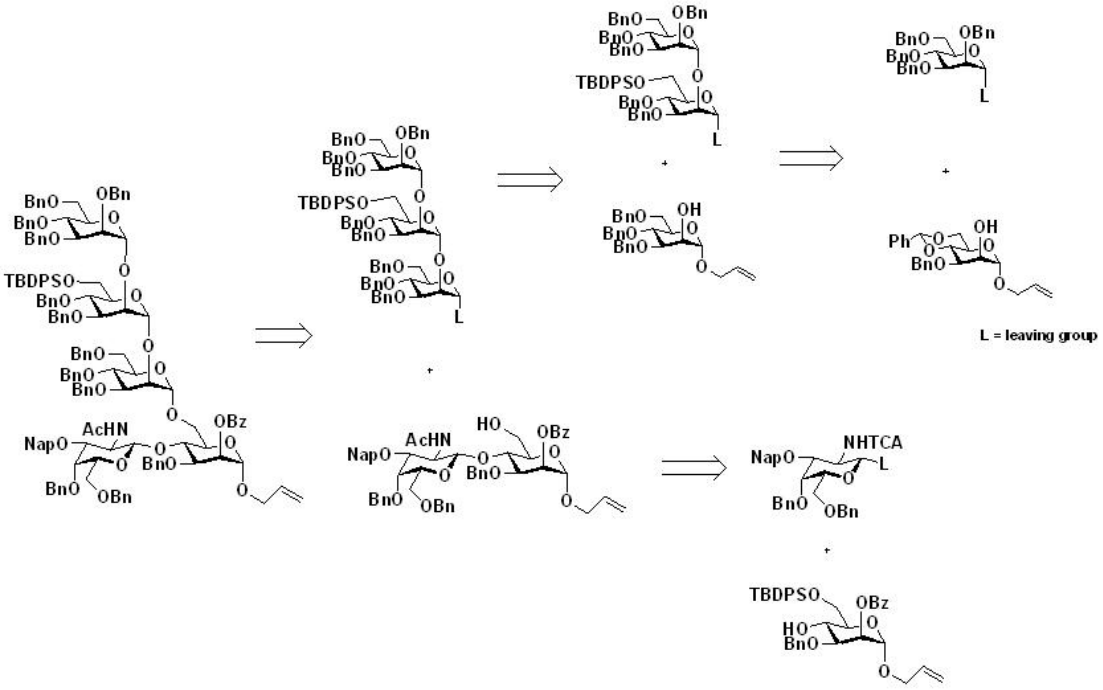
The Efficent Synthesis of a Pentasacchride Part in Glycosyl Phosphatidyl Inositol (GPI) Anchor of Scrapie Prion Protein.

김응곤, 김관수

연세대 화학과

A factor for Bovine Spongiform Encephalopathy (BSE, mad cow disease) is the prion protein which is anchored to membrane by glycosyl phosphatidyl inositol (GPI) anchor. The function of GPI anchors has been widely discussed and there is evidence that, besides the obvious one of anchoring proteins to membranes, there are a lot of different functions of GPI anchors and/or metabolites of them. The present work describes the synthesis of a pentasaccharide portion, {D-Manp-(1→2)-α-D-Manp-(1→2)-α-D-Manp-(1→6)-[β-D-GalNAcp-(1→4)]-α-D-Manp}, of the Scrapie proin protein. The three a-manosyl lingkages in the pentasaccharide were constructed stereoselectively without employing the neighboring group participation strategy.



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Synthesis and Cation Sensing Properties of 4, 4'-Bisthiazole Derivatives

이상훈, 김상현, **Aasif Helal**, 김홍석

경북대 응용화학과

A series of 4, 4'-bisthiazole derivatives with different substituents at the 2 position of the thiazole riing were prepared and their photophysical properties were investigated. Among these, the compound(3a) with phenolic substituent at the 2 position was found to be highly selective to Zn^{2+} and Cu^{2+} cations. The mechanism of fluorescence was explained based on the cation-induced inhibition of excited-state intramolecular proton transfer (ESIPT).

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Sodium Ion Selective Two-Photon Fluorescent Probe for Bio-imaging Applications

김미경, *임창수, 홍종태, **장혜영, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과 **아주대 에너지시스템 사업단*

Na^+ is one of the most abundant alkali ions in the cell and plays critical roles in many cellular processes such as nerve conduction and muscle and heart contraction as well as participates in the regulation of electrolyte level, cation transport, and cell volume. Herein, We report an efficient two-photon probe (ANa1) that shows strong TPEF enhancement in response to Na^+, a dissociation constant (K_d^{TP}) of 20 ± 1 mM, and that emits larger TPEF than SBFI and Sodium Green upon complexation with Na^+. Unlike the previously available probes, this novel probe can selectively detect dynamic levels of intracellular free Na^+ in live cells and living tissues without interference from other metal ions and from the membrane-bound probes.

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Photofunctional supramolecular assembly of diacetylene for patterned fluorescence imaging.

김주호, 이은영, 장우동

연세대 화학과

Diacetylene 분자는 254 nm 의 자외선 노광에 의해 광중합을 일으켜 polydiacetylene(PDA)를 만든다. 또한 PDA 에 외부에서 stress 가 주어지게 되면 fluorescence 를 발생한다. 이러한 성질을 바탕으로 본 연구에서는 내부에 diacetylene 을 가지는 dendritic supramolecular polymer 를 합성하였고, 이를 ^{1}H-NMR 과 MALDI-TOF-MS 를 통해 확인하였다. ^{1}H-NMR study 와 UV 및 Fluorescent spectroscopy 측정을 한 결과 합성된 화합물이 254 nm 자외선 노광에 의해 광중합이 일어남을 확인하였다. 합성된 화합물은 형광을 가지고 있지만, 광중합이 일어나게 되면 형광이 사라지게 된다. 또 광중합이 일어난 화합물에 heat 을 하게 되면 처음과 다른 형광을 갖게 된다. 이러한 특징을 이용하여 새로운 형태의 형광기록용 디바이스로서의 응용이 가능할 것으로 기대된다.

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Inhibitory Effects of Medicinal Plants on Prolyl Endopeptidase

한아름

경희대 화학과

Recent studies showed that prolyl endopeptidase (PEP) plays an important role in the degradation of biologically active proline-containing neuropeptides. PEP is a serine protease and has been suggested to participate in learning and memory process by cleaving peptide bonds on carboxyl side of prolyl residue within neuropeptides of less than 30 amino acids, and is abundant in brain of amnestic patients. And compounds from medicinal plants are expected to prevent memory loss and neurodegenerative diseases of the central nervous system. A variety of medicinal plants, mainly traditional stimulants and tonics (Phellinus linteus, Syzygium aromaticum Merrill et Perry, Cynomorium songaricum Ruprecht, Curcuma longa Linné and etc.) were selected and examined for their PEP inhibitory activities. In our research, each MeOH extracts of the medicinal plants were partitioned between hexane, EtOAc, butanol and H2O. Six fractions showed more than 90% PEP inhibitory activities. Other compounds are untder structure analysis.

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Two-photon absorption properties of naphthalene-derived dipolar molecules and application in biological imaging

김형중, *임창수, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과*

Optical imaging with fluorescence microscopy is a vital tool in bio-imaging studies. Recently, two-photon microscopy (TPM) is attracting much attention in biological imaging due to the capability of imaging deep inside the living tissues for a long period of time. For maximum utilization of TPM, it is essential to develop efficient two-photon probes. However, most of the fluorescent probes presently used for TPM have small TP action cross sections (Φδ), demanding impractically high concentrations of probe and/or laser power. Herein, we describe the synthesis and two-photon absorption properties of a series of naphthalene-derived dipolar molecules. These compounds can be easily synthesized, show appreciable water solubility, and emit strong two-photon fluorescence when excited by 780-800 nm fs laser beam in the physiological condition. Moreover, we have synthesized a new two-photon probe that can detect the calcium waves in intact tissue using TPM.

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Design and synthesis of K^+-selective two-photon fluorescent probe for bioimaging

백나영, *김형중, *김환명

*아주대 화학과 *아주대 에너지시스템학부*

In recent years, two-photon microscopy (TPM), which employs two lower energy, near-infrared photons for excitation, has become a vital tool for live-tissue imaging owing to the advantages of increased penetration depth (>500 μm), localized excitation, and prolonged observation time. However, most of the fluorescent probes presently used for TPM have small TP action cross sections (Φδ), demanding impractically high concentrations of probe and/or laser power. Therefore, there is a need to develop efficient two-photon probes that can visualize the biological events deep inside the live tissue.Intracellular K^+ ion plays crucial roles in many fundamental biological processes such as neuronal excitability and transmission of electrical impulse as well as regulation of ionic and volume homeostasis.An ideal TP sensor for K^+ should have i) significant TP cross section in the NIR ranges, ii) sufficient water solubility to stain the cells, iii) high selectivity for K^+ ions, iv) pH-resistance, and v) high photostability. Herein, we describe the design, synthesis, and bio-imaging application of a TP probe for K^+ ions derived from triazacryptand as the receptor. This sensor meets all of the requirements as outlined above.

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Microwave-assisted N-Arylation of Carbazole in CuI catalyzed coupling reacions with aryl halides

류영실, *김수광, 주혁종, *염을균

*충남대 고분자공학과 *충남대 화학과*

Microwave technique has become interesting method in the many organic reaction, because of significantly reduce reaction times and improve yields. N-arylated compounds including carbazole is important for organic chemical because of preparations of many compounds of interest in biological, pharmaceutical and materials sciences. We studied an efficient microwave-assisted synthesis of carbazole compared with normal heating reaction. N-arylation of carbazole derivatives were obtained using ligand-free CuI catalyst. N-arylated carbazole products were obtained with thiophen, anisole, phenyl and pyridine synthesised. The reaction provided a now hetero cyclic halide, N-arylated carbazole with high yield compared with normal heating reaction.

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Kinetic Studies of Solvolytic Reaction for Chloromethyl methtyl sulfide and Chloromethyl phenyl sulfide

류준하, *성대동, **Dennis N. Kevill

*동의대 화학과 *동아대 화학과 **Department of Chemistry and Biochemistry, Northern Illinois University, DeKalb. Illinois 60015-2862 USA*

AbstractKinetic data are determined conductimetrically under the solvolytic condition at various temperatures in more than 40 solvent systems including fluorinated solvents. The results are discussed appropriately along with the comparison with the earlier data obtained by previous works so far and we reach conclusion that are reasonable in the correlation analysis interns of Extended Grunwald-Winstein Equation, along with criteria available in literatures.

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Thiazole-based chemosensor for Chromogenic and Fluorogenic Sensing of Cu^{+2}

Aasif Helal, 김상현, 김홍석

경북대 응용화학과

A new highly selective, reversible, chromogenic and fluorogenic chemosensor based on thiazole – coumarin moiety for quantification of copper ion in ethanol-DMSO was designed and synthesized. Selectivity toward copper ion was not affected by the presence of representative alkali metals, alkali earth metals and other transition-metal salts. The mechanism of fluorescence was based on intramolecular charge transfer (ICT) of the coumarin moiety.

THE KOREAN CHEMICAL SOCIETY

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장소: 대전컨벤션센터
발표코드: **Ⅲ37P199포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Polymer-metal complex micelles combining drug delivery system and photodynamic therapy

윤희재, 장우동

연세대 화학과

A polymer-metal complex micelles (PMCMs) containing cisplatin (cis-dichlorodiammineplatinum(II); CDDP), anticancer drug, were prepared by coordination bond of CDDP with dendrimer phthalocyanine(DPc) and poly(ethylene glycol)-block-poly(L-aspartic acid) (PEG-PLAn; molecular weight of PEG segment = 12,000 g/mol; polymerization degrees of aspartic acid segment n = 68, 96). Transmission electron microscopy (TEM) and laser light scattering (LLS) exhibited formation of unimodal $PMCM_{68}$ and $PMCM_{96}$ with average sizes of 108 and 135 nm, respectively. PMCMs were very stable in 10 mM phosphate buffer solution (PBS) without NaCl to maintain their shape and size over a month. However, PMCMs slowly released CDDP when they were incubated in physiological saline PBS solution at 37 °C. The loading capacities of CDDP in $PMCM_{68}$ and $PMCM_{96}$ were determined to be about 23 and 25 wt%, where the loading efficacy was 59 and 53%, respectively. Upon the laser light irradiation, generation of singlet oxygen was detected by photo-luminescence observation. Further biological studies are undergoing. The PMCMs would be effective nano-device for anticancer drug carrier with sustained drug release and photodynamic therapy (PDT).

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ENANTIOMER SEPARATION WITH MAGNETIC SILICA NANO PARTICLES

이규정, 최희정, 현명호

부산대 화학과

Magnetic silica nano particles(MSNPs) have attracted quite attention because of their superparamagnetic property, low cytotoxicity, and chemically modifiable surface. Because of the superparamagnetic property, MSNPs are attracted to a magnetic field, but retain no residual magnetism after the field is removed. Consequently, MSNPs attached to specific molecules of interest can be removed from a medium using a magnetic field. In this study, we for the first time demonstrate that MSNPs can be used in direct chiral separations. MSNPs were modified with an appropriate chiral selector such as (S)-N-(2,2-dimethyl-4-pentanoyl)proline-3,5-dimethylanilide. The modified MSNPs [MSNPs/(S)-CS)] were utilized in taking only one enantiomer form the bulk solution of racemic N-(3,5-dinitrobenzoyl)- -amino acid N-propylamides by using a magnet. The chiral separation process looks like fishing and this new method is termed as 'chirality fishing'. When MSNPs/(S)-CS and nonmagnetic silica particles modified with the antipode of the CS [NMSPs/(R)-CS] were used at the same time, two enantiomers were separated from the bulk solution of racemic analytes.

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C_{3v}-Symmetrical triarylureidotrindane Receptor: Synthesis, Anion Binding and Hydrogen Bond Mediated Molecular Cavitand

방소희, 최홍진

경북대 응용화학과

Design and synthesis of artificial receptors for selective recognition of bioactive substrates have received considerable interest in recent years. Receptor molecules with preorganized ligands are useful for the effective binding of guest molecules. C_{3v}-symmetric trindane-triamine 9 reacts with isocyanates to produce anion receptor 10 with chromogenic moieties. This triurea receptor 10, that has three ligands fixed in the same side (all-syn form), can form stable molecular container through hydrogen bonding with hydroxyl-containing slovent molecules such as CH_3OH and HOH, and bind anionic guests such as F^-, Cl^-, Br^-, $H_2PO_4^-$, HSO_4^-, NO_3^- ions. Anion recognitions were examined by ^{1}H NMR titration method in DMSO-d_6. Complexation induced chemical shift and visible color change were observed.

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Strategy toward Improving Turn-On Time of Light-Emitting Electrochemical Cells Based on Neutral Iridium Complexes containing a pendant cation

노탁균, 홍종인

서울대 화학부

It is well known that cationic iridium complexes having PF6- counter anion can be used as light-emitting electrochemical cells (LECs). One way of improving the turn-on time of LECs based on cationic iridium complexes is to use a fast cation transport in neutral irididium complexes containing a pendant cation. LECs derived from a neutral iridium complex containing a pendant sodium ion showed a faster turn-on time compared to the ionic transition metal complex with PF6-, because sodium cation has a faster mobility in the solid film than bulky anions. In order to know the effect of pendant cations on the turn-on time, neutral iridium complexes having a pendant cation such as lithium, sodium, potassium, and cesium, have been synthesized, respectively. Photophysical and electrochemical properties of these complexes, and detailed device studies will be presented.

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Synthesis and anion recognition based on 3,7-diaminocholestane-anthracenyl-imidazolium receptor.

Jadav Jyoti, Md. Wasi Ahmad, 김홍석

경북대 응용화학과

The design of steroid-based receptors capable of selective recognition of anions is of particular interest, due to of their rigid frame work, facial amphiphilicty, and suitable oriented functional groups. A new fluorescent cholestane based imidazolium receptor bridged with 9,10-dimethyleneanthracene has been synthesized and assessed it's binding properties for anions.

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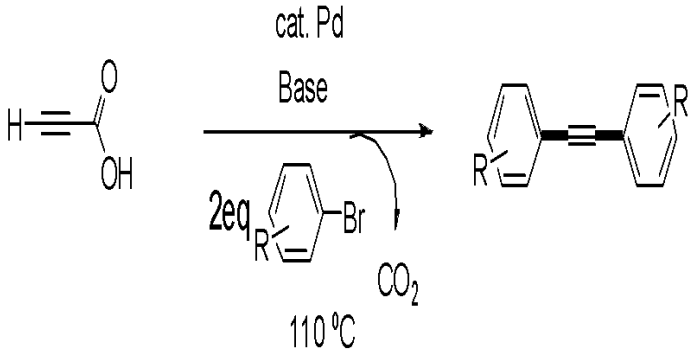
Synthesis of Symmetric Diarylalkynes from Propiolic acid using Pd-catalyst.

박경호, 이선우

전남대 화학과

Kyungho Park and Sunwoo Lee*Department of Chemistry, Chonnam National University, Gwangju 500-757, Republic of Koreasunwoo@chonnam.ac.krWe synthesized a variety of symmetric diarylalkynes from the reaction of arylbromides and propiolic acid using the combination of the Sonogashira reaction and decarboxylative coupling reactions. Two quivalent of aryl bromides were employed in this transformation. We found that one equivalent of aryl bromide involved in the Sonogashira coupling and the other one equivalent involved in the decarboxylative coupling reaction.



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New Deep Blue Emitting Materials Based on Indenopyrazine Core with High Thermal Stability

석창훈, 박영일, *이지훈, 박종욱

*가톨릭대 화학과 *충주대 나노고분자공학과*

New deep blue emitting materials 2,8-bis(3,5-diphenylphenyl)-6,6,12,12-tetraethyl-6,12-dihydro-diindeno[1,2-b:1',2'-e]pyrazine (DPP-EPY) and 2,8-bis(3',5'-diphenylbiphenyl-4-yl)-6,6,12,12-tetraethyl-6,12-dihydrodiindeno[1,2-b:1',2'-e]pyrazine (DPBP-EPY) were synthesized through introduction of m-terphenyl or triphenylbenzene bulky side groups in a new indenopyrazine core. These materials all showed high thermal stability and highly reduced intermolecular interaction. DPP-EPY and DPBP-EPY showed PL maxima of 456 nm and 460 nm in deep blue region and narrow PL spectra with full-width at half-maximum (FWHM) of 46 nm and 52 nm, respectively. As a result of making non-doped OLED devices using these synthesized materials as emitting layers, DPP-EPY showed EL spectrum of 452 nm, very narrow FWHM of 46 nm, luminance efficiency of 1.04 cd/A with current density of 10 mA/cm2 and CIE coordinate of (0.161, 0.104), creating a deep blue OLED close to the National Television System Committee (NTSC) blue standard.

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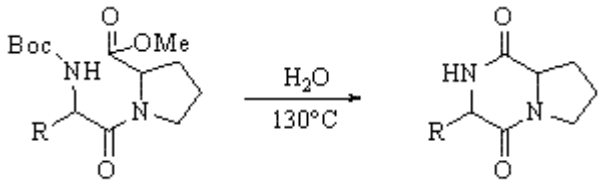
Water Mediated Efficient Synthesis of Proline Based Cyclic Dipeptides under Catalyst-Free Conditions

H. Thajudeen, *박경석, 문석식, 홍인석

*공주대 화학과 *농촌진흥청 국립농업과학원 농업미생물과*

Proline based cyclic dipeptides were synthesized from N-Boc protected dipeptide methyl esters under catalyst-free condition using water as a solvent. One-pot deprotection and cyclization has been used here as the key step which provides an efficient and environmentally friendly approach. Clean reaction conditions, easy isolation, and good yields of the cyclic dipeptides are the salient features of the methodology.



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Redox-sensitive and biocompatible cucurbituril-based vesicle : Efficient delivery and release of anticancer drugs in cytoplasm of target cells

박경민, *이돈욱, **Bijiay Sarkakr, *정현태, ***김지연, ****고영호, *****김기문

*포항공과대 첨단재료과학부 *포항공과대 시스템생명공학부*
***National Dong Hwa University, Taiwan ***포항공과대 화학과*
*****POSTECH, Division of Advanced Materials Science*
******포항공과대 지능초분자연구단, 화학과, 첨단재료과학부*

Nanomaterials as a promising drug delivery vehicle should be biocompatible, structurally stable enough not to lose drugs in unwanted sites before reaching the target sites, have biofunctionality on their surface to interact with specific cells or tissues for effective targeting, and release the drugs efficiently in the target cells. There are many reports about stimuli-responsive nanomaterials for the development of smart targeted drug delivery vehicles that can trigger the release of therapeutic agents such as drugs in response to specific cellular conditions after endocytosis. However, most of the nanomaterials are not structurally stable enough to prevent the loss of the drug in unwanted sites and require laborious chemical synthesis to have biofunctionality on the surface. Herein, we report novel redox-sensitive cucurbit[6]uril (CB[6])-based vesicles (SSCB[6]VCs) stably self-assembled by a new CB[6] amphiphile containing disulfide bonds between hexaethylene glycol units and a CB[6] core to be sensitively cleaved in reducing condition such as cytoplasm, the surface of which can be easily modified with wide variety of tag-attached polyamines using exceptionally strong host-guest chemistry. Remarkable features of SSCB[6]VCs including not only noncovalent surface modification using host-guest chemistry and stably self-assembled vesicle structures but also efficient release of entrapped drugs as a result of the vesicle collapse in cytoplasm of target cells provide a novel platform for efficient intracellular and cytoplasmic delivery systems for anticancer drugs such as doxorubicin, which opens possibility of practical applications of CB[6]-based nanoscale self-assemblies as targeted drug delivery systems.

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Ag-catalyzed Cascade Reaction to Substituted Indoles

오창호, 박효승, 안영천, 김정욱

한양대 화학과

Substituted indoles are core skeletons in a wide range of pharmaceutical drugs and naturally occurring alkaloids. To date, numerous elegant approaches via transition-metal catalysis have been devoted to generate such unique indole systems. However, only a few syntheses to indole derivatives have been successful by employing intra- or intermolecular cyclization of alkynes and imines. In this presentation, we report an atom economical and highly efficient approach for the construction of 2,3-substituted indoles via silver-transition complexes. During the course of our endeavors leading to 2,3-substitued indoles, we observed a highly unique behavior of silver-induced complex with novel 1,3-alkenyl shift to silver carbene.

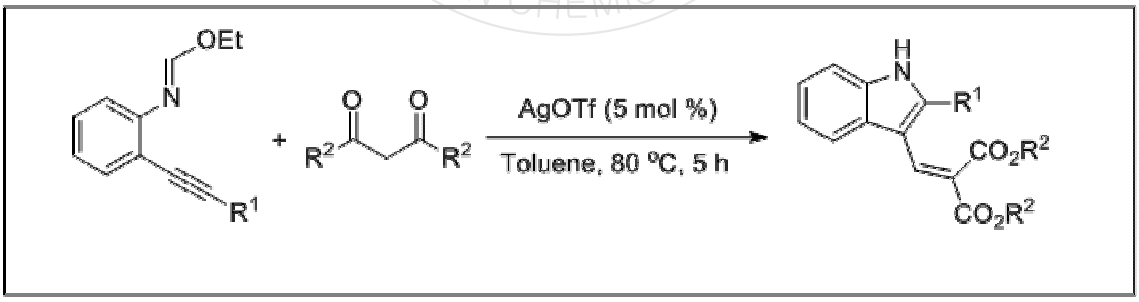

Fig. 1. Mechanism of 2,3-substituted indols

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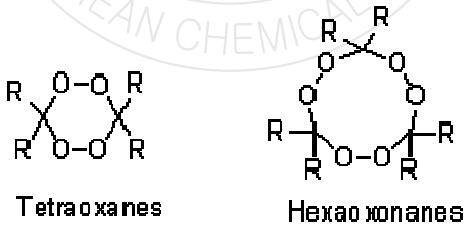
Synthesis and Evaluation of 1, 2, 4, 5 – Tetraoxanes and 1,2,4,5,7,8-Hexaoxonanes derivatives as Cetane Improvers

Ambadas B. Rode, 홍인석

공주대 화학과

Chemical synthesis and performances of a series of 1,2,4,5-tetraoxanes and 1,2,4,5,7,8 hexaoxonanes were investigated to evaluate for use as cetane improvers. Cetane Number (CN) performance of individual tetraoxanes, hexaoxonanes as well as with mixture compositions of other tetraoxanes and hexaoxonanes derivative is also studied. All individual as well as mixture compositions provided good cetane improving capabilities. In comparative study with conventional cetane number improver, 2-ethylhexyl nitrate (2-EHN), we found that tetraoxanes and hexaoxonanes derivatives are more superior.



R = same or different, cyclic or acyclic

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Synthesis, crystal and antibacterial studies of some tetrahydropyridin-4-ol derivatives

G.Aridoss, 박근수, 정연태

부경대 화상정보공학부

Antibacterial resistance to hospital-acquired Gram-positive bacterial pathogens, including methicillin-resistant Staphylococcus aureus (MRSA) and vancomycin-resistant enterococci (VRE), has been increasing at an alarming rate. Furthermore, these drug-resistant bacteria commonly infect healthy people in large communities, thus creating a serious health problem around the globe. To combat such drug-resistant bacterial strains, globally researchers are constantly trying to find novel therapies for the prevention and treatment of these infectious agents. Recently we started working on finding a better MDR antibacterial agent through structural optimization of biologically potent N-chloroacetyl-3-carboxyethyl-2,6-diphenyl-4-hydroxy-Δ3-tetrahydropyridine and also identified some pharmocophores that showed excellent in vitro activity against a wide range of Gram-positive and Gram-negative bacterial strains. In continuation, we have prepared some derivatives from this synthon and explored their in vitro antibacterial activity against both Gram-positive and Gram-negative organisms. This preliminary in vitro study concluded that compound with imidazole moiety in place of chlorine has emerged as good antibacterial agent.

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Combinatorial synthesis of quinoxaline library using o-azidoaniline building blocks

김용진

대구가톨릭대 화학과

A combinatorial solid-phase synthesis of quinoxaline library is reported. o-azidoanilines have been utilized as key building blocks in rodium-catalyzed N-H insertion reactions with resin bound α-diazo-β-ketoesters. The resin-bound N-H insertion products were then, cyclized in the presence TPP followed by oxidant (DDQ, Chloranil) to yeild the corresponding quinoxalines, which were then detached by diversity-building smart cleavage reaction.

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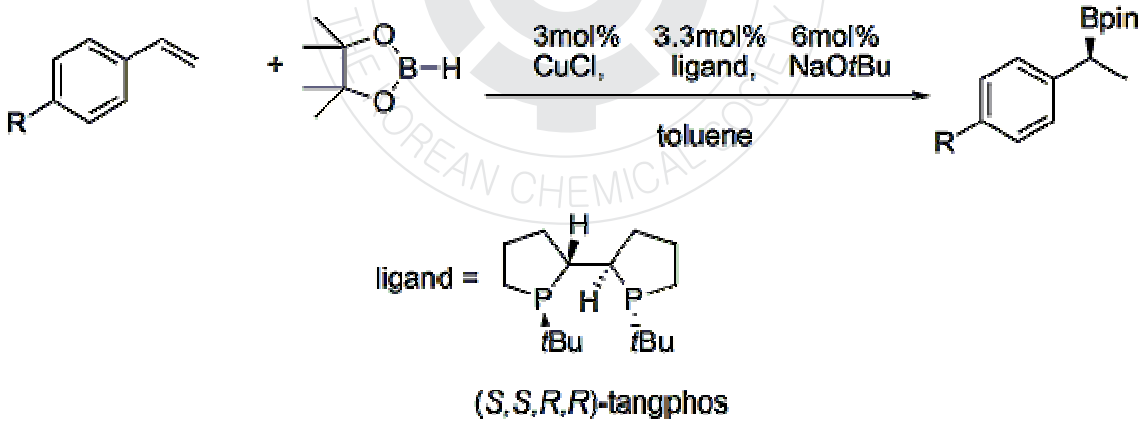
Copper-Catalyzed Asymmatric Hydroboration of Vinyl Arenes

노동완, 채희성, 윤재숙

성균관대 화학과

The development of efficient regioselective catalytic systems that are compatible with stable hydroboration reagents remains as a challenge. Herein, we present that copper(I) complexes with chelating phosphines catalyzes the regio- and enantioselective hydroboration of styrenes with pinacolborane (PinBH) at room temperature to afford the corresponding branched boronate esters.



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Synthesis and stereochemistry by spectral and crystal studies of various substituted 2,4-diaryl-3-azabicyclo[3.3.1]nonan-9-one oxime ethers

P. Parthiban, 정연태

부경대 화상정보공학부

3-Azabicyclononanes are important class of heterocycles due to their presence in a wide variety of naturally occurring diterpenoid/norditerpenoid alkaloids. The 3-azabicyclononane pharmacophore exhibits broad spectrum biological activities and various pharmacological actions. Since the stereochemistry plays a crucial role in biological activity, it is significant to establish the stereochemistry of the synthesized bio-active molecules. Hence, in the present study, we have reported the synthesis, complete spectral assignments and stereochemistry of the various substituted, biologically potent 2,4-diaryl-3-azabicyclo[3.3.1]nonan-9-one oxime ethers by their IR, Mass, 1H NMR, 13C NMR, 1H -1H COSY, NOESY, HSQC, HMBC and single crystal XRD data.

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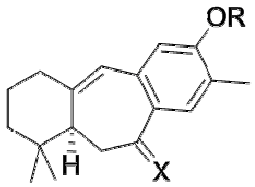
Total Synthesis of (±)-Faveline using Pt-catalyzed Cyclization of Enynebenzaldehyde.

오창호, 이성민

한양대 화학과

In 1991, a number of cytocidal compounds has been isolated from the bark of the Brazilian plant favela (Cnidoscolus Phyllacanthus). Faveline methyl ester 1, faveline 2, and deoxyfaveline 3 display significant activity against P-388 murine leukemia cells. Several groups were successfully synthesized faveline family. In 1992, Ghatak et al. was first total synthesis of these compounds. Majetich et al. synthesized 6,7,6-fused tricyclic compound using cycloalkylation of functionalized arene with a Lewis acid-activated conjugated dienone. In 2005, Banerjee et al. synthesized (±)-Komaroviquinone and (±)-Faveine methyl ester through intramolecular Heck reaction.Recently, our group developed Pt-catalyzed [3+2]-cyclization of o-alkynylbenzaldehydes with pendant unsaturated bond. This methodology could adapt to synthesis of natural compound (±)-Faveline bearing a [6,7,6]-fused cyclic system.



R=Me, X=O - Faveline Methyl Ether, **1**
R=H, X=O - Faveline, **2**
R=H, X=H - Deoxofaveline, **3**

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Intramolecular Triplet-Triplet Energy Transfer in Benzophenone-Phthalimide Dyads

김성식, *M. Sakamoto, *M. Fujitsuka, *T. Majima

*전북대 화학과 *Osaka University*

A series of benzophenone (BP)-*N*-methylphthalimide (MePI) dyads (Cn, n = 3, 6, and 9, where n denotes the number of methylene group in the linker) were synthesized. The photochemical properties and intyramolecular triplet-triplet energy transfer from BP(T_1) to MePI were investigated. Formation of two different intramolecular complexes was observed, that is, a ground-state complex and a singlet exciplex. The formation of the triplet-equilibrium between MeBP and MePI was observed. The triplet-equilibrium constant (1.0 and 1.1 for C6 and C9, respectively) and forward (3.8 x 10^7 and 3.9 x $10^7 s^-$ for C6 and C9, respectively) and back (3.8 x 10^7 and 3.6 x $10^7 s^{-1}$ for C6 and C9, respectively) energy transfer rates were estimated from the results of transient absorption measurements. From the van't Hoff plots, enthalpy and entropy change for the equilibrium formation were also estimated.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Studies on the Synthesis of Succinamide Backbone Derivatives as Prolyl Endopeptidase Inhibitors.

윤승빈

경희대 화학과

Prolyl endopeptidase (PEP: E.C. 3.4.21.26) is a serine protease first identified in 1971 in human uterus as a cleaving peptide bonds on the carboxylic side of prolyl residue. This enzyme plays as key role in degradation of proline-containing neuropeptides involved in the processes of learning and memory. Therefore compounds with PEP inhibitory activity are expected to prevent memory loss and neurodegenerative diseases of the central nervous system. We synthesized several compounds containing succiamide hackbone and measured the degree of PEP inhibitory activities

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Synthesis of carboranylbenzothiadiazolidines as Potential BNCT Agent

이채호, 임현화, 임정렬, *이종대, **강상욱

*원광대 생명나노화학부 *조선대 화학과 **고려대 소재화학과*

Carboranes are stable, lipophilic structures which resemble benzene in term of reactivity and bulkiness. Therefore it is not surprising that carborane-based biomolecules which an aromatic group is replaced by the boron cage have been prepared. Since carboranes which linked a biomolecule contain ten boron atoms, they theoretically may help deliver much higher concentrations of 10B atoms in cancer cells for boron neutron capture therapy (BNCT). Carboranylbenzothiadiazolidines containing water-soluble functional groups have been synthesized and evaluated growth inhibition of various tumor cell lines and boron corporation into B-16 melanoma cell.

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Synthesis of o-Carboranylphenols as Potential BNCT Agent

이채호, 임정렬, 임현화, *이종대, **강상욱

*원광대 생명나노화학부 *조선대 화학과 **고려대 소재화학과*

Born Neutron Capture Therapy (BNCT) was first proposed as a potential cancer therapy in 1936 but the successful application of BNCT to the treatment of cancer still presents a challenge in medical research. BNCT is a binary therapy, which is dependent on the selective deposition of 10B in the tumor prior to irradiation by slow thermal neutrons. The combination of 10B and thermal neutron produces 2.4 MeVmol-1 enough to destroy the tumor cells. We herein report on the synthesis of of o-Carboranylphenols as potential BNCT agent. They accumulate in B-16 melanoma cells with a significantly high level although its cytotoxicity is considerably low.

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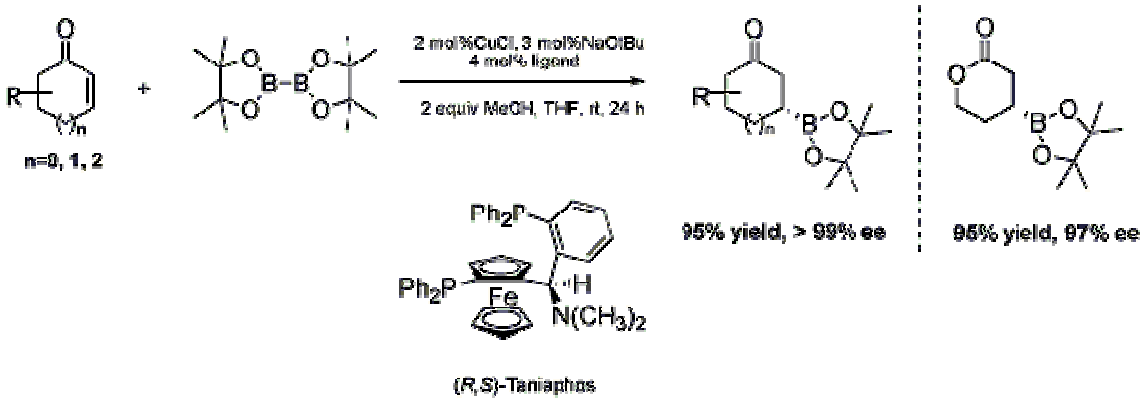
Efficient asymmetric synthesis of ß-borylated carbonyl compounds through catalytic boron conjugate addition to cyclic carbonyl substrates

풍신혜, 김혜령, 윤재숙

성균관대 화학과

The enantioselecitive ß-boration of various acyclic enones, esters and amides have been recently studied by using transition metal complexes coordinated with chiral ligands. However, there are only a few reports on cyclic starting materials. Herein, we describe a highly enantioselective copper-boryl (Cu-B) catalyst system that is effective for the boration of cyclic carbonyl compound including enones and unsaturated lactones. The desired products are obtained in good yields and excellent ee. This method provides a new catalytic synthetic route to chiral cyclic ß-hydroxy ketones, which are difficult to access otherwise.



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Synthesis and Optical Properties of New Single Black Pigments Based on Azo and Anthraquinone Moieties

정지윤, 박영일, 박종욱

가톨릭대 화학과

For full color expression of LCD, a color filter (CF) is necessary to change white back light into red, green and blue lights. In such CF, red, green and blue pigments are used with black matrix (BM) materials[1]. BM improves the contrast of red, green and blue lights converted from white back light through prevention of external light. BM is used to prevent malfunction of thin film transistor (TFT) by minimizing reflection of light[2]. Although Cr/CrOx with sputtering process has been in use as BM, Cr is a heavy metal that causes environmental problems. High cost and complicated sputtering process are increasing the necessity of an organic BM[3]. Based on azo and anthraquinone moieties, new black matrix pigment materials AAQ and DAAQ were synthesized for the first time by through Suzuki C-N coupling reaction. As a result of verifying UV-visible absorption spectra of the synthesized materials, DAAQ was found to absorb the entire visible region in 400 ~ 800 nm in solution state with high extinction coefficient of 8.1 × 103 L/cm·mol. Realization of black color using a single material is expected to be useful for black matrix application. Also in film state made by through spin coating, both AAQ and DAAQ absorbed the entire visible region. Synthesized materials AAQ and DAAQ respectively showed Td of 353 and 366 ℃. In case of AAQ, high thermal stability was verified with Tm measured at 267 ℃.[1] Y. D. Kim, J. P. Kim, O. S. Kwon, I. H. Cho, Dyes and Pigments, 2009, 81, 45[2] R. W. Sabnis, M. D. Stroder, R. E. Nichols and E. G. Hays, Soc. Inform. Display Digest., 1998, 29, 54[3] Y. Ugai, K. Nishimura, S. Aoki, Electronics and Communications in Japan, 1999, 83, 2

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The studies on the indium-mediated bisallylation of 4-bromocrotonates with aldehydes.

이주현, *강순방, 정낙철, *김유승, **금교창

*고려대 화학과 *KIST 생화학물질연구센터 **KIST 케모인포메틱스연구센터*

The reaction of methyl 4-bromocrotonate with benzaldehyde in the presence of indium metal in water afforded the homoallylic alcohol as a Barbier-type product. On the other hand, the reaction in DMF was proceeded to afford the bisallylated diol compound as a single diastereomer. The diol compound was generated by the indium-mediated Barbier-type allylation reaction of the crotonate with benzaldehyde followed by the second allylation of the intermediate homoallyic alcohol with the aldehyde. The chemical transformation of the diol compounds was studied to determine structure and stereochemistry of the diol compounds. In addition the mechanism of the reaction will be discussed.

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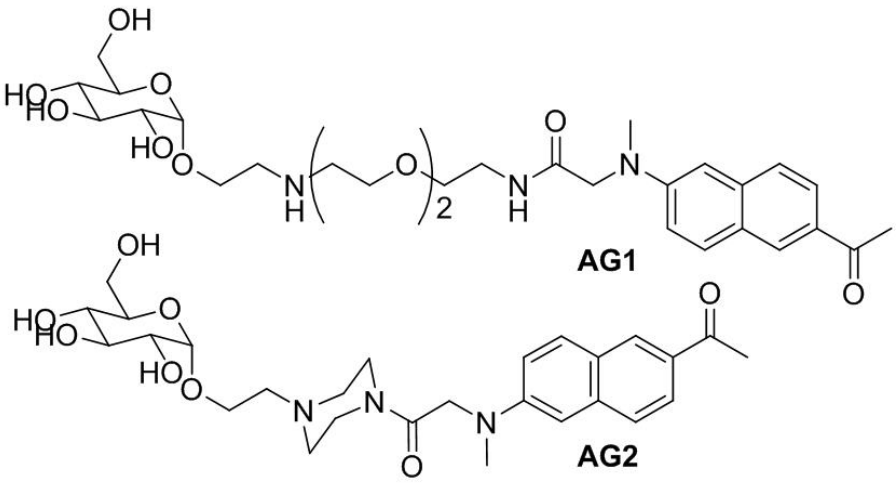
Two-Photon Tracers for the Glucose Uptake and Their Application in Screening of Anticancer Agents

임창수, *김환명, **Tian Yu Shun, 신유나, 황혜림, 조봉래

*고려대 화학과 *아주대 에너지시스템학부 **korea university*

Recently, We developed TP tracers (AG1, AG2) that can be excited by 780 nm fs laser pulses, easily loaded into the cancer cells and tissues, show high photostability and negligible toxicity, and can visualize the glucose uptake in live cells and tissues by two-photon microscopy (TPM). Moreover, AG2 can screen the anticancer agents in the cancer cells and cancer tissues at 75-150 μm depth by TPM.



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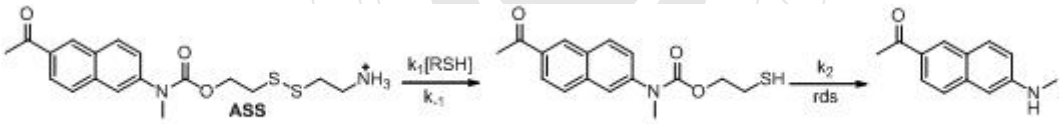
A Two-Photon Fluorescent Probe for Thiols in Live Cells and Tissues.

이준한, 임창수, *Yu Shun Tian, 조봉래

*고려대 화학과 *Korea Univ.*

We report a two-photon fluorescent probe (ASS) that can be excited by 780 nm femto-second pulses and can detect thiols in live cells and deep inside the intact tissues by two-photon microscopy. ASS derived from 2-methylamino-6-acetylnaphthalene (1, acedan) as the fluorophore and a disulfide group as the thiol reaction site.



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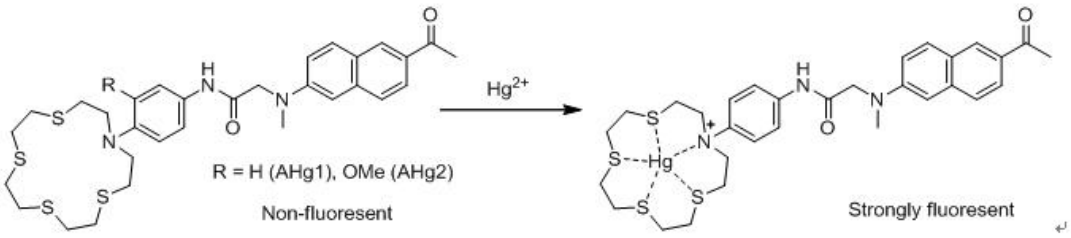
A Two-Photon Probe for Mercury Ions in Live Cell and Tissue

임창수, 강동원, 강민영, *Yu Shun Tian, 조봉래

*고려대 화학과 *Korea univ.*

Herein, we report a novel highly selective TP probe for intracellular free Hg^{2+} (AHg1-AHg2) derived from 2-acetyl-6-(dimethylamino)naphthalene as the TP chromophore and azathiacrown as the Hg^{2+} ion chelator. These probes can be excited by laser photons at 780 nm. It shows 30-8-fold enhancement in one- and two-photon excited fluorescence in response to Hg^{2+} respectively, emits strong TPEF upon complexation with Hg^{2+} K_d^{TP} = AHg1 (5.20 ± 0.03) μM - AHg2 (0.25 ± 0.02) μM, and can selectively detect intracellular free Hg^{2+} ions in the live cells and living tissues without interference due to other metal ions and the membrane-bound probes.



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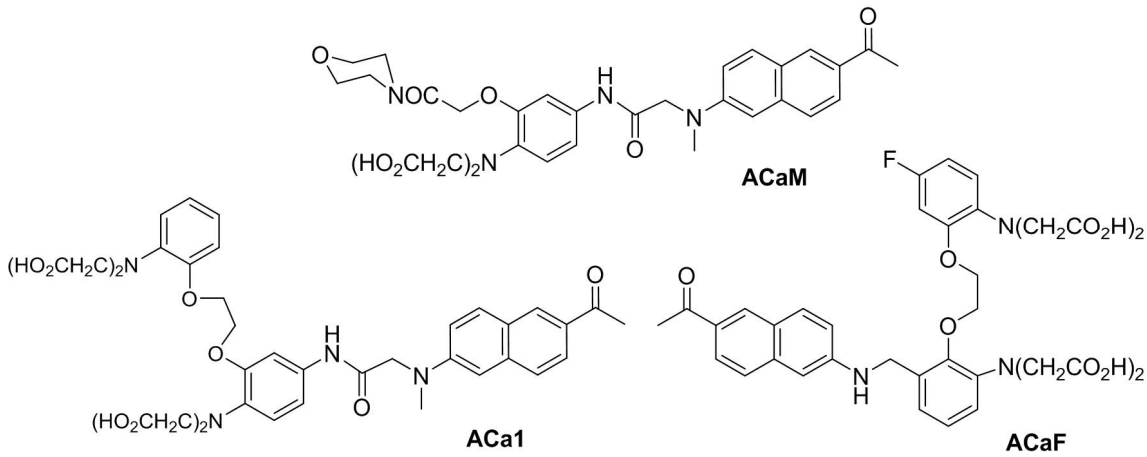
Two-Photon Probes for Long-Term Imaging of Levels of Ca^{2+} Ions

임창수, 노원영, 손지훈, *Tian Yu Shun, 조봉래

*고려대 화학과 *korea university*

Herein, we report an efficient two-photon probe that can visualize the calcium distribution in the live tissues. In this work, we extend our previous work and present a series of TP probe (ACa1-ACaF-ACaM) that can be excited by 780 nm photons, show 40-6-2-fold two-photon excited fluorescence enhancement (TPEF) in response to Ca^{2+}, and the dissociation constants (K_d^{TP}) were (0.23 ± 0.02)-(0.43 ± 0.03)-(116.20 ± 0.02) μM upon complexation with Ca^{2+}. Unlike the previously available probes, these novel probes can selectively detect dynamic levels of Ca^{2+} ions in live cells and living tissues without interference from other metal ions and from the membrane-bound probes, because of their different K_d value. Moreover, these probes are capable of monitoring the calcium waves about > 100 μm depth in live tissues for long time using TPM with no artifacts of photo-bleaching.



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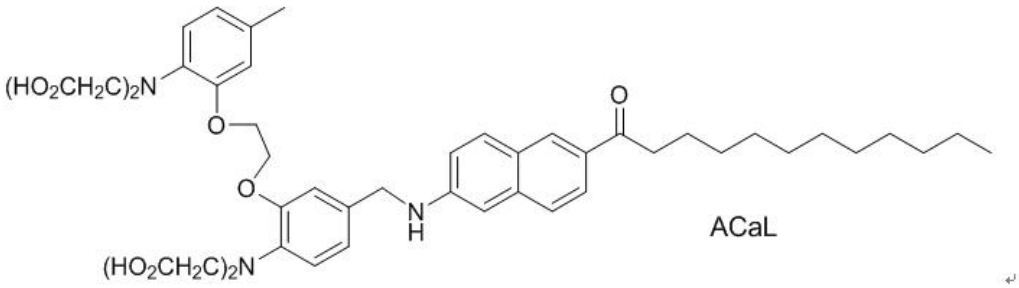
A Two-Photon Fluorescent Probe for Near-membrane Calcium Ions in Live Cells and Tissues

임창수, 노원영, 이준한, *한지희, **Tian Yu Shun, 조봉래

*고려대 화학과 *고려대 화학 **Korea Unviersity*

We recently reported an efficient two-photon probe that can visualize the calcium ions in the plasma membrain. In this work, we extend our previous work and present a series of TP probe (ACa1CL) that can be excited by 800 nm photons, show 12-fold two-photon excited fluorescence enhancement (TPEF) in response to Ca^{2+}, dissociation constants (K_d^{TP}) of (0.048 ± 0.003) μM upon complexation with Ca^{2+}. Unlike the previously available probes, these novel probes can selectively detect dynamic levels of membrain free Ca^{2+} in live cells and living tissues without interference from other metal ions and from the membrane-bound probes. Moreover, these probes are capable of monitoring the calcium waves about > 100 mm depth in live tissues for longer than 4,000 s using TPM with no artifacts of photo-bleaching.



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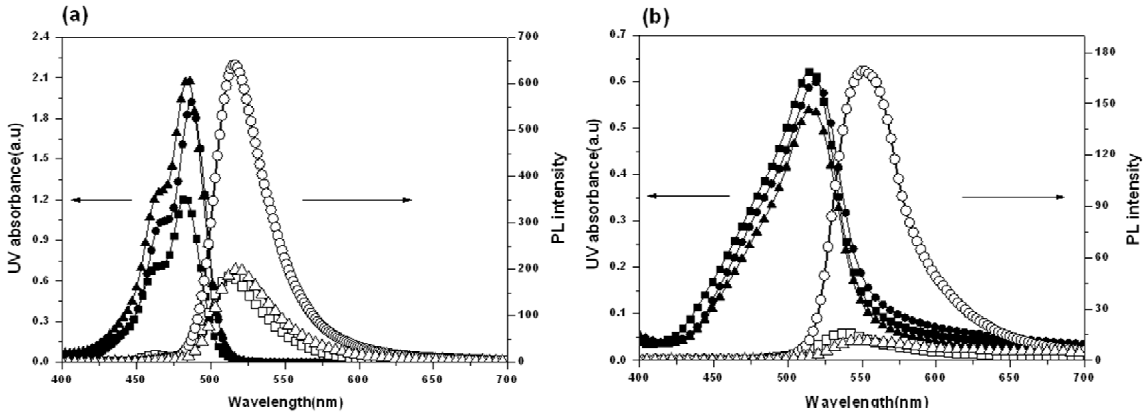
Relationship Between Luminescent Property and Connecting Position of Side Group in Bis(dipyrrinato)zinc Complex Derivatives

이소라, 석창훈, 박영일, 박종욱

가톨릭대 화학과

New yellow emitting materials were synthesized using bis(dipyrrinato)zinc complex moiety by substituting position 1 and 2 of naphthalene groups with position 5 of dipyrrinato. Phenyl group was substituted for use as comparison material. Bis[5-(1-naphthalenyl)-dipyrrinato]zinc complex ($Zn(1\text{-}NaPN)_2$) substituted at position 5 of dipyrrinato and naphthalene group showed about 10 times stronger luminescence property and sharper PL spectrum compared to bis[5-(phenyl)-dipyrrinato]zinc complex ($Zn(PPN)_2$) and bis[5-(2-naphthalenyl)-dipyrrinato]zinc complex ($Zn(2\text{-}NaPN)_2$). Optical properties in film state were shown identically in the result of non-doped organic light emitting diodes (OLEDs) device. Luminance efficiency (cd/A) of $Zn(1\text{-}NaPN)_2$ was 0.33 cd/A, which was about 4 ~ 8 times higher than $Zn(PPN)_2$ and $Zn(2\text{-}NaPN)_2$ respectively at 0.04 and 0.08 cd/A. Quantum efficiency was also about 2 ~ 3 times higher.



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A new fluorescent chemosensor for In^{3+} based on inhibition of excited-state intramolecular proton transfer

한도영, 김현정, 정효성, 김종승

고려대 화학과

we have presented calix[4]crown-6-diazaanthraquinone (CCA-6) bearing two amine group as both colorimetric and fluorescent selective chemosensors for In^{3+} ion in CH_3CN which operates by inhibition of ESIPT signaling mechanism. When the Cs+ ion is bound in crown moiety, inhibited ESIPT process based on $In^{3+}$is regenerated due to conformational change of (CCA-6). doesn't exist crown moiety synthesized (CPA) which carried out same TEST as (CCA-6) to prove such phenomenon

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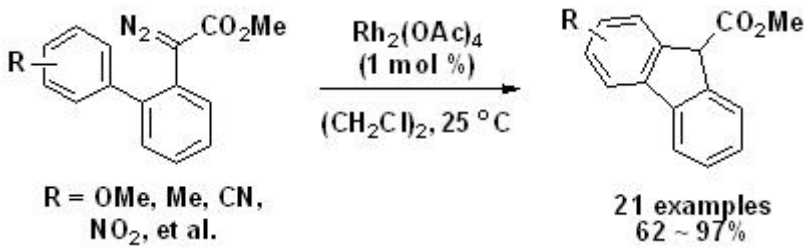
Transition metal Catalyzed Intramolecular C–H Insertion Reaction of Biaryldiazoacetate: Facile Synthesis of Fluorene Derivatives

김진호, 박세흠, 장석복

KAIST 화학과

α-Diazocarbonyl compounds has attracted attention owing to their versatile applications in organic synthesis. Their abilities to generate carbene with thermolytic, photolytic, or transition metal-employed condition made it possible to extend range of reactivities of α-diazocarbonyl compounds. In recent years, many groups reported inter-, intramolecular asymmetric transformation of α-diazocarbonyl compounds catalyzed by competent chiral metal complex. Recently, our group reveal that aryldiazoesters could be decomposed leading to indene in Cu(NHC)-catalyzed [NHC: *N*-hetero-cyclic carbene] system. In this context, we envisioned that fluorene or its derivatives could be synthesized through biaryldiazoacetate via intramolecular C–H insertion pathway. Fluorene derivatives have extensive applications as dyes or optical brightening agents in material chemistry. In addition, fluorene is a precursor of F-moc which is a proficient amine protectiong group of amino acids. Nevertheless, there are limited known methods to synthesize fluorene derivatives practically in laboratory system. It is more difficult to make *mono*- or *di*-substituted fluorene derivatives which have nonsymmetrical structure. Most synthesises for substituted fluorenes result from Friedel-Crafts reaction of fluorene, or substitutions of 9-carbon in strong base condition. Herein, we want to introduce an effective synthesis to various fluorene derivatives, including nonsymmetrical fluorene derivatives, by virtue of transition metal catalyzed diazo decomposition reaction.



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Chromogenic Bis-indole as a Selective & Sensitive Chemodosimeter for Mercuric Ion in Aqueous Solution

김현정, 김자형, 김종승

고려대 화학과

A water-soluble Bis-indole derivative (1) capable of chemodosimetric Hg^{2+} ion detection was synthesized. The color changes and UV/vis changes of 1 were eminently shown upon Hg^{2+} addition, from which chemodosimeter 1 exclusively detected the 1 equiv of Hg^{2+} ion within less than a reaction time of one minute. Compound 1 exhibited a high selectivity toward Hg^{2+} that was unimpeded by the presence of other metal ions. Chemodosimeter 1 and its selective and sensitive Hg^{2+} detection in aqueous systems gives a potential guideline in biological and environmental application-oriented chemodosimeter research.

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Fluorescence Enhancement through Intramolecular H-Bonding Blocking by Hg^{2+}

김현정, 김자형, 김종승

고려대 화학과

We designed and synthesized a new pyrene-based water-compatible fluorescence 'turn-on' sensor (1) for Hg^{2+} ion. The fluorescent sensor (1) shows a very significant fluorescence enhancement to the metal cations in a simple and efficient way. Complexation studies by NMR, UV and fluorescence spectroscopy were carried out towards different ions and it was found that the receptor shows excellent selectivity for Hg^{2+} ions. The Hg^{2+} ion selectivity is due to the blocking of hydrogen bond between the phenolic OH and the imine nitrogen atom in 1 and the Hg^{2+} ions.

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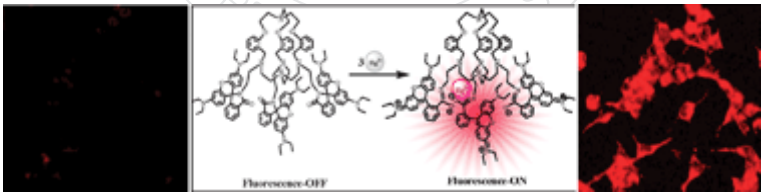
발표종류: 포스터, 발표일시: 금 10:30~12:30

A cryptand based Hg(II) selective fluorescence sensor in aqueous medium and its application in live cell imaging

정효성, 이재홍, 김종승

고려대 화학과

A novel cryptand based fluorogenic indicator bearing rhodamine was developed as a fluorescent OFF-ON chemosensor high selectivity towards Hg(II), but no significant response towards other biologically relevant metal ions. The fluorescent probe coordinates with Hg(II) ions with 1:3 complex stoichiometry as resulted in UV-Vis titration and ESI-MS results. We also have described cell line applications of 1·Hg(II), a new fluorescent indicator for imaging toxic Hg(II) in living biological samples (HEK 293 cell line).



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장소: 대전컨벤션센터
발표코드: **Ⅲ37P233포**
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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of 7-(Substitutedamino)coumarin Derivatives as the Fluorescent Brightner

임중철, 강용한

한양대 응용화학과

Coumarin derivatives are used as the Fluorescent Brightners effectively for animal textile materials, synthetic polyamide, and acetate fibers. Various 7-(substitutedamino)coumarin derivatives have been prepared from the reaction of 3-dialkylaminophenol with ethyl acetoacetate or methyl phenylformylacetate(methyl 3-hydroxy-2-phenylacrylate). Synthetic details and the whitness and fastness of the newly prepared compounds will be discussed.

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Synthesis and Properties of Bis(triazinylamino)stilbenes containing the β-amino acid derivatives as the Fluorescent Whitening Agent [1]

이정선, 신다롬, *강용한

*한양대 과학기술대학 응용화학과 *한양대 응용화학과*

Fluorescent whitening agent(FWA) are dyes that absorb light in the ultraviolet and violet region of the electromagnetic spectrum, and re-emit light in the blue region. These additives are often used to enhance the appearance of color of fabric and paper, causing a "whitening"effect, making materials look less yellow and by increasing the overall amount of light reflected to the eye. In this study, symmetrically substituted bis(triazinylamino)stilbenes containing a β-amino acid derivative were prepared as the fluorescent whitening agents. Synthetic details and the whitness and fastness of the newly prepared compounds will be discussed.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

A new general and one-pot synthetic method of ketones from esters

김민애, 안덕근

강원대 화학과

A useful and effective functional group transformation of various organic compounds is important in organic synthesis of natural products and materials with interesting properties. A ketone in the organic compounds is one of important functional group undergoing a wide variety of chemical transformations, and especially general one-pot transformation of common esters to ketones without isolation of intermediate have been reported only one method that was based on preparation of Weinreb amides as intermediate by the reaction of esters with magnesium amides.Recently, we have found that a useful and new one-pot synthetic method of ketones from esters in excellent yields

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Properties of Bis(triazinylamino)stilbenes containing the β-amino acid derivatives as the Fluorescent Whitening Agent [2]

박진기, 강용한

한양대 응용화학과

Disodium 4,4'-bis(triazinylamino)stilbene-2,2'-disulfonate derivatives are most widely used as the fluorescent brighteners for the whitening both cotton and wool. They increased the whiteness by a process of absorption of the light in ultraviolet ray (330~380nm) and emission of the visible blue lights (400~450nm). It is necessary for the fluorescent brighteners to show the high fluorescence activity a planner molecular structure with conjugated double bonds and electron–donating groups. Unsymmetrically substituted bis(triazinylamino)stilbenes containing a β-amino acid derivative were prepared as the fluorescent whitening agents by using 4-amino-4'-nitrostilbene-2,2'-disulfonic acid as a starting material. Synthetic details and the whitness and fastness of the newly prepared compounds will be discussed.

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A Quaternary Ammonium Triflate Catalyzed Biginelli Reaction

박수정, 곽영우

경북대 화학과

The one-pot assembly of an aldehyde with β-keto ester and urea pioneered by Biginelli allows the direct formation of hydropyrimidines. In this presentation we outline the design of a new piperidinium triflate, such as 1,1,3,5-tetramethyl-4-oxo-2,6-diphenylpiperidinium triflate which shows the highest catalytic activity, catalyzed Biginelli reaction that allows the production of a diverse range of new hydropyrimidines from respective aldehydes, β-dicarbonyl compounds, and urea/thio urea.

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Development of synthetic pathway of ethyl 3-cyclopropyl-3-oxopropionate

이혜미, 이지연, *강용한

*한양대 과학기술대학 응용화학과 *한양대 응용화학과*

Pitavastatin is a synthetic lipid-lowering agent that act as an inhibitor of 3-hydroxy-3-methylglutaryl-coenzyme A(HMG-CoA) reductase(HMG-CoA reductase inhibitor) and is chemically known as (3R,5S)-7-[2-cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl]-3,5-dihydroxy-6(E)-heptanoic acid. It is well-known the preparation of 2-cyclopropyl-4-(4-fluorophenyl)quinoline has been prepared from the reaction of 2-amino-4'-fluorobenzophenone and ethyl 3-cyclopropyl-3-oxopropionate. In this study, the synthetic pathway of ethyl 3-cyclopropyl-3-oxopropionate was developed and the details will be discussed.

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Cetane number improvers containing cyclic nitrate and carbonate derivatives

조창용, 김영준, *정근우

*충남대 화학과 *한국화학연구원 그린화학연구단*

Cyclic nitrate compounds (DHDP-R-NO2, DCPD-R-NO2, DCPD-2R-2NO2) and carbonate compounds (DHDP-R-Carbonate, DCPD-R-Carbonate, DCPD-2R-2Carbonate) were synthesized from norbornylene, tricyclo[5.2.1.0(2,6)]decan-3-ene, and dicyclopentadiene. They were added to diesel fuel and the cetane number were measured . The cetane number of the mixture with nitrate compounds and carbonate compounds were higher than that of diesel by 2~3 and 0.1~0.2, respectively.

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Formation of Polythiophene Nanorod/Au Nanoparticles and their Optical properties

김지수, 윤국로

한남대 화학과

Nano-materials were widely used in hybrid systems for electronics, optoelectronics, bioelectronics, photovoltaic cells, biosensors.We demonstrated that Polythiophene Nanorods were decoration with Au nanoparticles by the pores of anodized aluminum oxide (AAO) template. The resulting Polythiophene Nanorod/Au Nanoparticles were characterized by infrared spectroscopy, scanning electron microscopy, atomic force microscopy, and transmission electron microscopy.

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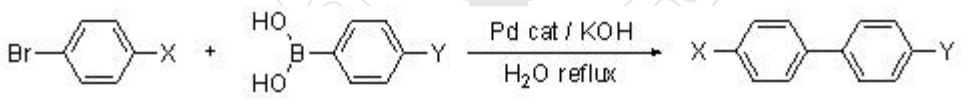
Pd Nanoparticle Immobilized on Resin: Effective Catalyst for Suzuki Reaction in Water Solvent

DeCastro Kathlia, 이학준

한양대 응용화학과

We report herein the preparation of Pd nanoparticle catalyst immobilized on commercially available macroporous resin having polyamine active group. This catalyst exhibits well to excellent catalytic activity in the Suzuki cross coupling reaction of various aryl bromides and aryl boronic acids using water as solvent in reflux condition. Our protocol offers a mild alternative to the several existing methods for Suzuki reaction. Furthermore, the catalyst can be recycled without significant loss of catalytic activity.



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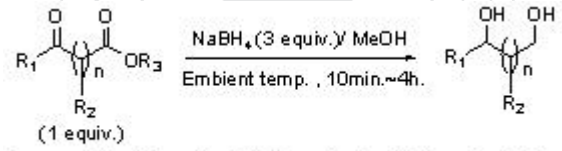
Reduction of Various Keto esters using Sodium Borohydride-Methanol System: A Comprehensive Study

김주령, *이학준

*한양대 바이오나노학과 *한양대 응용화학과*

Several ketoesters were reduced to their corresponding alcohols using sodium borohydride-methanol system. The reduction was completed within 10 minutes to 3 hours at room temperature. The alcohol products were isolated after aqueous work-up in well to excellent yield. Furthermore, we have found the excellent chemoselective reduction of keto esters in the presence of isolated ester functionality. This protocol is simple, easy, cost effective and applicable for industrial purposes



R_1 = arnyl, alkyl, R_2 = H, alkyl, R_3 = ethyl, methyl, n = 0, 1, 2, 3

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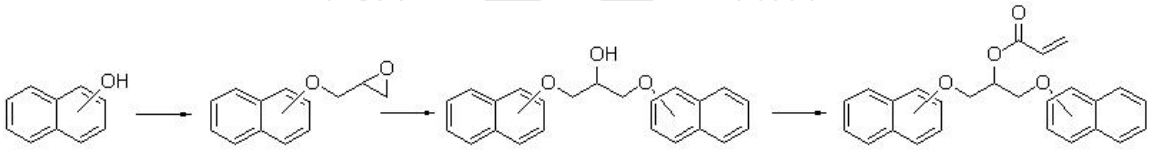
Fuctionalized Aromatic Glycidyl Ether : Plausible compound for better LCD Back Light Unit

배정은, 이학준, 김백선, *김동국

*한양대 응용화학과 *한양대 화학과*

High refractive acrylate monomers are used as material for LCD prism sheet. The higher its refractive index, the brighter the LCD panel. We found that the refractive index of 1-naphthyl and 2-naphthyl glycidyl ether are higher relatively. To further increase the refractive index we modified these ether by using acrylate, urethyl and another naphthoxy group. We found that indeed it has higher refractive index.



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발표코드: **Ⅲ37P244포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

An Efficient Synthesis of Optically Pure (1,2,3,4-tetrahydroquinoxalin-2-yl)methanol Derivatives

김종찬, 권지혜, 이백경, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

Various biological activities of substituted tetrahydroquinoxalin derivatives attracted attention from many chemists and biologists. The synthesis of various hydroxymethyl substituted tetrahydroquinoxalin was started from chiral 2-halo-N-((1-(1-phenylethyl)aziridin-2-yl)methyl)aniline, reductive amination products of the chiral 1-(1-phenylethyl)aziridine-2-carbaldehyde by various o-haloanilines. Regioselective aziridine ring opening with acetic acid and subsequent hydrolysis afforded 3-(2-halophenylamino)-2-(1-phenylethylamino)propan-1-ol. Intramolecular cyclization by Pd-catalyzed N-alkylation reactions of the 1-o-halophenoxy-2-amino-3-hydroxypropanes yielded (1,2,3,4-tetrahydroquinoxalin-2-yl)methanol derivatives in high yields.

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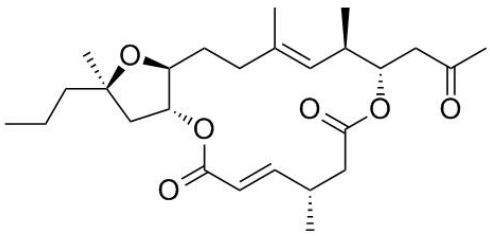
Expedient Synthesis of (-)-Amphidinolide X

정재훈

서울대 화학부

(–)-Amphidinolide X is one of the cytotoxic macrolides isolated by Kobayashi and co-workers from the laboratory-cultured dinoflagellates Amphidinium sp., which are symbionts of the Okinawan marine flatworms Amphiscolops sp.[1] Amphidinolide X is known to possess cytotoxic activity with IC50 values of 0.6 and 7.5 g mL–1 against murine lymphoma L1210 and human epidermoid carcinoma KB cells, respectively, in vitro. It is the only naturally occurring macrodiolide known to date that consists of a diacid and a diol unit, and it has been a popular target for synthetic studies because of its scarcity and unique structure. The most characteristic feature in the structure of amphidinolide X is the substituted 3-hydroxyoxolane structure, which is derived from a tertiary alcohol. The total synthesis of (–)-amphidinolide X was accomplished by employing a SmI2-mediated 5-exo cyclization of an aldehydo beta-alkoxyvinyl sulfoxide and a ring-closing metathesis reaction. [2]1.Tsuda, M.; Izui, N.; Shimbo, K.; Sato, M.; Fukushi, E.; Kawabata, J.; Katsumata, K.; Horiguchi, T.; Kobayashi, J. J. Org. Chem. 2003, 68, 5339-5345.2.Jung, J. H.; Kim, Y. W.; Kim, M. A.; Choi, S. Y.; Chung, Y. K.; Kim, T.-R.; Shin, S.; Lee, E. Org. Lett. 2007, 9, 3225-3228.



(–)-Amphidinolide X

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Absolute Configuration of Axial Chirality by Asymmetric Chiral Amino Alcohols

박현정, *김관묵

*이화여대 나노과학부 *이화여대 화학과*

Chiral recognition is particular importance in living systems which often show different activities toward a pair of enantiomeric drugs. The chiral recognition phenomena in solution have often been studied by NMR, UV, fluorescence, and circular dichroism spectroscopies. Among them, CD spectroscopy is used routinely in organic chemistry and biochemistry to determine structural differences arising from changes in chirality. A new type of biphenyl, in which 3-phenylurea units are attached to the 2,2'-biphenol group, has been synthesized. It exihibits axial chirality circular dichroism spectra upon intraction with asymmetric chiral amino alcohols. Thus, biphenyl is an excellent chirality sensor for amino alcohols. CD spectra obtained from the reactions with different amino alcohols are remarkably close. Uryl-based receptor showed the same tendency enantioselectivity toward the chiral amino alcohols. Energy calculation strongly supports complementary hydrogen bonding between alcoholic –OH and uryl two –NHs.

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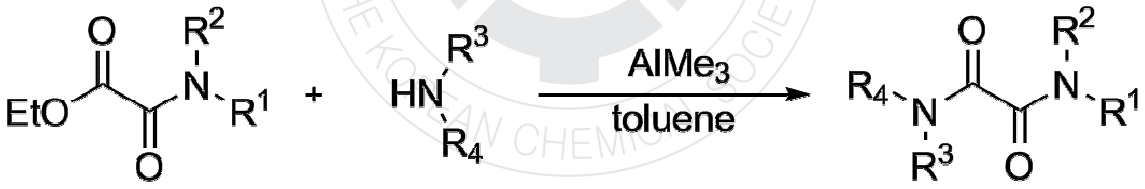
Aluminum amide mediated synthesis of unsymmetrical oxalyl bis-amide

이영석, *이상협

*대구가톨릭대 화학과 *대구가톨릭대 생명화학과*

Unsymmetrical oxalyl bisamide are found in many biologically active compounds both synthetic and natural. In this presentation, the conversion of oxalyl esters into unsymmetrical oxalyl bisamide using the aluminum amide reagents derived from a variety of amine species, including primary, secondary, aliphatic, and aromatic amines will be discussed.



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Enantioselective recognition of amino alcohols and chirality conversion of amino acids by carbonylurea-based imine receptor

Raju Nandhakumar, 김관묵

이화여대 화학과

Molecular recognition, especially chiral recognition, is one of the significant processes for diverse chemical and biological phenomena. The study of synthetic modeling systems for chiral recognition of amino alcohols, amino acids and amines is an area of ever increasing research activity. Although much progress has been made, it remains a challenge to develop highly stereoselective receptors for these substrates based on simple organic molecules. We designed novel chiral binol receptors based on uryl, thiouryl and guanidinium groups with additional phenylcarbonyl motif. These receptors enantioselectively binds an amino acid and converts L-amino acid to D-amino acid. The receptor binds the substrate via imine bond which is well known to be reversible. Resonance Assisted Hydrogen Bonding (RAHB) stabilizes the imine bond formed between the aldehyde of the receptor and amino group of the substrate. The uryl (thiouryl or guanidinium) group in the receptor binds carboxylate group of the substrate by another hydrogen bonding. The complementarity and directionality of those hydrogen bondings contribute substantially to the enantioselectivity. Furthermore, they are used to enantioselectively recognize various 1,2-amino alcohols. The synthetic details of these receptors and the molecular recognition properties studied by 1H NMR will be presented.

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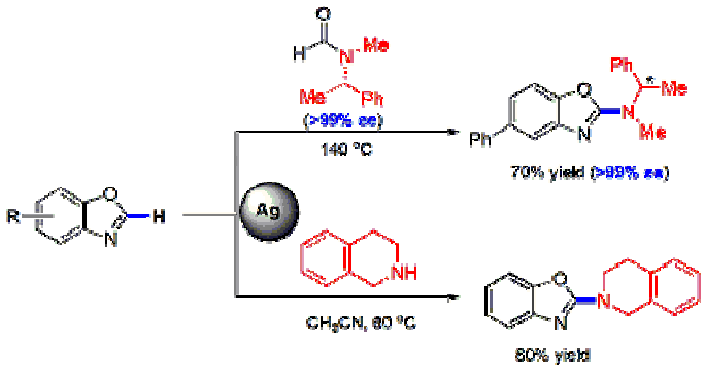
Silver-Mediated Direct Amination of Benzoxazoles: Tuning the Amino Group Source from Formamide to Parent Amines

조승환, 김지영, 장석복

KAIST 화학과

The construction of C–N bonds of (hetero)aromatic compounds are manifestly important transformation in synthetic chemistry since it can offer nitrogen-containing molecules of great interest in biological, pharmaceutical, and materials sciences. During the past decades, remarkable progresses have been made in the metal-facilitated C–N bond forming-reactions such as hydroamination or oxidative amidation of double or triple bonds as well as the Buchwald-Hartwig type cross couplings. Despite these significant advances, direct installation of amino groups or their surrogates on aryl- or alkyl C-H bonds is still highly challenging.In this poster, we will describe unprecedented Ag-mediated C–N bond formation of benzoxazoles by the decarbonylative coupling with formamides. On the basis of the mechanistic consideration, we also developed a direct amination protocol with parent amines under highly mild conditions.During the study of catalytic system for this reaction, we found that catalytic amount of other transition metal (eg. Co, Mn) with peroxide instead of using stoichiometric silver were employed for this amination reaction. Further insight into the scope and mechanism of catalytic system are now under investigation.



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Conformation and Fungicidal activity of Methoxyacrylate (MOA) Compounds

나춘섭, 박은묵, 김승태, *박규순

*영남대 화학과 *국민대 화학과*

Synthesis, conformational analysis and fungicidal activity of methoxyacrylate compounds (3-4) based on the natural product, Strobilurin A is described. Fungicidal activities of 3-4 against six representative fungal diseases and their comparative conformational analyses vs Strobilurin A are accounted.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **Ⅲ37P251포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Stereochemical Mechanism of Selenium Dioxide – Mediated Allylic Oxidation of Substituted Alkenes

박규순, *윤지훈, *심윤수, *나춘섭

*국민대 화학과 *영남대 화학과*

Stereochemical mechanism of the allylic hydroxylation of substituted alkenes with selenium dioxide was investigated by a combination of experimental and theoretical studies. A comparative analysis of two results showed that the overall transformation is controlled by two competing pathways: the major path corresponds to an anti-exo mode ene step followed by a stereospecific [2, 3]-sigmatropic rearrangement and the minor is via the rotation of allylselenic acid initially formed by the anti-endo attack of selenium oxide prior to the sigmatropic rearrangement.

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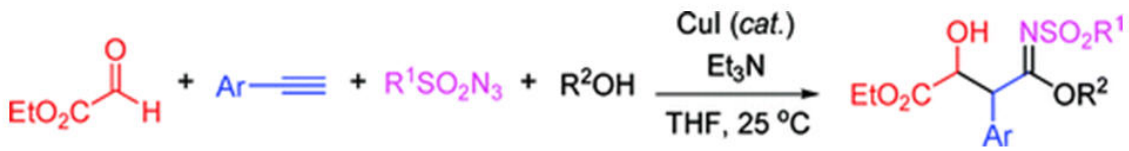
A New Entry of Copper-Catalyzed Four-Component Reaction: Facile Access to α-Aryl β-Hydroxy Imidates

박세흠, 조승환, 장석복

KAIST 화학과

α-Aryl β-hydroxy imidates are efficiently obtained by the four-component reaction of ethyl glyoxylates, aryl acetylenes, sulfonyl azides, and alcohols using a copper catalyst. The developed procedure is characterized by high selectivity, mild reaction conditions, a wide substrate scope, and an excellent functional group tolerance. Facile transformations of the obtained sulfonylimidate moiety to other carbonyl groups such as sulfonamides or esters were also demonstrated.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

A One-pot Synthesis of Pyrazolo[3,4-b]Pyridinyl Hetero-Biaryls

이상희, 박승범

서울대 화학부

Hetero-biaryl(HB) compounds are widely detected in numerous bioactive compounds, phamacophore of potential drugs. To obtain HBs, a large number of coupling methods, such as Kumada, Negishi, Stille and Suzuki coupling, have been developed over the past years. Although these reactions provide a lot of advantages like wide reaction scope, functional group compatibility and relative good yield, they have several limitations as follows; low efficiency with bulky substrate, toxicity from dealing with transition metal, extra effort for screening proper catalyst or additive, expense and safety issue. Therefore, we considered that development of another synthetic approach for HBs in convenience should be meaningful. Here in, synthetic method to afford pyrazolo-pyridinyl HBs from indole derivates as electrophile with aminopyrazole in one-step is described. Most of starting materials are commercially available or easily prepared. Through optimized reaction condition, we can synthesize various pyrazolo-pyridinyl derivates in moderately yield. Our strategy shows broad reaction scope and can be applied the substrate with various functional groups. We observed HBs containing not pyrimidyl but pyridinyl structure regioselectively, resulted from possibility of attacking aminopyrazole. As well as, it provides highly bulky ortho-substituent biaryls, which are usually regard as difficult to synthesize by widely used methods.

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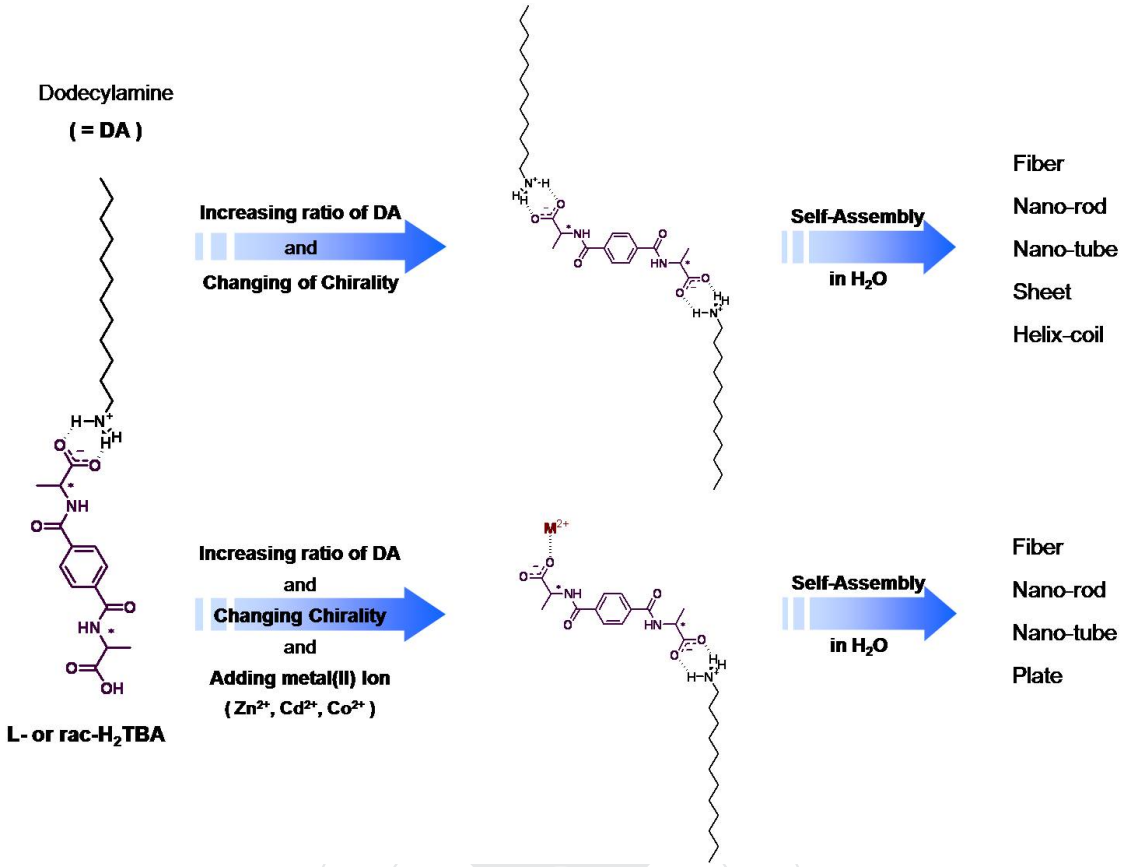
발표종류: 포스터, 발표일시: 금 10:30~12:30

Nano- and microstructure fabrication using three components system

장동학

서울대 화학부

Charged H-bonding complex between terephthaloylbisalaine (H_2TBA) and dodecylamine (DA) can self-assemble into nano- and micro-sized superstructures in aqueous solvent. These self-assembled superstructures were obtained by changing composition of complex between H_2TBA, DA, and metal ions. Composition of complex can be replaced with changing ratio of the component, chirality, and adding another component. Replacement of composition of complex could influence aggregation pattern to mutate self-assembled structures. It was confirmed with FT-IR spectra and powder-XRD analysis. As a result, two- and three-component complex between H_2TBA, DA, and metal ion can be simply fabricated various nano- and micro-sized superstructures. Especially, changing composition of amphiphiles such ratio, chirality can induce different self-assembled structure.



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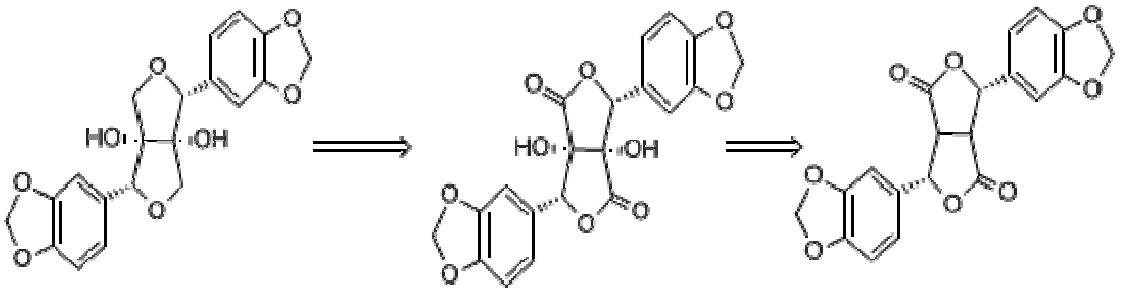
Synthetic Approach For (-) Wodeshiol

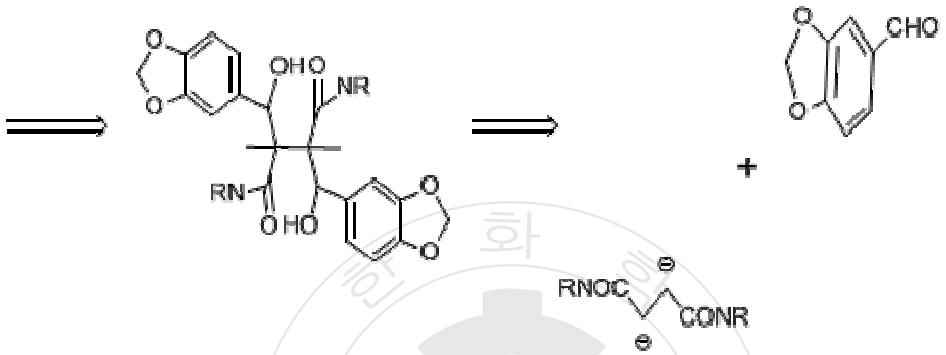
이순호, 박외숙

충북대 화학과

The goal of this research is to synthesize (-)-wodeshiol in its optical active form, which is a furofuran lignan possessing a variety of biologically active properties such as antitumor, antihypertensive, antioxidant, inhibition of platelet-activating factor (PAF), phosphodiesterase inhibitory, microsomal monooxygenase inhibitory effects for insects and pyrethrins insecticidal. In addition to its various of biologically active properties, It has an interesting structural features; four continuous stereogenic centers and two tertiary hydroxyl functions at the bridgehead carbon C-1 and C-5. The summary of synthetic method is as follows. Succinyl chloride is treated with freshly prepared S-(-)-4-benzyl-2-oxazolidinone to form the chiral auxiliary in the presence of n-BuLi to afford 1,4-bis-(4S-benzyl-2-oxo-oxazolidin-3-yl)butane-1,4-dione. Aldol reaction of boron Z-enolate (generated by treatment of N-acyloxazolidinone with Bu2BOTf and DIPEA) with piperonal affords the aldol product. The aldol product is subjected to intramolecular ring cyclization by treatment of KH_2PO_4 and H_2O_2 to give dilactone. Oxygenation of the lithium enolate generated from dilactone with MoOPH gives the dihydroxy dilactone which possesses two tertiary -OH functions. The reduction of the dihydroxy dilactone with DIBAL and subsequent treatment of triethylsilane affords (-)-wodeshiol.



(-) - Wodeshiol



NR = chiral auxiliary

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Design and Synthesis of Novel Polyphenolic compounds and Evaluation of their Biological activities

이보현, 우연지, *신용순, *연고흠, 이정은, **이봉호, **박정호

*한밭대 응용화학생명공학과 *한밭대 응용화학과 **한밭대 응용화학생명공학부*

Essential energy for living is derived from foods by the action of digestive oxidants, which also simultaneously generate harmful free radicals as Reactive Oxygen Species (ROS). Natural antioxidants reduce the risk of cancer, Alzheimer's disease, inflammatory-immune injury by ROS. They also protect body from damages. We have synthesized a series of polyphenolic compounds by connecting the two compounds through a amine linker. The new compounds were evaluated for their synergic effect in biological system such as antioxidant, AChE, BuChE and tyrosinase inhibition. The great synergic effect of new compound is shown on both antioxidant effect and anticholinesterase activity, but we could not observe the synergic effects on tyrosinase and elastase inhibition activities.

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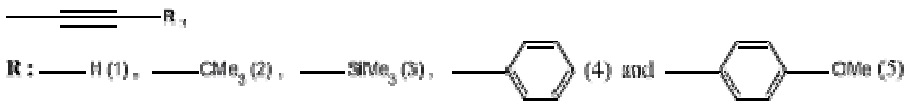
Optical Properties of 5,5'-Bis[(alkyl or aryl)ethynyl]-2,2'-bithiophene

전보람, 곽영우

경북대 화학과

The heteroaromatic systems containing the thiophene ring that have been reported are of great interest due to their luminescence and non-linear optical properties, as well as their liquid crystalline phase behaviour, which they owe to the bent nature of the thiophene moiety. In this presentation, we report the synthesis and optical properties of 5,5'-Bis[(alkyl or aryl)ethynyl]-2,2'-bithiophene. The target molecules were prepared by the Sonogashira cross-coupling of two equivalents of the substituted terminal acetylene with 2,5-dibromothiophene. All the compounds were characterized by NMR, IR, mass spectroscopy. Their absorption, emission spectra and quantum yields were also measured. The absorption maxima of the target molecules are moved to longer wavelength in DCM in the order 1 < 2 < 3 < 4 < 5. The HOMO-LUMO energy gaps of the target derivatives are theoretically calculated in the range of 0.10-0.13eV. There is a significant increase of the stretching absorption of C≡C bond of target molecules by the change of substituent in the order 1 < 3 < 4 < 5 < 2.



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Development of siRNA delivery system based on controlled release by photoirradiation

나희경, 유수윤, *이지언, 장홍제, 민달희

*KAIST 화학과 *KAIST 화학과*

Synthetic siRNAs have been considered as a new class of nucleic acid therapeutics for treatment of various infectious and genetic diseases. Even though it has been spotlighted as promising therapeutics with high potential, its application for clinical use is still limited due to the lack of efficient delivery system. In an attempt to overcome the drawback of the conventional delivery system, great deals of research have been done by many research group using nanomaterial-based delivery system. The tracking and controlled release of drug at the targeted site can be the main issues in the development of this delivery technique. In this presentation, we'll discuss a synthesis and efficiency of new siRNA delivery system based on inorganic nanoparticles which enable both controlled release at the specific site and novel tracking of drug loaded nanoparticles. With this delivery system, fine control over spatio-temporal release of siRNAs was achieved while modulating effective siRNA dose and minimizing off-target effect.

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Synthesis and characterization of organic thin-film transistors (OTFTs) based on quaterthiophene.

강문성, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

Conjugated oligomers and polymers represent one of the most important classes of advanced materials in recent years. The extensive amounts of research in the field are driven by the promise of low-cost processing applications that are typical of organic materials over their inorganic counterparts. The greatest advantage of organic materials is the diversity of structures and tunability of properties offered through molecular design. Recently, great studies have been made in areas such as thin-film transistors, light-emitting diodes, photovoltaic cells, and nonlinear optical devices. Thiophene-based materials have drawn considerable attention for their potential applications in the area of organic semiconductors because of their excellent chemical stability, high carrier mobility, and the ease of structural tuning to adjust the electronic, optical, and morphological properties. We synthesized new organic thin-film transistor material by Sonogashira reaction and Stille coupling reaction.

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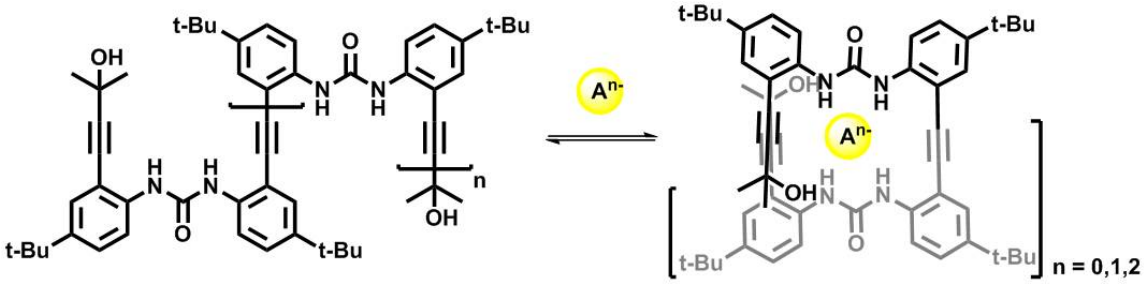
Synthesis and Anion-binding Properties of Bis(4-t-butylphenyl)urea Oligomers.

이혜원, 정규성

연세대 화학과

We have synthesized three bis(4-t-butylphenyl)urea oligomers consisting of one to three bis(4-t-butylphenyl)urea units that fold into helical structures and serve as synthetic foldamers. The bis(4-t-butylphen yl)urea oligomers were prepared by sequentially connecting the bis(4-t-butylphenyl)urea scaffold through ethynyl linkers. Upon folding, the bis(4-t-butylphenyl)urea form a tubular cavity where anion binding can occur through hydrogen bonding to the urea NHs and butynol OHs. We hypothesized that the number of bis(4-t-butylphenyl)urea determines the binding structure and subsequently, the anion binding affinity and selectivity. The structural properties of the bis(4-t-butylphenyl)urea derivatives were characterized by 1H NMR. The binding of anions within the helical cavity will be confirmed by a crystal structure of the bis(4-t-butylphenyl)urea derivatives with sulfate or chloride. Physical measurements detailing the folding and anion binding are reported here.



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Synthesis and Reaction of 1,5,3,7-Diazadiphosphocine-1,5-dicarboxylic acids

구제민, 송주현, 이도훈, 김윤영, 최순규, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

In order to synthesize new bioactive compounds and contrasting agents, reaction of glycine, aspartic acid and glutamic acid as an acidic amino acid with para formaldehyde and hypophosphorous acid were executed respectively. Products obtained as white solids were hydroxy-3,7-dioxoperhydro-1,5,3,7-diaza diphosphocine-1,5-diacetic acid, 2-[5-(1,2-dicarboxyethyl)-3,7-dihydroxy-3,7-dioxo-315.715-[1,5,3,7]-diazadiphosphocan-1-yl]-succinic acid and 3,7-dihydroxy-3,7-dioxoperhydro-1,5,3,7-diazadiphos-phocine-1,5-di-(2-glutaric acid). And esterfications of their acids by treatment of ethanol or benzyl alcohol were executed. We tried the synthesis of pyrrole by treatment of amine and 2,5-dimethoxy tetrahydrofuran with 1,5,3,7-Diazadiphosphocine-1,5-dicarboxylic acids.

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Synthesis and Decomposition of Imidazolidine-2,4,5-Trione derivatives

전은혜, 김용환, 이언진, 이용균, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

Generally ureas were widely used as starting materials for the synthesis of various pharmacologically active compounds. 2,4,5-Imidazolidinetriones are known for their germicide, plant growth regulator, and fungicide properties. In order to obtain a new agrochemical and bioactive Materials, we planned to synthesize 2,4,5-Imidazolidinetriones, and then will obtain new Di-ureas from decompose of 2,4,5-Imidazolidinetriones. Herein we report a facile one-pot and high-yield procedure for the decomposition of 2,4,5-Imidazolidinetriones under basic condition.

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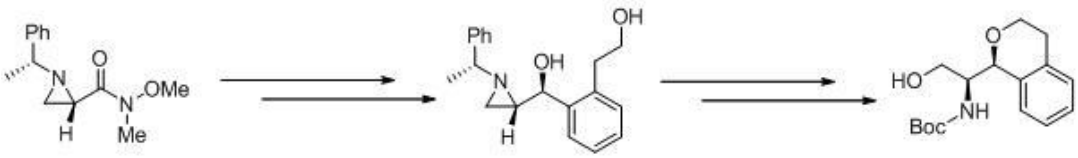
An Efficient Synthesis of Enantiomerically Pure isochroman-Derived Cyclic Amino alcohol scaffold from Aziridine

이상빈, 송혜경, 이백경, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

Various enantiomerically pure 2-acylaziridines were prepared efficiently from the corresponding aziridine-2-carboxylate via Weinreb's amide and the subsequent treatment of TBS protected 2-bromo phenethyl alcohol and n-BuLi. The carbonyl group of those 2-acylaziridines was stereoselectively reduced to give 1,2-amino alcohols with high diastereoselectivities and chemical yields. Then isochroman was synthesized via intramolecular cyclization by secondary alcohol and tosylated primary alcohol.



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A Study on the Carbonylative Suzuki Reaction by a Palladium Catalyst

방경모, 신은혜, 안현정, 변석인, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

The cross-coupling reaction is considered one of the most straightforward and general methods for the formation of carbon-carbon bonds. In this area, the transition-metal catalyzed three-component cross-coupling reaction between organometallic reagents, carbon monoxide, and organic halides is now considered a useful tool for ketone synthesis. Aryl, 1-alkenyl, 1-alkynyl, allyl, benzyl, and alkyl halides have been shown to be suitable electrophiles for this carbonylative cross-coupling reaction. We studied reactivities of alcohols through change of alcohols like phenol, benzyl alcohol, and 4-(hydroxymethyl)phenol by Suzuki carbonylation according to palladium catalyst.

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Synthesis of the ester derivatives of glucosamine

남선미, 이영행, 채규윤

원광대 화학과

The use of trifluoroacetic anhydride as a promoter for the acylation of glucosamine is reported. In this research, glucosamine in a pre-mixed solution of trifluoroacetic anhydride and carboxylic acid was heated at 70℃ with mechanical stirring. The ester derivatives of glucosamine were synthesised between glucosamine and various carboxylic acid derivatives.

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Preparation of chitosan esters derivatives in organic phase

안채영, 이영행, 채규윤

원광대 화학과

The trifluoroacetic anhydride is an effective promoter for the preparation of chitosan. Efficient acylation in a homogeneous solution is attained when the carboxylic acid of interest and trifluoroacetic anhydride are added, the latter in at least twice molar excess to the hydroxyl groups of the residues. The reaction necessitates prior heating of chitosan in acetic acid before the acylation reagent is added.Complete dissolutin is achieved whithin 1 h when powdered chitosan is heated at 70℃ in a mixed solution of carboxylic acid(s) and trifluoroacetic anhydride.Chitosan esters prepared are chitosan acetate, chitosan propionate, chitosan butylate, chitosan valerate, each from a solution of the respective reactants.

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Indolocarbazole-Amide Hybrid Foldamer Based on Intramolecular Hydrogen Bonding

석재민, 정규성

연세대 화학과

We synthesized indolocarbazole oligomers capable of folding into an ordered conformation to generate helical internal cavity in water. Now, we expanded this system by introducing amide linkers between indolocarbazole building blocks. By intramolecular hydrogen bonding between amide C=O and indolocarbazole N-H, the indolocarbazole oligomer folds into a pre-organized helical structure reminiscent of an alpha-helix. Synthesis and structural details will be described in poster.

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Preparation of highly stable folic acid conjugated manganese ferrite nanocrystals by one-pot reaction

록치충, 이영행, 채규윤

원광대 화학과

Magnetic colloidal nanocrystals have the potential to be utilized as probes and vectors for next-generation diagnosis and therapy. However, rendering these nanocrystals biocompatible has remained a challenge. Here, biocompatible water-soluble superparamagnetic manganese ferrite (MnFe2O4) nanocrystals with reactive moieties were prepared via a one-pot synthesis protocol by thermal decomposition of metal acetylacetonate precursor. We have achieved these carboxylic acid functionalized nanocrystals coupled with 9-aminoacridine and folic acid through 2,2'-(ethylenedioxy)-bis-ethylamine using carbodiimide. Utilizing Mössbauer spectroscopy, we show that these nanocrystals exhibit unique superparamagnetic behaviors. In addition, we demonstrate that nanocrystals are no significant toxicity and suggesting the biocompatibility. Based on this exploration, this high quality biocompatible manganese ferrite nano-platform can be potentially developed for application in MR imaging and drug delivery systems.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Application of Polymeric Retention Aid to Sheet Farming Process

임운식, *김성권, *이영행, *채규윤

*원광대 생명나노화학 *원광대 화학과*

Retention aids plays the leading role to improve papermachine performance and paper quality. Especially, the papermaking machine speed has ever been increasing to comply with the demand of higher productivity under maintaining high quality of paper. Thus, different types of the polymers as retention aids were applied to sheet farming process. To compare the retention efficiency of them, first-part retention ratio, solid and ash contents, and cationic demand(CD) were measured. The results of a comparative analysis between retention ratio and anion trash removed efficiency are also discussed.

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Enzymatic Assaying Using (glyco)peptide microarrays

성정원

연세대 화학과

The majority of proteins are posttranslationally modifide, the most abundant modification being the attachment of carbohydrates to the side chains of asparagine, serine and threonine. By far one of the most abundant carbohydrate is found in naturally occuring O-glycopeptide is the 2-acetamido-2-deoxy-D-glucose(GlcNAc) residue, which is α-O-glycosidically bound to serine or threonine. Based on this research, the (glyco)microarrays are fabricated for studying (glyco)peptide substrate specificity for O-GlcNAc transferase(OGT) and OGlcNAcase(OGA). For this study, FmocSer(β-GlcNAc$(OAc)_3$)-OH, FmocSer(β-GlcNAz$(OAc)_3$)-OH, UDP-OGlcNAz were successfully synthesized. And (glyco)peptide library were synthesized manually. we first studied (glyco)peptide substrate specificity for OGT and OGA using (glyco)peptide microarrays for prepared several (glyco)peptides. The (glyco)peptide substrate specificity could be studied through click chemistry of fluorescence linked triple bond and azido group of O-GlcNAz.

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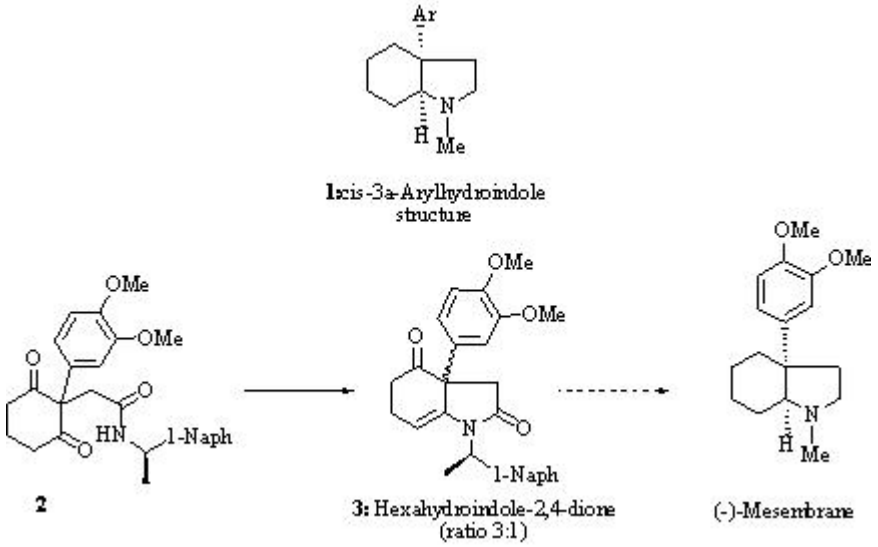
Diastereoselective Route to cis-3a-arylhexahydroindole Structure:Synthesis of (-)-Mesembrane

Le Anh Tuan, 김건철

충남대 화학과

Over the years, the Sceletium alkaloids have still gained much attention from synthetic chemists due to the interesting cis-3a-arylhydroindole skeleton (1).1 The problematic challenge needed to overcome is the stereoselective construction of the sterical quarternary carbon center (C3a). During the syntheses of members of this alkaloid family, a number of methods have been published,2 however, a more efficient, stereoselective strategy still needs to develop.In our research, the key intermediate 1,3-diketone amide (2) prepared by palladium-catalyzed coupling reaction followed by Claisen rearrangement and amide synthesis, provided a (3:1) diasteroisomeric mixture of tetrahydroindole-2,4-diones (3) under thermodynamically controlled-condition. Deoxygenation of the ketone group and reduction with Et3SiH in CF3COOH furnished the cis-3a-aryloctahydroindol-2-ones, which led to the synthesis of (-)-mesembrane.References:1) a) Jeffs, P. W. In the Alkaloids; Rodrigo, R. G. A., Ed.; Academic Press: New York, 1981; Vol. 19, 1-80. b) Hoshino, O. In the Alkaloids; Brossi, A., Ed.; Academic Press: New York, 1987; Vol. 51, 251-376.2) a) Saito, M.; Matsuo, J.; Ishibashi, H. Tetrahedron 2007, 63, 4865. b) Padwa, A.; Brodney, M. A.; Dimitroff, M.; Liu, B.; Wu, T. J. Org. Chem. 2001, 66, 3119. c) Mori, M.; Kuroda, S.; Zhang, C. S.; Sato, Y. J. Org. Chem. 1997, 62, 3263.



대한화학회 THE KOREAN CHEMICAL SOCIETY

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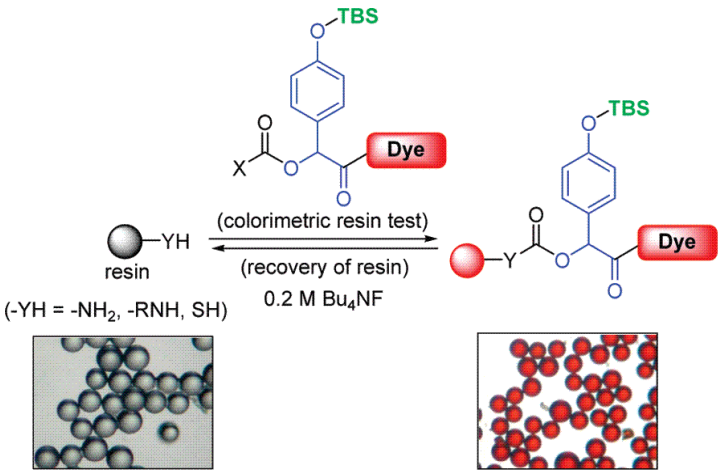
Nondestructive, Colorimetric Monitoring of Amines and Thiols on a Solid Support

양세진

연세대 화학과

To develop simple and rapid methods for monitoring functional groups on the resin-supported molecules without the need for specialized instrumentation,colorimetric monitoring tools have been explored.Colorimetric resin tests have been successfully employed to monitor the progress of on-resin reactions, most of these methods are limited by the fact that samples can not be reused for the next reactions after resin tests, and as a consequence, the need for repetitive colorimetric resin testscauses a large sample loss. Therefore, the development of a rapid, simple, and nondestructive method to detect the progress of on-resin reactions remains as a significant challenge. A new, nondestructive, highly sensitive method for colorimetric monitoring of primary amines, secondary amines, and thiols on a solid support was developed. The resin used in this method is simple regenerated for the repetition of the reaction or an ensuing reaction. By using this new method, several peptides containing secondary amide linkages and C-terminal hydrazide groups were prepared in high purities and yield.



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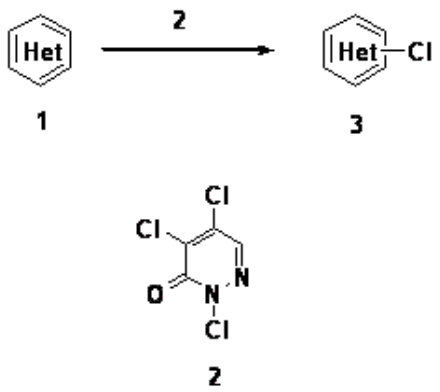
Chlorination of Aromatics Using 2-Chloropyridazin-3(2H)-ones

박송은, 김보람, 이형근, 김은정, 윤용진

경상대 화학과

An aromatic compounds involving halogens are very important in synthetic chemistry. Electrophilic halogenations agents are useful for the halogenations of aromatic compounds. Recently, 2,4,5-trichloropyridazin-3(2H)-ones as electrophilic chlorination agent reported. We attempted to chlorination of some aromatic compounds such as pyridine, thiophene and phenol, etc. using this compound. In this poster, we report the results for the chlorination of some aromatic compounds using 2,4,5-trichloropyridazin-3(2H)-ones.



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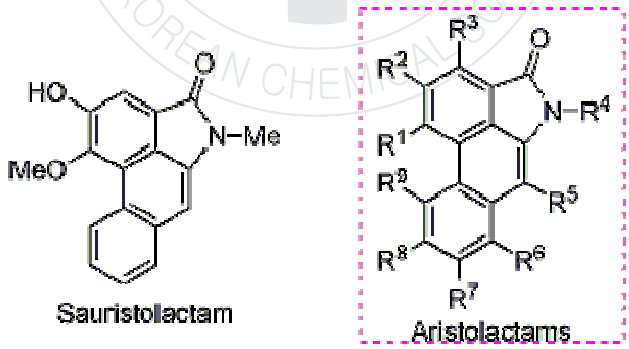
A Concise and Practical Synthesis of Sauristolactam

김태정, *김좌겸, *김범태, *허정녕

*한국화학연구원 의약화학 *한국화학연구원 신약연구단*

Sauristolactam belongs to a large family of aristolactam alkaloids, which consist of a core phenanthrene lactam ring system. Sauristolactam was isolated from the aerial part of *Saururus chinensis*. Theses aristolactam alkaloids including sauristolactam possess an interesting array of biological properties such as anticancer, anti-inflammatory, antiplatelet, and neuro-protective activities. In the present study, we describe the efficient synthetic route toward sauristolactam employing a one-pot Suzuki-Miyaura coupling and aldol-type condensation reaction.



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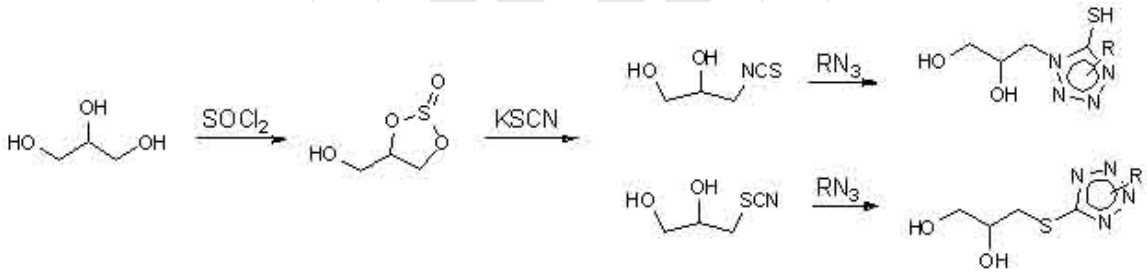
Tetrazole Synthesis of Diol and Triol *via* Cyclic Sulfites

이헌정, *이제우, 경영수

*강릉대 화학과 *강릉대 화학신소재학과*

Diols and triols are easily prepared and found as natural resources such as glycerine. These alcohols can be transformed to cyclic sulfites in high yield with thionyl chloride. Reaction of cyclic sulfites with nucleophies such as thiocyanate, isothiocyanate and halides gave products of substitution in good yield. Thiocyanate and isothiocyanate substituted compounds can be used synthesis of tetrazoles with azide.



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Isolation, synthesis, and structural assignment of Boletulactol: new natural product from Boletus pseudocalopus

tittov, 문석식

공주대 화학과

Two new bioactive stereo isomers named boletulactol A and boletulactol B were isolated from the ethyl acetate fraction of mushroom Boletus pseudocalopus by chromatographic methods. The relative stereo structures of the isolates were established by 1D and 2D-NMR techniques along with UV, IR, HRTOFMS, and specific rotation. The absolute stereochemistries of these Boletulactols were confirmed by synthesize of all possible stereoisomers of boletulactols. Boletulactols were synthesized in three steps from Farnesol. The absolute stereochemistry of the boletulactol A and boletulactol B were confirmed by comparing the specific rotation of synthesized boletulactols with the isolated boletulactols.

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Research on Stereoselective Acylation of Aminodiol Derivatives by the Neighboring Effect of *N*-Protecting Groups

강선영, 김현아, 최문실, 조다혜, 전근호

숭실대 화학과

We research on the selective acylation reaction of amino-1,4/5-diol with different types of N-protecting groups. In the acylation reaction, 4-OH was preferred when chloroacetyl chloride, stronger acylation reagent, was used with N-protecting groups such as p-nitrobenzen sulfonyl (Nosyl), p-toluene sulfonyl(Tosyl), t-butoxycarbonyl(Boc) . On the other hand, benzoic anhydride, weaker acylation reagent, has tendency to produce ester with 1-OH using the same N-protecting groups. Here, Steric hindrance seems to have larger influence on the selection of the hydroxyl group position with stronger acylating reagent. Therefore, less crowded 4-OH was preferred. However, in case of weaker reagent, 1-OH is dominantly acylated because it can be aided from the electrowithdrawing effect of neighboring N-protecting group. In this point of view, benzothiazole sulfonyl (Bts), a recently introduced N-protecting group, is expected to give stronger stereoselectivity to 1-OH because it has higher electrowithdrawing neighboring effect than Nosyl, Tosyl, and Boc.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Selective Anion Binding Induces Helical Folding in Indolocarbazole Oligomers

김준일, **juwarker**, 정규성

연세대 화학과

An ambitious goal of supramolecular chemists is the mimicry of structure and function of biomacromolecules such as proteins and enzymes. One strategy involves the design of synthetic, modular molecular building blocks and their implementation in the formation of stable, higher order structures such as helices. We describe the success achieved by the indolocarbazole moiety in generating synthetic helical structures known as foldamers. Rational design of an indolocarbazole monomer containing NH and OH hydrogen bond donors, followed by synthetic extension results in the formation of a functional oligomer. Hydrogen bonding to anions within the cavity formed upon folding drives subsequent aromatic stacking and a helical conformation. Here, structural confirmation and anion binding studies are reported and discussed. Selective sulfate binding is observed in the solution and solid state due to complementarity of the foldamer cavity with the anionic guest geometry.

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Isolation and Characterization of Bioactive Compounds from the Seeds of Angelica acutiloba

Mozahidur Rahaman, Md.Maniruzzaman Manir, 문석식

공주대 화학과

Activity-directed fractionation and purification were employed to identify cytotoxic active compounds from the seeds of Angelica acutiloba. Air-dried seeds of A. acutiliba were extracted with methanol and then separated into hexane, n-butanol, and water layers. Among them, only the hexane layer showed strong cytotoxicity against human lung cancer cell line A549 and subjected to separation and purification using various chromatographic techniques. Nine compounds showing cytotoxic activity were isolated through a series of silica, reversed phase C18 column chromatography, preparative C18 HPLC and characterized by IR, UV, HR-TOF-MS, specific rotation and 2D-NMR.

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Synthesis and spectroscopic properties of 9,9-dibutyl-7-(phenylamino)-9H-fluorene-2-sulfonic acid

정혜미, 고광희

충남대 화학과

Molecules that can have photoinduced intramolecular charge transfer (ICT) excited states usually exhibit a large dependence of their fluorescence properties on the environment, and have drawn a great deal of interest in their use as fluorescent probes, sensors, and components of light activated switches. Here, we report the synthesis of various novel water-soluble 9,9-dibutyl-7-(phenylamino)-9H-fluorene-2-sulfonic acid as candidates for highly sensitive fluorescent probes for applications with biological molecules. Their absorption and fluorescence behaviors are also investigated.

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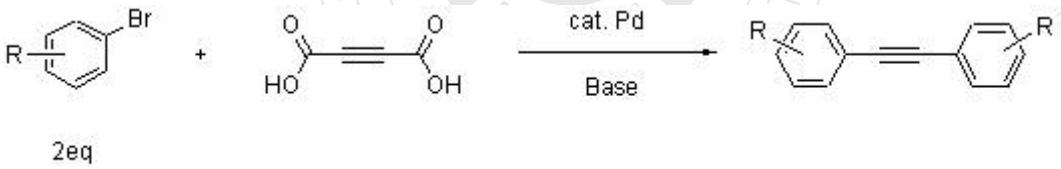
Palladium-Catalyzed Decarboxylative Coupling Reation with Acetylene dicarboxylic acid

배고운, 이선우

전남대 화학과

Goun Bae, and Sunwoo Lee*Department of Chemistry, Chonnam National University, Gwangju 500-757, Republic of Koreasunwoo@chonnam.ac.krWe synthesize a symmetric diaryl alkyne derivatives from acetylene dicarboxylic acid. Decarboxylative coupling of sp-sp2 carbon is possible by palladium-catalyst. The desired products were obtained in moderate to good yield.



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Synthesis of Bis(4-substitutedphenyl)ethynylene by palladium catalyzed cross-coupling

손종우, 김수광, 염을균, *김경만

*충남대 화학과 *한국화학연구원 에너지소재센터*

Bis(4-substitutedphenyl)ethynylene derivatives are interesting compounds, which have delocalized electrons, pi-conjugation systems through the carbon skeletal. These compounds are monomers of semiconducting materials, molecular sensors, molecular wires, and fire-retardant additives. We obtained symmetrical and unsymmetrical bisphenylethynylene compounds by using palladium and copper catalysts. In our study, we attempted Sonogashira reaction to obtain not only unsymmetrical bisphenylethynylene derivatives which are expected to have fire-resistant property but also diphenylbutadiyne compounds.

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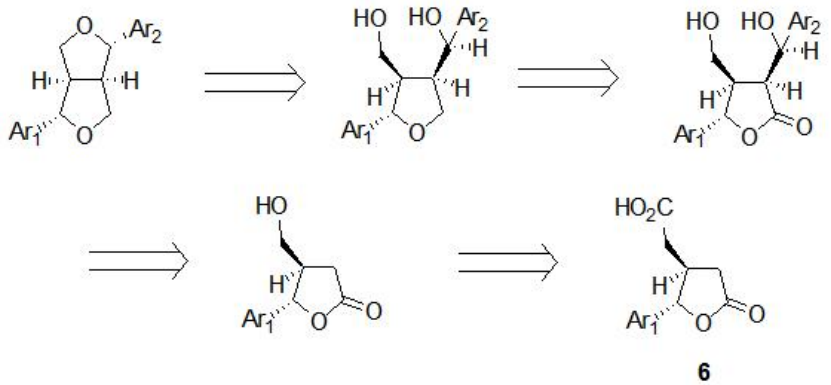
Synthetic Approach For (+) Fargesin

박수용, 박외숙

충북대 화학과

The purpose of this research is to deverop an asymmetric total synthesis of (+)-Fargesin. (+)-Fargrsin which is an unsymmetrically substituted axial-equatorial furofuran lignan has anticancer, antiypertensive and antioxidant effect. Its synthetic method is an follows. S-(-)-4-Benzyl-2-oxazolidinone was deprotonated with n-butyl lithium and reacted with β-carbomethoxypropionyl chloride to give 1-(4S-benzyl-2-oxazolidin-3-yl)-4-methoxybutane-1,4-dione. This 1,4-dione was treated with Bu_2BOT_f and DIPEA to form z-boron enolate which was reacted with piperonal to obtain (2S,3S)-2-piperonyl-5-oxotetrahydrofuran-3-carboxylic acid. This acid was reduced with BMS to the corresponding alcohol. This alcohol was transformed to silyl ketene acetal. The silyl ketene acetal was reacted with 3,4-dimethoxybenzaldehyde in the presence of (R)-BINOL-Ti(IV)Cl_2(catalytic enantioselective Mukaiyama aldol reaction) to produce diol-lactone compound. This diol-lactone compound will be transformed to (+)-Fargesin after reduction and cyclization.

Retrosynthetic Analysis



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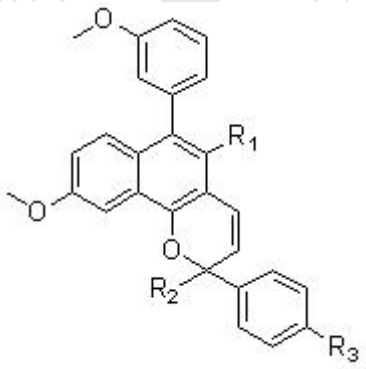
A synthesis of novel photochromic naphthopyran-spiro compounds, and its spectroscopic characteristics

도준호

홍익대 화학시스템공학

The photochromic dyes exhibit a reversible change in color thereby enable their application in the field of molecular switches and UV screening glass. In an effort to develop a novel photochromic dye, the naphtopyran-spiro structural system have been designed and synthesized; whereR1 is alkyl group, R2 is aryl group, and R3 is amino group. The structures were elucidated through NMR spectra and X-ray crystallography and their physical and spectroscopic properties were characterized.



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Bioactive (alcohol dehydrogenase inhibitory and antioxidant active) compounds from Green tea leaves.

Md.Maniruzzaman Manir, Mozahidur Rahaman, 문석식

공주대 화학과

A Phytochemical investigation of the methanolic extract and its n-butanol-soluble fraction of Green tea leaves led to the isolation of highly alcohol dehydrogenase (ADH) inhibitory and antioxidant active compounds through a series of reversed phase column chromatography and preparative C-18 HPLC. The structures of these compounds (flavanols and flavonoids like quercetins, kaemferols, myricetins and their derivatives) were determined using spectroscopic analyses (UV, IR, and NMR), with comparison of their spectral data with previously reported values. Isolated compounds showed good inhibitory activities (IC50) of 0.39-35 ug/mL whereas ADH inhibitor, 4-methylpyrzole, showed the IC50 of 326.6 ug/mL against alcohol dehydrogenase (ADH). ADH and radical scavenging activity against DPPH will be presented during presentation..

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발표코드: **Ⅲ37P286포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Cytotoxic compounds from the roots of Lycopus rasissimus (Lamiaceae)

V.S.Jamal Ahamed, 김영섭, 문석식

공주대 화학과

Nine homologous triterpenoid derivatives were isolated from the roots of Lycopus ramosissimus (Lamiaceae) by the chromatographic methods such as silica gel open column and C18 HPLC. The stereo-structures of the isolates were established by 1D and 2D-NMR techniques along with UV, IR, HRTOFMS, and specific rotation. Especially, direct and long range heteronuclear analysis (HMQC and HMBC NMR experiments) confirmed the connectivity in their structures. Compounds 1-6 showed strong cytotoxicity against human lung cancer cell line A549 with the IC50 of 5.1, 6.75, 3.2, 15.5, 5.79, and 5.0 g/mL, respectively.

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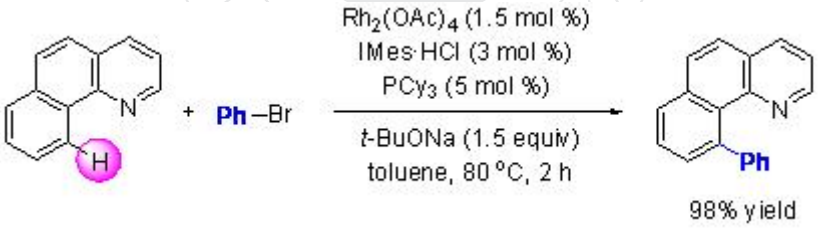
발표종류: 포스터, 발표일시: 금 10:30~12:30

Rh(NHC)-Catalyzed Direct Intermolecular Arylation of sp^2 and sp^3 C-H Bonds with Chelation Assistance

김민, 곽재성, 장석복

KAIST 화학과

A new catalyst system of rhodium was developed for the chelation-assisted direct intermolecular arylation with the help of electron-rich N-heterocyclic carbene (NHC) and phosphine ligands. The reaction is operationally simple, and proceeds smoothly under mild conditions to afford mono- or diarylated products in excellent yields. The present protocol could be readily applied for the arylation at the sp^2 or sp^3 C-H bonds of 2-pyridyl-containing aryl, vinyl, or alkyl moieties.



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Synthesis of diarylacetylene derivatives by palladium catalyzed crosscoupling reaction with Pd-NaY zeolite catalyst.

김수광, 손종우, 염을균, *김경만

*충남대 화학과 *한국화학연구원 에너지소재센터*

Condensed polyaromatic compounds have been estimated as promising fire-proof material for the pollution issues. Therefore, much attention has been paid to the development of efficient methods for preparing diarylacetylene derivatives. In this research, we studied efficient and economically synthetic method for the diarylacetylene compounds. We will discuss reaction conditions and palladium catalyst recycle test.

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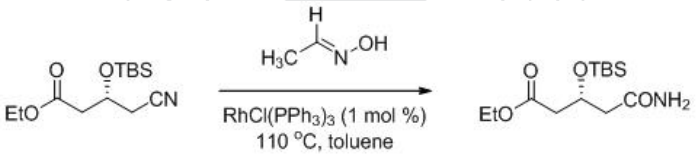
Anhydrous Hydration of Nitriles to Amides using Aldoximes as Water Surrogate

이진우, 김민, 장석복, 이희윤

KAIST 화학과

Based on the mechanistic insight from our report of the effect of nitrile additives in the rearrangement of aldoxime into amides, we speculate a possibility of utilizing aliphatic aldoxime as the water surrogate for the anhydrous hydration of nitriles. As the result, we developed anhydrous and neutral hydration protocol that is mild enough to accommodate base or acid sensitive functional or protective groups.(1) M. Kim, J. Lee, H.-Y. Lee, S. Chang, *Adv. Synth. Catal.* 2009, *351*, 1807-1812.



일시: 2009년 10월 28~30일(수~금) 3일간
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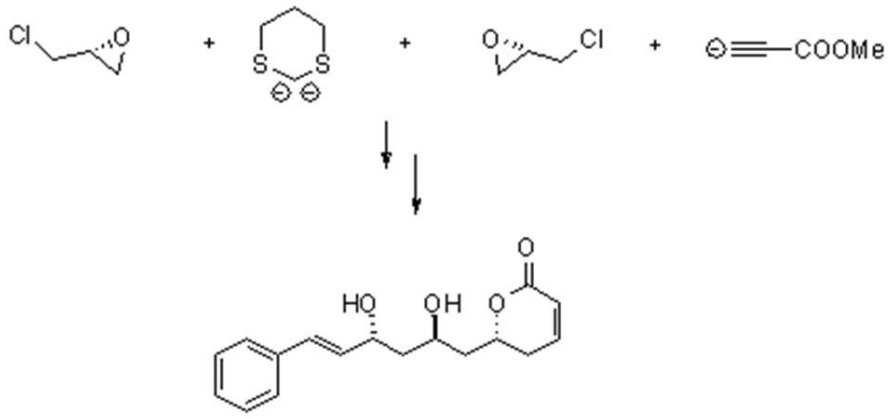
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Epichlorohydrin in Versatile Synthesis of Polyol Natural Products

Murugan R.N., 이희윤

KAIST 화학과

Natural products that contain α, β-unsaturated δ-lactones moiety possess a wide range of biological activities presumably due in part their electrophilic nature as Michael acceptors. Recently, we have established a simple synthetic route for the synthesis of δ-lactones enantioselectively using the cheap, commercially available enantiopure epichlorohydrin as a starting material. Herein we describe the synthesis of Cryptomoschatone D2 and its diastereomers using 11steps. The triol backbone could be made from the carbonyl dianion equivalent like dithiane anion that reacts with the two epichlorohydrin together to produce 1,3,5-triols stereoselectively and depending on the reaction order and subsequent reactions, all the diastereomers of 1,3,5-triols can be synthesized. References: (1) Lee, H-Y et al. *SynLett*, **2009**, *2*, 249.



Cryptomoschatone D2

일시: 2009년 10월 28~30일(수~금) 3일간
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발표종류: 포스터, 발표일시: 금 10:30~12:30

Labeled Pyronaridine Tetraphosphate for Metabolic Studies

박상현, 정연준

한국원자력연구원 방사선생명공학연구부

Pyronaridine tetraphsphate (PNDP) is being developed for the treatment of malaria. The antimalarial activity of PNDP has been attributed to both blood schizontocidal and gametocytocidal activities. An efficient reaction has been devised for H-2 and C-13 labeled PNDP using a microwave irradiation technique resulting in the significant rate enhancements and the high product yields. Instrumental analysis showed satisfactory results. The labeled compounds should be useful for preparing internal standard for mass spectral quantification and for metabolic studies.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

A new Highly selective Al(III) ion chemosensor using triazole ring

김상훈, 김종승

고려대 화학과

We have synthesized a new fluorescent compound 1 containing two 1,2,3-triazole rings, and measured its optical properties upon the metal ions. The complexation of Al(III) ion induced a broad new absorbance band and fluorescence enhancement. Furthermore, compound 1 was also selective to Al(III) over other metal ions.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

pi-Extended, Expanded porphyrins : Synthesis of Rubyrin, Rosarins and Sapphyrins

이창희, 기세영

강원대 화학과

New expanded porphyrins analogues with pi-system extended, have been synthesized and characterized. The synthesis is accomplished by acid-catalyzed condensation of naphthobipyrrole, aromatic aldehydes and pyrrole. It was found that the product was dominated by the ratio of the three starting material. When naphthobipyrrole and aromatic aldehyde was condensed, the rosarin was the only isolatable product. On the other hand, the condensation of naphthobipyrrole, aromatic aldehyde and pyrrole resulted in the formation of two different products; rubyrin and pyrrole-inverted sapphyrin. The product ratio (rubyrin/sapphyrin) varies depending on the ratio of the starting material. The two reversible pyrrole-ring flipping was observed depending on the acid concentration. This transformation of the macrocycle involves flipping of one pyrrole unit and dramatic shifts of N-H signal and beta-pyrrole-H.

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Design and synthesis of fluorescent nucleotide 3'-*O*-allyl linked dye as a reversible terminator for DNA sequencing

김택수

KIST 케모인포매틱스

To overcome the limitations of the Sanger sequencing technology, a variety of new methods have been investigated. SBS (Sequencing By Synthesis) is an effective method as the next generation DNA sequencing. We design and synthesis of 3'-*O*-allyl linked fluorescent nucleotide analogue, 3'-*O*-allyl-dTTP and 3'-*O*-allyl-dATP as a reversible terminator. The nucleotide is efficiently incorporated by DNA polymerase into a growing DNA strand to terminate the polymerase reaction.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and properties of phosphorescent heterocyclic Ir(III) complexes

송민호, 염을균

충남대 화학과

Conventional fluorescent OLEDs have low efficiencies and limitation of the practical use in panel display. Recently many research groups are interested in developing new phosphorescent OLED materials, which in principle could be three times more efficient, thus displaying enhanced performance and greater energy efficiency. we synthesized new phosphorescent Ir(III) complexes and characterized electroluminescent properties for the synthesized Ir complexes.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Syhthesis of Halogenated Pentacene Derivatives for the Patterning on the Solid Surface

구현서, 황광진

홍익대 화학시스템공학과

The research of organic semiconductor vased on the hetero-compound has been proceeded for the application in Organic Field Effect Transistors(OFETs). Pentacene derivatives that consists of six membered plane ring have high mobility based in the conjugation of π electron and studied as the material of the p-channel. However, pentacene derivatives has low solubility and, limits to synthesize or applicate the functional products. To solve this problem and provide a new potential patterning materials, halogenated pentacene derivatives were designed and synthesized. Halognenated pentacenequinone with Tetrabromo xylene derivatives are reacted with , 1,4-benzoquinone and subsequently deoxygenated to give 2,3,9,10-tetrabromopentacene.

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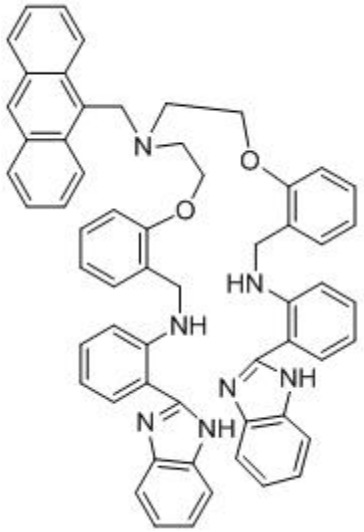
발표종류: 포스터, 발표일시: 금 10:30~12:30

Benzimidazole-based dipodal receptor as a highly selective fluorescent probe for Fe(III)

이두연, 장두옥

연세대 화학과

The synthesis of fluorescent sensors for transition metal ions is gaining impetus because of their biological and environmental importance. There are numerous reported examples of fluoroionophores which show excellent selectivity for transition metals.In the present investigation, we have developed a new benzimidazole-based mixed donor dipodal receptor. The rationale behind the design of this receptor is that it bears mixed donor groups and is flexible, bearing an anthracene moiety on one pod as a fluorophore was synthesized. These characters of present receptor will provide that variable coordination modes for different metal ions and expected for highly fluorescence selectivity.The receptor exhibited fluorescence emission which is quenched upon addition of Fe(III), but it showed no significant changes on addition of other metal ions such as Ag(I), Ca(II), Co(II), Cu(II), Mg(II), Ni(II) and Zn(II).



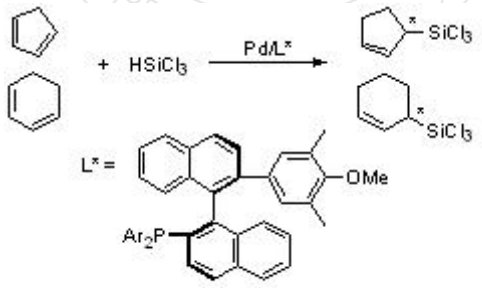
일시: 2009년 10월 28~30일(수~금) 3일간
장소: 대전컨벤션센터
발표코드: **Ⅲ37P298포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Asymmetric hydrosilylation of conjugated 1,3-dienes with chiral palladium catalysts with chiral Ar-MOP ligands tuned electronically

박훈서, 김종훈, 한진욱

한양대 화학과

Hoon Seo Park, Jong Hoon Kim, Jin Wook Han*Department of Chemistry, Hanyang University, Seoul 133- 791, Koreajwhan@hanyang.ac.krPalladium-catalyzed asymmetric hydrosilylation of olefins provides one of the most efficient routes to enantiomerically enriched organosilicon compounds. Enatioselectivities of the hydrosilylation is highly dependent upon chiral ligands coordinated with palladium. Chiral Ar-MOP derivatives with different electron-donating ability were tested for asymmetric hydrosilylation of conjugated 1,3-dienes in this study.



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발표코드: **Ⅲ37P299포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

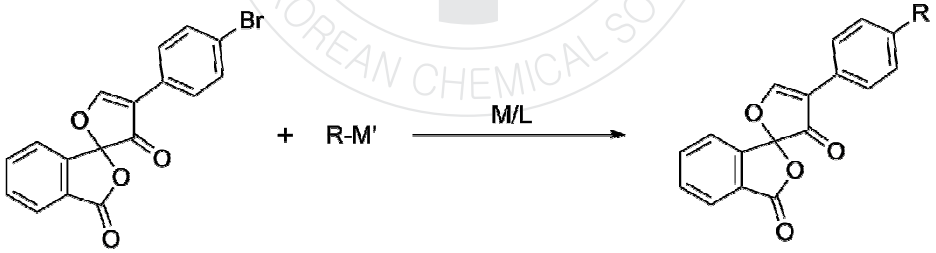
Transition metal-catalyzed synthesis of new fluorescamine derivatives[발표취소 10-12]

신동근, 한진욱, *유호정, 진휘원

*한양대 화학과 *한양대 화학*

Fluorescamine has been widely [illegible] detection of primary amines and peptides. Fluorescamine, which is [illegible] nary amines to form pyrrolinones which yield strong fluorescence at [illegible] vatives were prepared by various cross-coupling reactions catalyzed [illegible]

발 표 취 소



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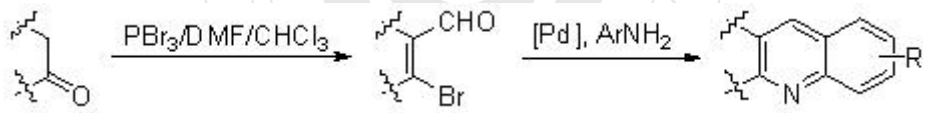
발표종류: 포스터, 발표일시: 금 10:30~12:30

A Palladium-Catalyzed Expedient Synthesis of Quinolines from β-Bromovinyl Aldehydes and Anilines

김효보, 김태균, 조찬식

경북대 응용화학과

β-Bromovinyl aldehydes, which are readily prepared from ketones via the bromo analogue of Vilsmeier reaction, are arylaminated and cyclized with anilines in DMF at 110 ℃ in the presence of a catalytic amount of a palladium catalyst to give the corresponding quinolines in good yields.



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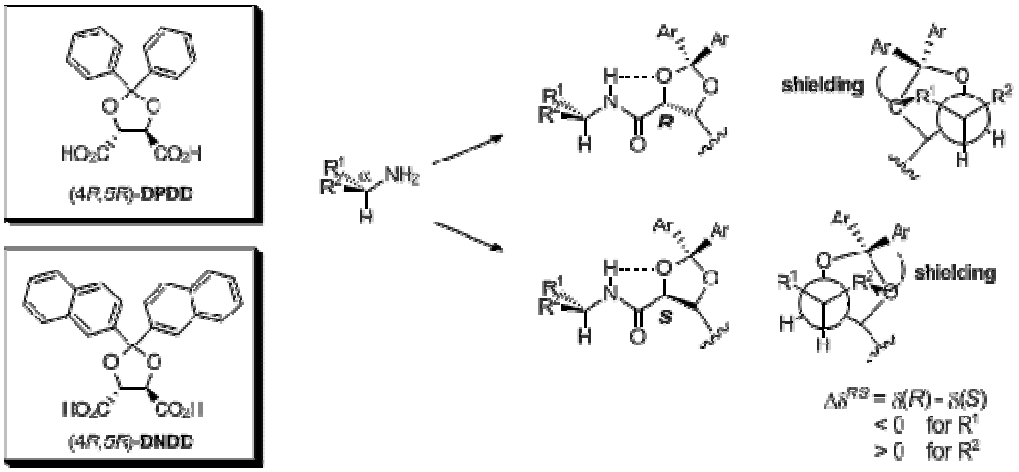
발표종류: 포스터, 발표일시: 금 10:30~12:30

Chiral Derivatizing Agents Drived from Tartaric Acid: A Simple and Tunable Approach for the Determination of the Absolute Configuration of Primary Amines

심유진, 최기항

고려대 화학과

A new chiral auxiliary reagent, 2,2-diphenyl-[1,3]dioxolane-4,5-dicarboxylic acid (DPDD) has been prepared from dimethyl tartrate and benzophenone through a simple two-step synthesis. DPDD amides of α-chiral primary amines showed significantly different 1H NMR chemical shift values depending on the stereochemistry of the derivatizing agent. The chemical shift difference (DdRS) between (4R,5R)- and (4S,5S)-DPDD amides could be correlated to the absolute configuration of the chiral amine on the basis of the molecular conformation stabilized by intramolecular hydrogen bonding. Unlike other reagents developed so far, preparation of more efficient reagents with enhanced anisotropic effect was very simple and straightforward. The amides of DNDD, which was prepared from 2,2'-dinaphthyl ketone instead of benzophenone, showed significantly larger DdRS than the corresponding DPDD amides making more error-free assignment of the absolute configuration possible.



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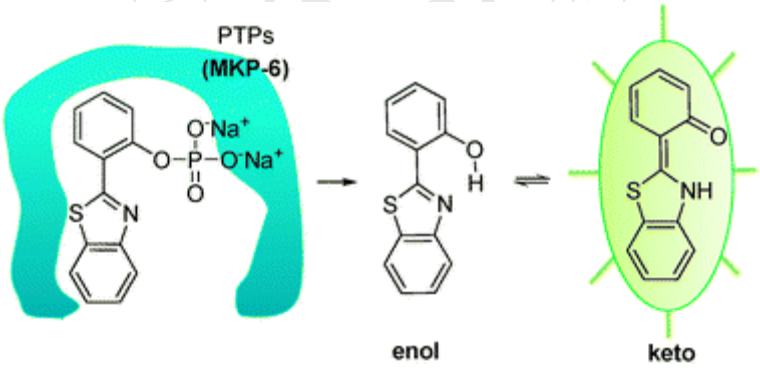
발표코드: **Ⅲ37P302포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A highly selective fluorescent ESIPT probe for the dual spcificity phosphatase MKP-6

김태일

단국대 화학과 유기화학전공

A highly selective fluorescent probe for a protein tyrosine phosphatase(PTP) was designed by a simple phosphorylation of the 2-(2'-hydroxyphenyl)benzothiazole(HBT) chromophore: upon selective enzyme hydrolysis, an exctited-state intramolecular proton transfer(ESIPT) process occurs, resulting in a large Stokes shift.



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CB[6]-Based Glycopseudopolyrotaxanes: Towards Antiadhesion Therapy

김지연, 안영주, *이돈욱, **박경민, 김기문

*포항공과대 화학과 *포항공과대 시스템생명공학부 **포항공과대 첨단재료과학부*

Extracellular carbohydrate-protein interactions are critical in cellular communication processes such as fertilization, immune response, tumor cell metastasis, and bacterial or viral infection. Therefore, various types of carbohydrate clusters have been investigated to control the biological system by enhancing or inhibiting such interactions. Recently, we reported new carbohydrate clusters using CB[6] as a new multivalent scaffold, and demonstrated their specific and multivalent interactions with a lectin. Furthermore, we demonstrated that the carbohydrate clusters form a host-guest complex, which was delivered into a specific cell by receptor-mediated endocytosis. Here we report polypseudorotaxanes formed by CB-based mannose clusters (ManCB[6]) threaded on a polyviologen (PV) polymer to increase the multivalent effects. Mannose units on the glycol-polypseudorotaxane selectively bind to the FimH protein on the ORN 178 *E. coli* strain and thus efficiently agglutinate the bacteria. The hemagglutination inhibition assay (HIA) experiments showed that the ManCB[6]@PV exhibited a valency-corrected 300-fold enhancement over monomeric methyl mannopyranose. The ability of ManCB[6]@PV to inhibit ORN178 bacterial binding to UROtsa cell (urinary epithelial cell) was investigated in vitro by flow cytometry. In the absence of the ManCB[6]@PV, the FITC-labeled ORN178 strains significantly interact with the UROtsa cell and thus give strong fluorescence signal. However, after pre-treating of ManCB[6]@PV to the ORN178, the fluorescence signal was reduced by inhibiting the binding of FITC-labeled bacteria into the UROtsa cells. The results suggest glycopseudopolyrotaxanes are potentially useful in antiadhesion therapy by inhibiting infection of pathogens into the host cell.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of Blue-Light-Emitting Materials Based on Boron Complex.

곽민정

단국대 화학과

Boron complexes based on N, O-chelating ligands, 2-(2'-hydroxyphenyl)benzoxazole (HBO) and 2-(2'-hydroxyphenyl)benzothiazole (HBT), have been prepared and their detail photophysical properties were investigated in solution and in the solid state. Boron complexes are a deep blue fluorophore with high fluorescence efficiency and photostability, suggesting their potential materials science applications.

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Enheanced emission by aggregation of cyano-stilbene derivative

한가람

단국대 화학과

Most often the aggregation of pi-conjugated organic chromophores with a planar and rigid structure induces a remarkable decrease of fluorescence efficency in comparison with that of dilute solutions. However, recently several materials having enhanced emission rather than fluorescence quenching in aggregates or solid states have been reported. In order to get insight on highly fluorescent compounds in solid states, we synthesized a series of asymmetric cyano-stilbene derivatives containing benzothiazole unit and investigated their detail photophysical properties in diluted solution and aggregate states.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Facile One-Pot Synthesis of 1-Alkyl-3-polyfluoroalkyl Imidazolium Ionic Liquids

이방숙, *권오준, *김훈식, 이현주

*KIST 청정에너지연구센터 *경희대 화학과*

Imidazolium-based ionic liquids bearing a polyfluorinated alkyl group on the cation were efficiently synthesized in excellent yields and selectivities from the one-pot reaction of a fluoroolefin with [1-alkyl-3*H*-imidazolium]X, where X = Cl, NO_3, CF_3CO_2, BF_4 or $(CF_3SO_2)_2N$, formed in situ from the interaction of an alkylimidazole with an acid, HX.

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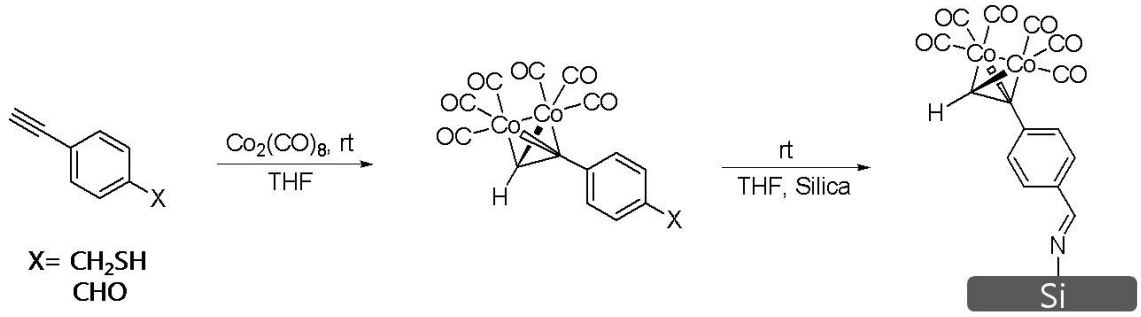
Synthesis and SAMs Formation of Alkyne-Cobalt Complex for Photolysis on the Solid Surface.

이영배, 조성기, 강혜영, 김영근, 황광진

홍익대 화학시스템공학과

The alkyne functional group on the solid surface can be a linker with the DNA, fluorescent substance, protein and various compounds thus enable its application for diagnosis, sensor. Especially, Site selective alkyne formation by the photolysis of alkyne precursor on the gold or silica surface might be applicable for micro-array or patterning. We have designed and synthesized the alkyne-cobalt complex as a potential alkyne precursor in which aldehyde or thiol group was introduced in consideration of the formation of self-assembled monolayers(SAMs). Via imine reaction of amino silane and aldehyde complex, SAMs of cobalt complex were prepared and their analysis will be presented.



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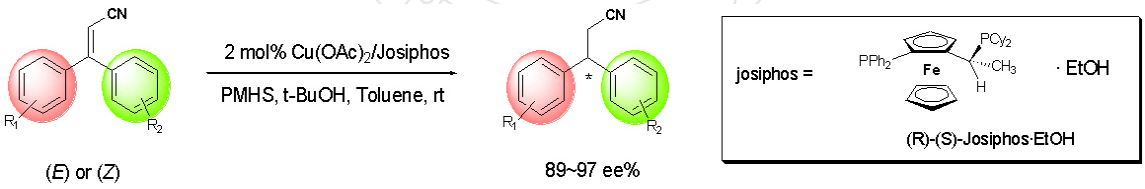
Enantioselective Conjugate Reduction of 3,3-Diarylacrylonitriles Possessing Two Sterically Similar Aryl groups

김효현, 윤재숙

성균관대 화학과

1,1-diarylalkyl moieties are important units in a number of physiologically active compounds. We have developed an efficient enantioselective conjugate reduction of β,β-diaryl-substituted-α,β-unsaturated nitriles with copper(II)-Josiphos catalyst in the presence of polymethylhydrosiloxane(PMHS) as the stoichiometric reducing agent. We synthesized a range of substrates with bearing sterically similar aryl groups via copper-catalyzed hydroarylation reaction, and successfully reduced them in high yields with excellent enantioselectivity (up to 97% ee).



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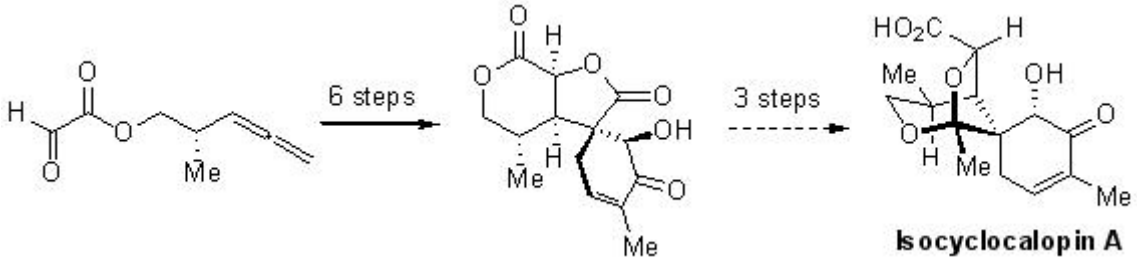
Synthetic Approach to Isocyclocalopin A: Diastereoselective Construction of the Tricyclic Core from a Furopyran-2,7-dione

김재한, 유범선, 양대석, 유찬모

성균관대 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of transition metals are some of the most attractive methodologies since reactions can directly construct complicate molecules from relatively simple starting materials. We would like to present herein several crucial points that have emerged from our recent investigations: 1) novel cyclization of allene-glyoxyaldehydes mediated by Pd or Ru complex to afford the bicyclic lactones; 2) synthetic studies toward an enantioselective synthesis of isocyclocalopin A.



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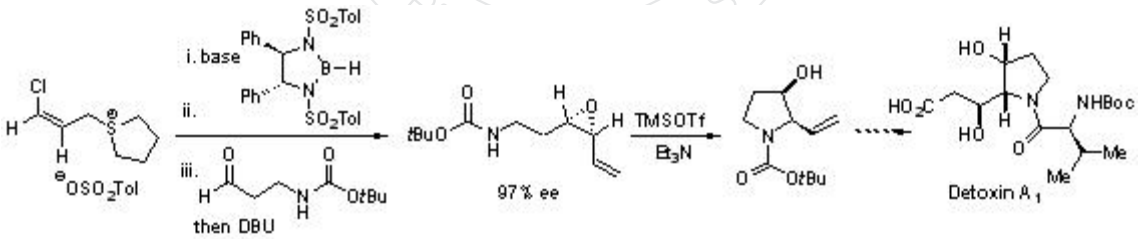
Diastereoselective Endo-cyclization of Vinyloxiranes Under Acidic media: Enantioselective Synthesis of 3-Hydroxy-1-Vinyl Pyrrolidine Unit

공수연, 성원제

성균관대 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity via catalytic process in the production of enantiomerically pure compounds is of considerable current interest in the field of synthetic chemistry. We would like to present herein several crucial points that have emerged from our recent investigations: 1) new method for the preparation of functional allylic boranes from reaction of a sulfur ylide with chiral boranes 2) enantio- and diastereoselective synthesis of 3-vinyloxiranes in high levels of stereoselectivity 3) synthetic applications to the piperidine alkaloids.



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Evidence for General Base Catalysis by Protic Solvent and Solvolysis of 1-(Phenylmethoxycarbonyl)pyridinium Ion

최송희, 성미혜, 경진범, *Dennis N. Kevill

*한양대 응용화학과 *Department of Chemistry, Northern Illinois University*

The kinetics of nucleophilic substitution reactions of 1-(phenylmethoxycarbonyl)pyridinium ion, prepared with the essentially non-nucleophilic/non-basic trifluoromethanesulfonate as the counterion, have been studied increasing concentration of methanol in acetonitrile as a solvent. Experimental second-order rate coefficients(k_2^{exp}) and calculated second-order(k_2) and third-order(k_3) rate coefficients were observed. A Grunwald-Winstein equation treatment of the specific rate of solvolysis for the 1-(phenylmethoxy-carbonyl)pyridinium ion could be carried out in terms of variations in solvent nucleophilicity, and an appreciable sensitivity to changes in solvent nucleohilicity was found.$\log(k/k_0)=lN_T+mY_{Cl}+c$, $\log(k/k_0)=lN_T+c$

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Syntheses of Ozonides from α β-unsaturated 5-Ring Ketones

liwei, lina, 이은희, 구본석, 정인찬

한서대 화학과

For a long time Ozonides were only of academic interest. In resent years, however, they attract considerable interest as potential novel antimalarials. The Synthesis of ozonides could be rationalized by cycloaddition of carbonyl oxide and the carbonyl compounds which are derived from the primary ozonide of olefins. Then they get corresponding ozonide by recombination of cycloaddition. All of the ozonides have been isolated by column chromatography on silica gel. The structures of all isolated Ozonides were established by 1H-NMR and 13C-NMR spectroscopy, and their reduction with triphenylphosphin to give the expected carbonyl compounds.

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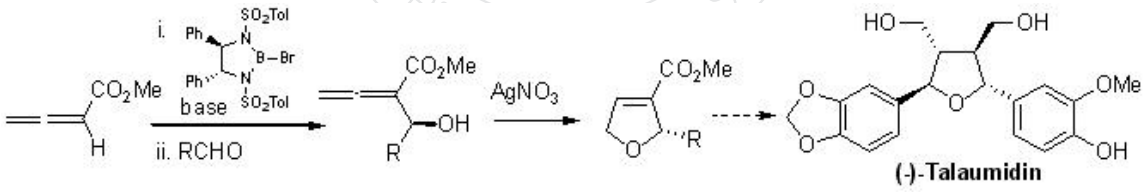
A Highly Enantioselective Aldol Process of an allenoate with Aldehydes Using Chiral Ligand

권지숙, 이보빈

성균관대 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity via catalytic process in the production of enantiomerically pure compounds is of considerable current interest in the field of synthetic chemistry. We would like to present herein several crucial points including stereochemical pathways and absolute and relative stereochemistry that have emerged from our recent investigations: 1) an aldol condensation of allenoate with aldehyde in the presence of chiral boron bromide 2) Synthesis of dihydrofurans. Stereoselectivity and mechanistic details will be presented.



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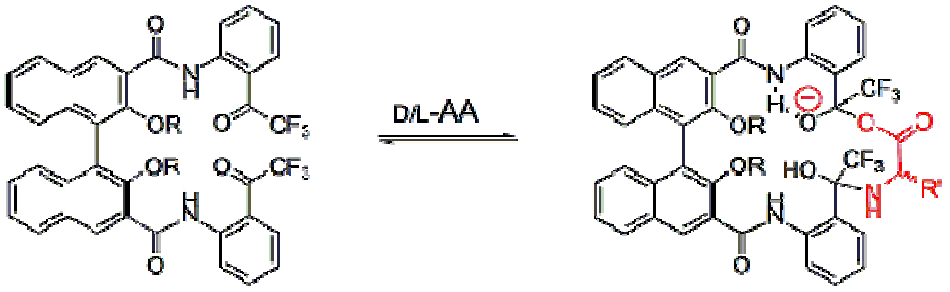
Binaphthyl based bis (CATFA) homoditopic receptor for chiral discrimination of α-aminoacids

sunderraman, 안교한

포항공과대 화학과

The development of structurally simple chiral hosts for the enantioselective recognition of α-amino acids by an unified approach still represents an open challenge in the field of molecular recognition and sensing. Successful chiral hosts developed hitherto1 depend on two different binding motifs for the recognition of the amine moiety and the carboxylate moiety of α-amino acids. Herein, we report the design and synthesis of a simple homoditopic binaphthyl based chiral receptor 1 for the chiral discrimination of α-amino acids. The chiral receptor 1 utilizes o-(carboxamido)trifluoroacetophenone2,3 motifs for both carboxylate and amine recognition. The chiral discrimination of various α-amino acids by receptor 1 can be conveniently monitored by proton coupled 19F NMR of the trifluormethyl groups of the receptor 1-amino acid adducts. The unique 1:1 binding mode was further confirmed by Isothermal Titration Calorimetry.References1) Park, H.; Kim, K.M.; Lee, A.; Ham, S.; Nam, W.; Chin, J. J. Am. Chem. Soc. 2007, 129, 1518.2) Kim, Y.K.; Lee, Y.-H.; Lee, H.-Y.; Kim, M.K.; Cha, G. S.; Ahn, K. H. Org. Lett. 2003, 5, 4003.3) Ryu, D.; Park, E.; Kim, D.-S.; Ham, S.; Yan, S.; Lee, J.S.; Chang, B.-Y.; Ahn, K. H. J. Am. Chem. Soc. 2008, 130, 2394.



(S)-1 (R = Me, Alkyl) (S)-1-AA adduct

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Stitching of Aldehyde-Fréchet Dendrons with Tripodal Azide Using Staudinger/aza-Wittig Reactions

이재욱, 한승철

동아대 화학과

A new convergent synthetic method for the synthesis of Fréchet-type poly(arylether) dendrimers will be described. Staudinger/aza-Wittig reactions are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Taking advantage of these facts, herein we will disclose the general and efficient strategy for the convergent synthesis of Fréchet-type poly(arylether) dendrimers by the trimerization reaction of Fréchet-type dendrons via Staudinger/aza-Wittig reactions (new click reaction) between azide and aldehyde.

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Synthesis of the Homolytic and Heteroleptic Cyclometalated Iridium(III) Complexes for OLEDs

이재욱, 이언엽, 한승철

동아대 화학과

The organic light-emitting diodes (OLEDs) using phosphorescent materials have attracted much attention due to their high external quantum efficiency in recent years. We will study novel homolytic and heteroleptic iridium(Ⅲ) complexes containing carbazole at main ligand. Herein the 9-[2-(2,4-difluoro-phenyl)-pyridin-4-yl]-9H-carbazole was synthesized as main ligand. The homolytic and heteroleptic cyclometalated iridium(III) complexes with a main ligand were prepared. The homolytic and heteroleptic iridium(Ⅲ) complexes will be investigated by ^{1}H and ^{13}C NMR spectroscopy, mass spectra, UV, and PL.

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Synthesis of Dendronized Linear Polymers between Polystyrene with Side-Chain Azide Moieties(Polystyrene-Azide) and Fréchet Dendrons

이재욱, 김병기, 한승철

동아대 화학과

Our strategy for the synthesis of dendritic polymers utilized the Cu(I)-catalyzed Huisgen [2 + 3] dipolar cycloaddition reaction between an organic azide and a terminal alkyne. To apply the click chemistry concept in the construction of the dendronized linear polymers, we synthesized the polystyrene having pendent azides which was reacted with the propargyl functionalized Fréchet-type polyether to provide the dendritic polymers. The dendritic polymer was characterized by ^{1}H-NMR spectroscopy, IR spectroscopy, and GPC analysis.

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Synthesis of Unsymmetrical Fluorescent Diblock Codendrimers via Double Click reaction

이재욱, 강화신, 한승철

동아대 화학과

The synthetic strategy of the convergent synthesis of diblock codendrimer by the double click reaction between 2 types of dendrons (the propargyl functionalized Frechet-type polyether and the propargyl functonalized Tomalia-type PAMAM dendrons) and the 3,6-diazido-9-octyl-8*H*-carbazole will be disclosed. We will use the first click reaction leading to the PAMAM monodendrons containing the chromophore at a core, and then will use the second click reaction with Frechet-type polyether dendrons leading to the formation of fluorescent diblock codendrimers. The unsymmetrical fluorescent diblock codendrimers will be characterized by ^{1}H and ^{13}C-NMR spectroscopy, IR spectroscopy, and mass spectra and GPC analysis.

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Synthesis and Characterization of fluorescent Fréchet Amine Dendrimers Containing a 9,9'-Dialkylated Fluorene Unit at Core

이재욱, 성새름, 한승철

동아대 화학과

The convergent synthesis of emissive Fréchet-type dendrimers containing a chromophore via Staudinger/aza-Wittig reaction between azide and aldehyde will be disclosed. The dendrimers with fluorene unit at core were synthesized from the Staudinger/aza-Wittig reaction (new click reaction) between the azide-dendrons and 9,9'-dialkylated-2,7-dialdehydefluorene. These reactions are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing dendrimer. The absorption and emission of the dendrimers will be disclosed.

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Convergent Synthesis of UnSymmetrical Diblock Denderimers via Double Click of the Fréchet-type Dendrimers

이재욱, 지원호, 한승철

동아대 화학과

The click chemistry, which is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition, proved to be an ideal reaction that used as the most practical and reliable chemical transformations and has found in many applications in organic chemistry and synthesis of dendrimer. Taking advantage of these facts, herein we present the efficient strategy for the convergent synthesis of unsymmetrical diblock dendrimers containing the propargyl-functionalized Fréchet-type polyether dendrons via double click reaction.

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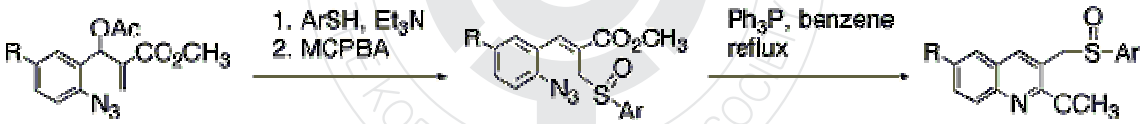
3-Arylsulfinylmethylquinolines from Baylis–Hillman acetates of 2-azidobenzaldehydes

한은구, 김혜정, 이기정

한양대 화학공학과

A simple method for synthesizing several 2-methoxy-3-arylsulfinylmethylquinolines using an aza–Wittig type reaction of 3-(2-azidophenyl)-2-(arylsulfinylmethyl)propenoates, which were readily obtained from the Baylis–Hillman acetates of 2-azidobenzaldehydes, has been developed.



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동맥경화성 혈관 질환치료제로서의 stilbene유도체의 합성

손지영, 이용남, 임은영, 정만길

연세대 화학과

동맥경화증의 발생에는 혈관 평활근 세포와 혈관 내막 세포가 관여하는 것으로 알려져 있다. 이에 천연물인 단삼의 유효성분 LAB(lithospermic acid)가 혈관 평활근 세포와 혈관 내막 세포에 대한 효과를 갖고 있음을 확인하였다. 따라서 본 연구에서는 이러한 LAB 의 caffeic acid moiety 를 가지면서 보다 합성이 쉽고 낮은 분자량과 높은 생리활성을 가질 것이라 예측되는 새로운 형태의 (E)-stilbene 유도체를 제안하였다. 이에 새로운 stilbene 유도체의 효율적인 합성을 수행하였고 stilbene 의 B-ring 의 위치에서 다양한 작용기를 도입해봄으로써 SAR 연구 및 새로운 동맥 경화성 혈관 치료제로서의 가능성을 확인해보고자 하는 바이다.

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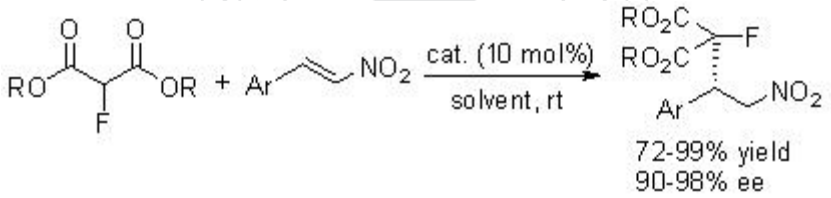
Highly enantioselective conjugate addition of fluoromalonates to nitroalkenes using chiral catalysts

권보경, 강승희, 김대영

순천향대 화학과

The enantioselective conjugate addition of fluoromalonates to aromatic nitroalkenes catalyzed by chiral catalysts generated a stereocenter at the carbon bearing the aromatic group and an adjacent prochiral center from the fluoromalonate. Treatment of fluoromalonates with aromatic nitroalkenes under mild reaction conditions afforded the corresponding 2-fluoro-2-(2-nitro-1-arylethyl)malonates with high yields (72–99%) and excellent enantioselectivities (90–98% ee).



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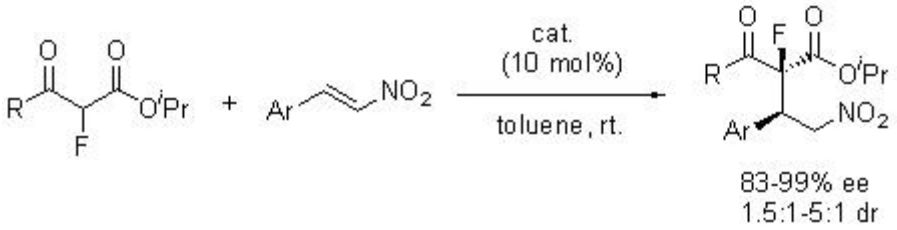
장소: 대전컨벤션센터
발표코드: **Ⅲ37P324포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Organocatalytic synthesis of quaternary stereocenter bearing a fluorine atom: enantioselective conjugate addition of α-fluoro-β ketoesters to nitroalkenes

김선미, 김대영

순천향대 화학과

The catalytic enantioselective conjugate addition reaction of α-fluoro-β ketoesters to nitroalkenes promoted by chiral bifunctional organocatalysts is described. The treatment of α-fluoro-β ketoesters with nitroalkenes under mild reaction conditions afforded the corresponding Michael adducts containing a fluorinated quaternary stereogenic center with excellent enantioselectivity (up to >99% ee).



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Enantioselective α-hydrazination of β-ketoesters catalyzedby chiral nickel complexes

이나리, 권대길, 김대영

순천향대 화학과

The catalytic enantioselective electrophilic α-hydrazination promoted by chiral nickel complexes is described. The treatment of β-ketoesters with azodicarboxylates as electrophilic amination reagents under mild reaction conditions afforded the corresponding α-amino β-ketoesters with high yields (80–96%) and enantioselectivities (up to 88% ee).

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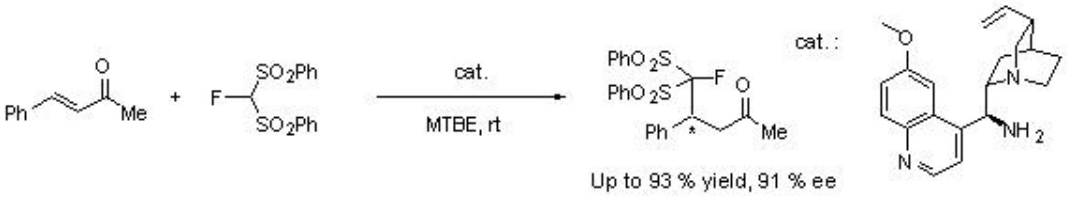
발표종류: 포스터, 발표일시: 금 10:30~12:30

Enantioselective conjugate addition of fluorobis(phenylsulfonyl)methane to α,β-unsaturated ketones catalyzed by chiral bifunctional organocatalysts

문형욱, 김대영

순천향대 화학과

The catalytic enantioselective conjugate addition reaction of fluorobis(phenylsulfonyl)methane to α,β-unsaturated ketones promoted by chiral bifunctional organocatalysts is described. The treatment of fluorobis(phenylsulfonyl)methane to α,β-unsaturated ketones under mild reaction conditions afforded the corresponding Michael adducts with high enantioselectivity. The conjugate addition adducts are useful for the synthesis of chiral monofluoromethylated compounds.



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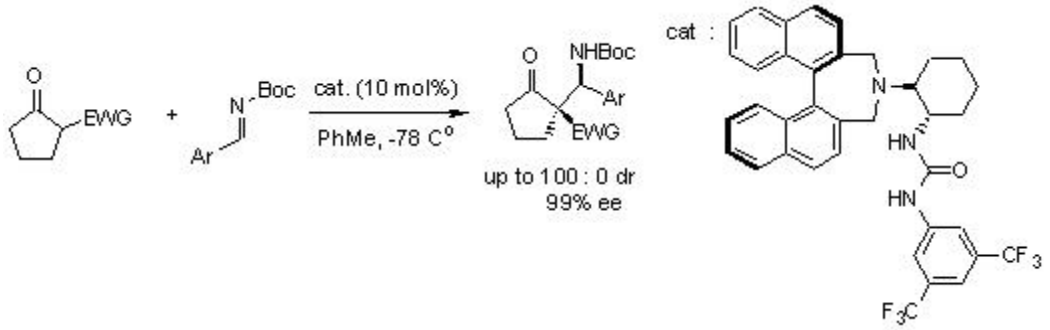
발표종류: 포스터, 발표일시: 금 10:30~12:30

Organocatalytic Highly Enantio- and Diastereoselective Mannich Reaction of Active Methine Compounds with N-Boc-aldimines

강영구, 이주희, 김대영

순천향대 화학과

The catalytic enantioselective Mannich reaction promoted by chiral bifunctional organocatalysts is described.The treatment of active methine compounds with N-Boc-aldimines under mild reaction conditions afforded the corresponding β-amino acid derivatives with excellent diastereoselectivities(up to 100:0 dr) and excellent enantioselectivities(up to 99% ee).



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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

방향족 화합물의 고리화반응을 이용한 불소이온 감지용 형광 및 비색 센서의 개발

한소정, 김태현

인천대 화학과

방향족 화합물의 고리화 반응을 이용하여 새로운 불소이온 감지용 화학센서를 개발하였다. 개발된 센서는 실리콘과 불소이온과의 친화력을 이용하여 매우 높은 선택성을 나타내었으며, 또한 수용액 상에서도 효과적으로 불소이온을 감지 할 수 있다. 불소이온의 고리화 반응에 의한 형광의 변화 뿐만 아니라, 색의 변화를 통해서도 불소이온의 감지를 모니터 할 수 있는 장점을 가졌다. 센서의 합성, 선택성, 감도, 불소이온에 대한 반응속도 등이 발표될 것이다

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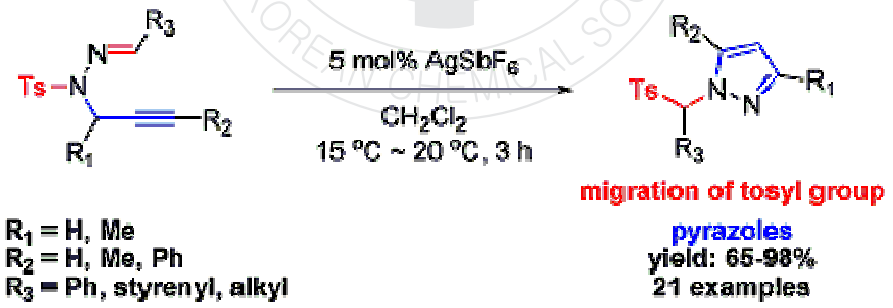
발표종류: 포스터, 발표일시: 금 10:30~12:30

Silver(I)-Catalyzed Facile Synthesis of Pyrazoles From Propargyl N-Sulfonylhydrazones

이영탁, 정영근

서울대 화학부

A silver(I)-catalyzed facile formation of pyrazoles from propargyl N-sulfonylhydrazones has been disclosed. During the reaction, a migration of sulfonyl groups (Ts, Ms) was observed. Good functional group compatibility was observed under mild reaction conditions (at room temperature for 3-5 h). This methodology allows for the efficient and regioselective synthesis of 1,3- and 1,5-disubstituted and 1,3,5-trisubstituted pyrazoles.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of New Blue Light Emitting Iridium Complex Containing Trimethylsilyl group

강현희, 소기호, 박현태, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Organic light-emitting diodes (OLEDs) are currently attracting a lot of attention owing to their potential application in the field of full-color flat panel displays as an efficient and low cost alternative to the widely used liquid crystal displays. Phosphorescence materials are generally based on heavy metal complexes with the most effective being those based on iridium. Iridium complexes can emit light from both singlet and triplet excitons, enabling the fabrication with close to 100% internal quantum efficiency.In this research, we designed and synthesized new iridium complex with trimethylsilane group. The new iridium complex containing tremethylsilyl group is expected to have improved efficiency and stability due to inhibited triplet-triplet annihilation.Moreover, trimethylsilyl group can improve the process ability due to high vapor pressure and high solubility.The physical properties of new iridium complex will be discussed.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and Characterization of Novel Purpurin-18 derivatives as Target-Specfic Photosensitizers for Photodynamic Therapy

Cui Bing Cun, *Li Jia Zhu, *차민욱, **박호성, **이우경, **심영기

*인제대 나노공학과 *인제대 나노시스템공학과 **인제대 나노공학부*

A novel series of 3-(11-O-alkyl), 3-(11-N-amino) and 132-N-amino purpurinimides have been synthesized. Treatment of purpurin-18 methyl ester with various alkyldiamine gave the corresponding purpurinimides, reaction these purpurinimides with 2-dimethylaminoethanol and hexanol produced the 3-(1'-hexyloxy)ethyl-3–devinyl purpurin-18-N-aminoimides and 3-(1'-dimethyl aminoethyloxy)ethyl-3-devinyl purpurin-18-N-aminoimides, respectively. All the structures of new compounds were characterized by UV-Vis and 1H-NMR spectra accordingly.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis, Structure and Spectroscopic Properties of Methyl 2-(1,1'-pentyl)-2-devinyl pyropheophorbide-a Derived from methyl Pyropheophorbide a

Cui Bing Cun, [*]**Li Jia Zhu**, [*]차민욱, [**]박호성, [**]윤일, [**]이우경, [**]심영기

인제대 나노공학과 [*]인제대 나노시스템공학과 [**]인제대 나노공학부

Methyl pyropheophorbide a was used as a starting material, the aldehyde chlorin was obtained by the protection of ring-E and oxidation of vinyl group at 3-position, Grignard reaction with pentyl magnesium bromide converted the formyl group into the acyl group. The hydroxyl group of sec-alcohol chlorin was oxidized by mixed oxidizing agent consisting of tetrapropylammonium perruthenate and N-methylmorpholine N-oxide to generate 3-acyl pyropheophorbide-a derivative. The Grignard reaction of which with pentyl magnesium bromide was carried out to yield tertiary alcohol chlorin as nucleophilic adduct. The following dehydration of tertiary alcohol chlorin was performed in the dry benzene at reflux and the pentenyl group at 3 position was hydrogenated by using Pd/C as a catalyst to yield Methyl 2-(1,1'-pentyl)-2-devinyl pyropheophorbide-a. The structures of all new compounds were characterized by UV-Vis and 1H-NMR spectra.

Keywords: Methyl pyropheophorbide-a ; Methyl 2-(1,1'-pentyl)-2-devinyl pyropheophorbide-a ; Photodynamic therapy

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of isoxazoline-linked chlorins and their in vitro cell viabilities

Li Jia Zhu, *Cui Bing Cun, 차민욱, **이우경, **심영기

*인제대 나노시스템공학과 *인제대 나노공학과 **인제대 나노공학부*

A concise synthesis of isoxazoline-linked chlorins is described. This approach is carried out from methyl pyropheophorbide-a as the starting material via 1,3-dipolar cycloaddition of a vinyl group on the periphery with nitrile oxide to give regioselective products with excellent yields. This method represents an extensive and efficient entry into the functionalization of chlorins with a chlorophyll-α skeleton. Moreover, we have examined a preliminary in vitro effect of these new derivatives on mouse sarcoma S-180 cell line in photodynamic therapy.Keywords: photodynamic therapy, photosensitizer, chlorin, methyl pyropheophorbide-a, isoxazole, 1,3-dipolar cycloiddtion, mouse sarcoma S-180 cell.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of New Catechin-Conjugated Chlorophyll-a Derivatives

Li Jia Zhu, *Cui Bing Cun, 차민욱, **이우경, **심영기

*인제대 나노시스템공학과 *인제대 나노공학과 **인제대 나노공학부*

The synthesis of a series of Catechin-conjugated chlorins is done by modification of 3-vinyl group or 17-methyl ester group of chlorophyll-a derivatives such as methyl pyropheophorbide-a (Mppa) and purpurinimide. The structures of new chlorophyll derivatives were characterized by UV, IR, 1H NMR spectra and elemental analysis. New derivatives will show potent photodynamic activities via Type III mechanism which is characterized having radical scavenger.Keywords: chlorin, catechin, chlorophyll-a derivative, photodynamic therapy (PDT)

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of 3-pyrazol Methyl pyropheophorbide-a derivative and its anti-cancer activity in vitro.

박호성, *차민욱, *Li Jia Zhu, 윤일, 이우경, 심영기

*인제대 나노공학부 *인제대 나노시스템공학과*

새로운 Methyl pyropheophorbide-a 유도체, Methyl pyropheophorbide-a 3 번 위치에 pyrazol 을 치환시킨 물질을 합성한 뒤, 합성된 물질을 UV, NMR 을 이용하여 확인한다. 합성된 Methyl pyropheophorbide-a 유도체들은 암세포에 선택적으로 Up-take 되고 특정 파장을 조사하면 물질이 활성화 되어 암세포를 apoptosis 나 necrosis 를 유도한다. Methyl pyropheophorbide-a 유도체들을 이용하여 암세포인 A549 cell 과 Hela cell 에 in vitro test 를 하여 Methyl pyropheophorbide-a 와 비교한다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Anti-cancer activity of 3-pyrazollinyl Chlorin derivative in vitro.

박호성, *차민욱, **Cui Bing Cun, 이우경, 심영기

*인제대 나노공학부 *인제대 나노시스템공학과 **인제대 나노공학과*

Photodynamic therapy 는 암을 치료하는 한 가지 방법으로서 암세포에 선택적으로 Up-take 되는 Photosensitizer 를 이용하여 암을 치료하는 방법이다. 새로운 Chlororin 유도체, Methyl Pheophorbide-a 3 번 위치에 pyrazol 을 치환시킨 물질을 합성한 뒤, 합성된 물질을 UV, NMR 을 이용하여 확인한다. Methyl Pheophorbide-a 유도체들을 이용하여 암세포인 A549 cell 과 Hela cell 에 in vitro test 를 하여 Methyl Pheophorbide-a 와 비교한다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of new water soluble chlorin e6 derivatives having cyclopropyl at 3-position and halogen at 20-position

차민욱, *박호성, Li Jia Zhu, **Cui Bing Cun, *윤일, *이우경, *심영기

*인제대 나노시스템공학과 *인제대 나노공학부 **인제대 나노공학과*

Chlorin e6 derived from the methyl pheophorbide-a that is a kind of water soluble photosensitizers has widely used for photodynamic therapy. For the development of extended wavelength of chlorin e6 derivatives, we performed that the 20-bromo-3-devinyl-3-cyclopropyl chlorin e6 and 20-chloro-3-devinyl-3-cyclopropyl chlorin e6 which were substituted by cyclopropyl moiety at 3 position and halogen moieties at 20- position were synthesized, respectively, and their chemical structures were analyzed by infrared spectroscopy (IR) and UV-Vis spectroscopy

Key Words: methyl pheophorbide-a, chlorin e6, photosensitizer, photodynamic therapy

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis of New Polyoxometalates-Conjugated Chlorophyll-a Derivatives

차민욱, *박호성, **Cui Bing Cun, Li Jia Zhu, *윤일, *이우경, *심영기

*인제대 나노시스템공학과 *인제대 나노공학부 **인제대 나노공학과*

The synthesis of New Polyoxometalates that are the kinds of anticancer agents conjugated chlorins is done by modification of chlorophyll-a derivatives such as purpurinimide. The structures of new chlorophyll derivatives were characterized by UV, IR, 1H NMR spectra and elemental analysis.

Key Words: chlorophyll-a, Polyoxometalates, purpurinimide

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Synthesis and characterization of water-soluble Sodium pheophorbide-a and gold nanoparticles stabilized by sodium pheophorbide-a.

Lkhagvadulam, 차민욱, *이우경, *심영기

*인제대 나노시스템공학과 *인제대 나노공학부*

For the broad application in Photodynamic Therapy (PDT) combined with Photothermal Therapy (PTT) to cancer and a diagnosis of cancer cell, a new type of water soluble ionic photosensitizer Sodium pheophorbide-a based on the pheophorbide-a and sodium were synthesized. And it was transformed into a small gold (Au) nanoparticles stabilized by the photosensitizer without adding any particular reducing agents and surfactants. UV-Vis spectroscopy, Transmission Electron Microscopy (TEM) were used for characterization of photosensitizer and gold nanoparticles

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Synthesis and characterization of Purpurinimide derivative photosensitizer and gold nanoparticles stabilized purpurinimide derivatives

Lkhagvadulam, *박호성, *이우경, *심영기

*인제대 나노시스템공학과 *인제대 나노공학부*

For the broad application in Photodynamic Therapy (PDT) combined with Photothermal Therapy (PTT) to cancer and a diagnosis of cancer cell, a new type of water soluble ionic photosensitizer of Purpurinimide derivative photosensitizer based Purpurin-18 and N,N-dimethylethylenediamine were synthesized and converted to the corresponding cationic water-soluble photosensitizer.And it was transformed into a small gold (Au) nanoparticles stabilized by the photosensitizer without adding any particular reducing agents and surfactants. 1H-NMR ,UV-Vis spectroscopy, Transmission Electron Microscopy (TEM), a preliminary in vitro photodynamic effect of the compound on A549 cancer cell were used for characterization of photosensitizer and gold nanoparticles

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발표코드: **Ⅳ38P160포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and evaluation of heteroaryl group substituted phthalazinone as MCH receptor 1 antagonist

임채조, 왕수미, 서무영, 김낙정, 이규양

한국화학연구원 대사증후군치료제연구센터

The melanin-concentrating hormone receptor (MCH-R1) as a G-protein-coupled receptor expressed in the brain and peripheral tissues have a great attention in treatment of obesity, due to regulation energy storage and body weight. In continuation of our efforts to search for new scaffolds of MCH-R1 antagonists, we have found phthalazinone derivatives as MCH-R1 antagonist, and examined the effect of diverse heteroaryl group instead of aryl group in the 4-position of phthalazinone derivatives on the MCH binding affinity. The details of structure-activity relationships (SAR) will be further disclosed.

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Synthesis and evaluation of naphtho[1,2-b]furan derivatives as MCH receptor 1 antagonist

임채조, 김지영, 김낙정, 이규양

한국화학연구원 대사증후군치료제연구센터

Antagonists of the melanin-concentrating hormone receptor (MCH-R1) have great potential utility for the treatment of obesity. As part of our ongoing project in the development of MCH-R1 antagonists, a series of naphtho[1,2-b]furan derivatives were designed, synthesized and evaluated. Among them, several analogs showed excellent MCH-R1 binding affinity in vitro assay. The detailed results of structure-activity relationships (SAR) will be presented.

THE KOREAN CHEMICAL SOCIETY

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Antitubercular Activity of Triazole Derivatives

김수현, *윤창수, **이상호, ***이용섭, ****박태호, *****조상래, *****오태권, ******김필호

*경희대 약학과 *한국화학연구원 신물질연구단 난치성질환치료제연구센터*
***한국화학연구원 신약연구단 ***경희대 약학과 ****한국화학연구원 화학물질연구단*
******연세대 의과대학 ******한국화학연구원 감염증치료제연구센터*

Tuberculosis (TB) remains one of the most deadly infectious diseases over the past few decades, infecting 8 million and killing 2 million people annually. However, novel antitubercular drugs have not been developed since 1960s. Thus, there is an urgent need for discovery of new drugs against Mycobacterium tuberculosis (Mtb), which causes TB. Recently, it has been shown that antifungal azoles are active against Mtb. Triazoles are also used very often in the pharmacological and medicinal applications. The present study focuses on biological activities of triazloes against Mtb. The majority of triazole derivatives have been prepared by click chemistry. Structure-activity relationship of triazoles will be presented.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Discovery of Antitubercular Natural Products from Steptomyces[발표 취소 10-15]

김수현, *윤창수, **이상호, ***이용섭, ****조상래, *****박태호, ******이종석, ****오태권, *******김필호

*경희대 약학과 *한국화학연구원 신물질연구단 난치성질환치료제연구센터*
***한국화학연구원 신약연구단 ***경희대 약학과 ****연세대 의과대학*
******한국화학연구원 화학물질연구단 ******국제결핵연구소 기초연구부*
********한국화학연구원 감염증치료제연구센터*

It has been shown that numerous natural products from plants, fungi, and marine organisms have antitubercular activity. Among current tuberculosis (TB) drugs, rifampicin, isoniazid, and streptomycin were indeed derived from natu[illegible]ies toward discovery of novel antitubercular natural products, o[illegible]olites from Streptomyces, which were obtained from Extract Colle[illegible]JM), have been screened against Mycobacterium tuberculosis. Considering activity and cytotoxicity, bioassay-guided fractionations have been performed and active fractions have been further purified. Our research progresses and efforts on discovery of antitubercular natural products will be presented.

발 표 취 소

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and Anti-angiogenic Activity of Deoxoartemisinin Trimer

박지현, 이용남, 임은영, 정만길

연세대 화학과

Artemisinin 은 항말라리아 및 항암성 등 높은 약효를 지니고 있다. 본 연구실에서는 항암성에 관한 연구를 수행하고 있으며 특히 항신생혈관기전에 관한 연구를 하고 있다. 또한 용해도와 산에 대한 낮은 안정도를 개선시키기 위해 12 번 탄소위치의 acetal type 을 변형시켜 non-acetal type 인 deoxoartemisinin 유도체를 합성하였다. Artemisinin 으로부터 합성된 Deoxoartemisinin 유도체에 대해 여러 가지 biological test 를 수행하여 높은 Antiangiogenic activity 를 가지는 것을 확인하였고 이 화합물들이 새로운 항암물질의 가능성을 가지는 것을 발견하였다.

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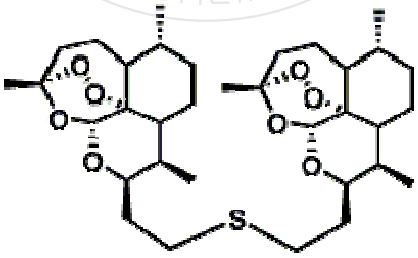
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and Biological Evaluation of Deoxoartemisinin Derivatives for Oral Cancer Therapy

이용남, 박지현, 임은영, 정만길

연세대 화학과

Artemisinin is of special biological interest because of its outstanding antimalarial activity. Recently, it was reported that artemisinin has antitumor activity. Its derivatives, artesunate, arteether, and artemeter, also have antitumor activity against melanoma, breast, ovarian, prostate, CNS, and renal cancer cell lines. We synthesized monomers and dimers of deoxoartemisinin and evaluated the antitumor activity of artemisinin and its various derivatives deoxoartemisinin, in comparison with paclitaxel (Taxol), 5-fluorouracil (5-FU), cisplatin in vitro. In this study, the sulfur linked dimer had the most potent antitumor effect (IC_{50} = 9.3 μM), even better than paclitaxel (IC_{50} = 13.1μM), on oral cancer cell line (YD-10B).



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Synthesis of Novel Phosphonate Analogs of Diclofenac

김태우, 김미현, 정강연

강릉대 환경응용화학공학과

Diclofenac is a non-steroidal anti-inflammatory drug (NSAID) showing potent anti-inflammatory, analgesic and anti-pyretic activities. However, it has several side effects such as acute kidney failure, bone marrow depression, and liver damage. Towards the discovery of novel NSAID, which are expected to have improved drug efficacy and better toxicity profile than diclofenac, we have synthesized new derivatives of diclofenac phosphonates efficiently from commercially available 2-aminobenzyl alcohol using click chemistry and Arbuzov reaction in good yields. These synthetic compounds are tested for in vitro anti-inflammatory and antiviral activities and one of the compounds showed promising results, which allowing us to pursue further studies.Keywords: diclofenac phosphonate, triazole compounds, NSAID.

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3,4-Dihydroquinazoline derivatives as T-type calcium channels blockers and anticancer agents

정수연, 주동준, 이재열

경희대 화학과

Calcium plays an important role in cell growth. For example, it has also been shown that calcium signaling is required for cell cycle progression from G1/S phase through to mitosis. It has been demonstrated that depletion of intracellular calcium arrests the cell cycle in the G0/G1 and S interphases. Regulation of the changes in intracellular calcium ion has been proposed to be via a T-type calcium channel. Therefore, novel T-type calcium channel blocker shows the possibility as new anti-cancer agent. Based on this finding, we have recently found that DWKH0090 shows the comparable potency to Doxorubicin against 5 human cancer cell lines as well as high channel blocking activity. In addition, this compound showed the potent growth inhibition of tumor on A549 cell- xenographed mice. This result implied that DWKH0090 as T-type calcium channel blocker would be used as a novel anti-cancer agent.

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Arylpiperazine-Containing Pyrrole 3-Carboxamide Derivatives for Treating Depressive Disorders

강석연, 박은정, 송광섭, 이석호, 김민주, 서희정, *배애님, **박우규, 김정민, 이진화

*(주)녹십자 *KIST 생체과학연구본부 **한국화학연구원 약리활성연구센터*

Modern treatment for depression, which focuses exclusively on agents that modulate monoamine neurotransmission, began with a monoamine oxidase inhibitor (MAOI). MAOIs increase serotonin and norepinephrine concentrations in the brain by inhibiting the MAO enzyme. The SARI (serotonin antagonist/reuptake inhibitor) drugs that block both the serotonin 5-HT_2 receptors and the serotonin transporters have been developed. We have relate to novel arylpiperazine-containing pyrrole 3-carboxamide derivatives of formula (I) or a pharmaceutically acceptable salt thereof which is useful for preventing or treating depressive disorders. And also provides a method for preparing the arylpiperazine-containing pyrrole 3-carboxamide derivatives or a pharmaceutically acceptable salt thereof, a pharmaceutical composition containing same, and a method for preventing or treating depressive disorders.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis, SAR and biological evaluation of 1,2,4-triazole-containing diarylpyrazolyl carboxamide as CB1 cannabinoid receptor ligands

서희정, 김민주, 이석호, 김정민, 이진화

(주)녹십자

Since the CB1 receptor antagonist SR141716 (rimonabant) was previously reported to modulate food intake, CB1 antagonism has been considered as a promising therapeutic target for the treatment of obesity. In the present study, various derivatives based on 1,2,4-triazole including diarylpyrazolyl carboxamide were synthesized and tested for CB1 receptor binding affinity. Further SAR studies were carried out to optimize the substituents of caboxamides. These SAR studies introduced several novel CB1 ligands with $IC_{50} \approx 2$ nM for the rat CB1 receptor binding. Based on these results, further lead optimization studies resulted in more potent compound with $IC_{50} < 1$ nM. Our discovery efforts including these results will be reported herein.

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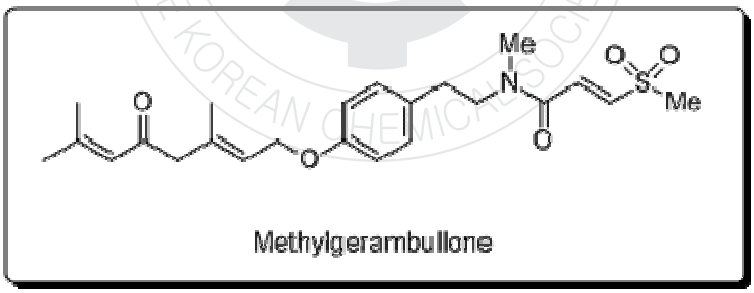
First total synthesis of methylgerambullone and improvement of gastrointestinal dyskinetic diseases

이소형, 하성훈, 문종택, 주동준, 이재열

경희대 화학과

Methylgerambullone is an one of the compounds that were isolated from the methanolic extract of Glycosmis angustifolia collected in Sri Lanka.We have firstly carried out the synthesis of methylgerambullone through convergent synthetic ways using three blocks. We described the biological activity such as the improvement of gastrointestinal dyskinetic diseases.



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Medical Radioisotope ^{64}Cu Production with ^{64}Ni(p,n)^{64}Cu Nuclear Reaction and Target Material Recycling

전권수, *박현

*한국원자력의학원 방사성의약품 개발실 *한국원자력의학원 방사성의약품연구팀*

^{64}Cu($T_{1/2}$=12.7h, β^- decay: 40%, β^+ decay:19%, E.C. decay:41%) is one of the most useful radioisotope, diagnostic and therapeutic, in nuclear medicine due to its multiple decay mode and the intermediate half-life. Several nuclear reaction, i.e., ^{64}Ni(p,n)^{64}Cu, ^{68}Zn(p,αn)^{64}Cu and ^{64}Ni(d,2n)^{64}Cu have been investigated for ^{64}Cu production. For mass and routine production, the ^{64}Ni target fabrication using electroplating, the reliable chemical separation of ^{64}Cu from the proton irradiated ^{64}Ni target using dithizone in CCl_4-HCl solvent extraction and anion exchange resin and the effective recovery process for the very expensive ^{64}Ni material($20,000/g) recycling were established. In this work, we report our mass production method of ^{64}Cu with enriched ^{64}Ni and Cyclone-30 accelerator.

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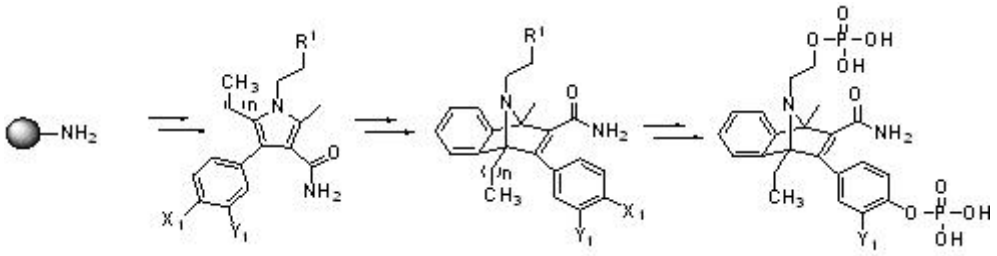
Solid-Phase Syntheses of 7-Azabicyclo[2.2.1]Hept-2-ene that Function as PP2Cδ Inhibitors

방정규, *박재훈, 곽옥금, *강신원, 전영호

*한국기초과학지원연구원 자기공명연구부 *부산대 화학과*

The phosphatase PP2Cδ indirectly suppresses the activity of the turmor suppressor protein p53. After DNA damage, such as ionizing radiation or UV light, several cellular pathways combine to increase the activity of p53, which in turn controls cell cycle arrest and apoptosis. Within the network of p53 activation, Wip1 inactivates p38 MAP kinase via dephosphorylation of a phosphothreonine. In its own role, phosphorylated p38 MAP kinase phosphorylates and activates p53. Therefore, Wip1 controls a negative feedback loop within the p38 MAP kinase-p53 signaling pathway. The growing evidence of the biological functions of Wip1 indicated that inhibition of its enzymatic activity could be an effective strategy for combating certain types of cancer. In this presentation, we show that using a 7-azabicyclo[2.2.1]hept-2-ene based scaffold, we developed a series of small molecules that mimic the three-dimensional arrangement of the polar and hydrophobic functional groups of the best cyclic-peptide inhibitor c(MpSIpYVA). The [4+2] cycloaddition reaction between pyrroles and diennophiles has been shown to be a method for the synthesis of the 7-azabicyclo[2.2.1]hept-2-ene derivatives.



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Prediction of CYP3A4 inhibitions by Quantum-Mechanical Calculations

이주연, *강영기, **강남숙

*한국화학연구원 신약플랫폼기술팀 *충북대 화학과 **한국화학연구원 분자설계실*

The active site of the cytochrome P450 (CYP450) is composed of an iron(III)-porphyrin moiety. Iron(III) is axially coordinated through the sulfur atom of cysteine residue in the backbone and the oxygen atom of a water molecule. The P450 catalytic reaction cycle is initiated by coordinating the substrate to the iron(III) and releasing the water molecule. Here, we are interested in knowing which kinds of substrates can coordinate to the CYP3A4 enzyme and explaining it with the correlation between the inhibitory activity (IC_{50}) of the substrate for CYP3A4 and the binding free energy (ΔG_{tot}) for the iron-porphyrin and substrate complex. In particular, we may get the information for the spin state of iron(III), the charge, and the calculation levels as well as the optimized structures of iron-porphyrin moiety ligated with a sulfur atom of cysteine and a substrate. The binding free energies are calculated at the hybrid density functional B3LYP/LanL2DZ level in the gas phase and at the B3LYP/6-31+G(d) level with the conductor-like polarizable continuum model in water. The correlation coefficients between the inhibition activity (IC_{50}) and the free binding energy (ΔG_{tot}) of iron-substrates complex are 0.69 and 0.42 in the gas phase and in water at 25℃, respectively. Further considerations are in progress.

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Synthesis and Inhibition of PGE_2 Production of 1H-Furan-2,5-dione and 1H-Pyrrole-2,5-dione Derivatives

박항아, 문종택, 주동준, 이재열

경희대 화학과

We synthesized and investigated the effect of 3,4-diphenyl-substituted 1H-furan-2,5-dione and 1H-pyrrole-2,5-dione derivatives on LPS-induced PGE_2 production in RAW 264.7 macrophage cells. Both 1H-furan-2,5-dione and 1H-pyrrole-2,5-dione rings as main scaffolds were easily obtained using one of three synthetic methods. Among the compounds investigated, 1H-3-(4-sulfamoylphenyl)-4-phenyl-pyrrole-2,5-dione (6l) showed a strong inhibitory activity (IC_{50} = 0.61 μM) of PGE_2 production.

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Acetylcholiesterase [발표취소 9-25]

김혜미, 강영기, *강남숙

*충북대 화학과 *한국화학연구원 분자설계실*

Acetylcholinesterase

발 표 취 소

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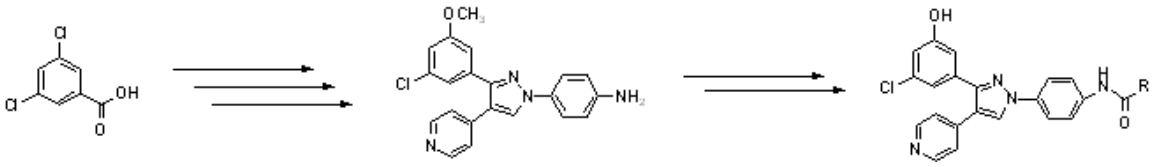
Synthesis and antiproliferative activites of 1-substituted-3-(3-chloro-5-methoxyphenyl)-4-pyridinylpyrazole derivatives for melanoma cell.

최원경, *심태보, *유경호, *조정혁, 최기항, **오창현

*고려대 화학과 *KIST 생체과학연구본부 **KIST 바이오소재연구센터*

Melanoma is the most aggressive form of skin cancer and is the fastest growing cancer in the United States. In this study, the synthesis of a new series of 1-substituted-3-(3-chloro-5-methoxyphenyl)-4-pyridinylpyrazole scaffold is described. Their *in vitro* antiproliferative activities against human melanoma cell line A375 were tested and the effect of substituents on the phenyl ring was investigated.



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장소: 대전컨벤션센터
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Efficient construction of 1,2,3-triazole library using by microwave-assisted reaction.

곽주명, 이정국, *서용완, 고훈영

*인하대 화학과 *인하대 자연과학대학 화학과*

Huisgen's 1,3-dipolar cycloaddition of alkynes and azides yielding triazoles is a prominent example of click chemistry reactions. The heterocyclic triazole structure as the well established bioisostere in the field of medicinal chemistry can be shown a wide range of biological activity. In general, the harsh condition such as high temperature and long reaction time could be required for the preparation of 1,2,3-triazole ring structure.New efficient synthetic protocol for construction of 1,2,3-triazole library via a fast one-pot microwave assisted reaction will be discussed.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Preparation of a 3'-azido-3'-deoxythymidine (AZT) derivative, which is blood-brain barrier permeable

임정균, 정성기

포항공과대 화학과

The blood brain barrier (BBB) is composed of densely packed endothelial cells which are connected through tight junctions. Thus it can prevent most molecules in blood plasma such as chemicals or pathogens from their entering the brain. In addition to killing of CD4+ T cells in the HIV infected patients, one of the most destructive aspects of AIDS is encephalopathy associated with infection of the brain by the virus. Penetration of anti-AIDS drugs into BBB thus gaining an access into the patient's brain is a highly desirable but unfulfilled property of anti-AIDS drugs such as AZT. With the help of recently reported sorbitol-based molecular transporter, we designed and synthesized AZT conjugates, which have also been found to readily cross BBB in mouse. AZT was covalently attached to the sorbitol-G8 transporter via the succinate ester linkage. To verify that the resulting conjugates contain AZT, the structures of the intermediates were further confirmed by IR to observe the characteristic azide band (around 2100 cm^{-1}) of AZT. The uptake property of the AZT conjugate was investigated by confocal microscopy in live HeLa cells. When the AZT conjugate (10 μM) was incubated with HeLa cells for 30 min, it was found to target nucleoli as well as mitochondria. The AZT-conjugate was injected intraperitoneally (ip) to mice and it displays an affinity toward brain, liver and also to some extent spleen. It is quite clear that our conjugates readily cross the BBB and also show somehow variant tissue selectivity. This prodrug methodolgy is applicable to virtually all other NRTIs including stavudine and lamivudine. Studies are in progress to further demonstrate that the sorbitol G8 carriers can be utilized in delivering a number of important drugs and potential drug candidates to brain and central nervous system.

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Highly efficient routine production of [^{18}F]fallypride with fully automated synthesis system

문병석, 김지선, 이병철

분당서울대병원 핵의학과

[^{18}F]Fallypride exhibits an effective radiotracer for the study of dopamine D2/D3 receptor occupancy, neuropsychiatric disorders and aging in humans. Despite this tracer has the potential for clinical use, automated labeling efficiency showed low radiochemical yields about 5-20% with relatively long incorporation time of fluorine-18. In present study, we describe an automated radiochemical synthesis of [^{18}F]fallypride varying different base concentration and incorporation time of fluorine-18 using GE Healthcare FX-FN for potentially utilizable in routine production sites. The optimal labeling condition of [^{18}F]fallypride in the automated synthesis was that 2 mg of tosyl-fallypride in acetonitrile (1 mL) was incubated at 100 °C for 10 min with 40% $TBAHCO_3$ (10 μL). [^{18}F]Fallypride was obtained with high radiochemical yield about 68 ± 1.6% (decay-corrected, n = 8) within 51 ± 1.2 min including HPLC purification and solid-phase purification for the final formulation. [^{18}F]Fallypride was prepared with a significantly improved radiochemical yield with high specific activity and shorten synthetic time.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and biological evaluation of pyrazol-based molecules as calcium channel blockers

문두현, *김정현, *최경일, *남길수

*한양대 화학과 *KIST 생체과학연구본부*

A novel series of piperidine contained pyrazole derivatives were designed, synthesized and evaluated on their calcium channel inhibitory activity. We previously described a series of piperazine contained pyrazole derivatives as potent calcium channel inhibitors. As continuous study, we introduced piperidine ring instead of piperazine ring. Here we will describe synthesis and structure activity relationships (SAR) in detail.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and evaluation of clotrimazole derivatives for inhibitory effect on nitric oxide production

정순재, *박정훈, *김상욱, *허민구, *김인종, *최상무, *양승대, 유국현

*동국대 화학과 *한국원자력연구원 방사선공업환경연구부*

Nitric oxide reacts with superoxide radical formation of peroxynitrite. The NO synthase inhibitors decrease free radical concentration. Clotrimazole [1-{(2-chlorophenyl)-diphenylmethyl}-1*H*-imidazole, CLT] has antitumor properties and also inhibits microsomal peroxidation. Therefore, we hypothesized that CLT derivatives would protect the cells suffering from LPS (lipopolysaccharide) induced expressions of various inflammation-associated genes. In this study, we synthesized *N*-(ω-fluoroalkyl)clotrimazolium salts and *N*-(ω-hydroxyalkyl)clotrimazolium salts to test the effect on the cells suffering from oxidative stress was examined by using a RAW 264.7 macropharge cells by quantitative RT-PCR analysis. CLT derivatives have been found to inhibit nitric oxide (NO) synthesis.

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Novel polyprenyl derivatives from the tropical marine sponge *Dactylospongia* sp.

이종욱, *이연주, **신희재, ***이희승

*한양대 응용화학과 *한국해양연구원 해양바이오센터 **한국해양연구원 천연물연구실*
****한국해양연구원 해양천연물연구실*

Marine invertebrate have provided a large number of hydroquinone derivatives which have been found through many articles. In accordance with these researches, we have searched for bioactive metabolites from tropical marine sponges. As a result, new derivatives of polyprenyl hydroquinone were isolated from the tropical marine sponge *Dactylospongia* sp., from Chuuk, Federated State of Micronesia. The structures were proposed by means of spectroscopic methods including 2D NMR and MS.

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Synthesis and neuronal differentiation of N-hydroxybenzamide derivatives in mesenchymal stem cells

권성욱, *강승규, **정희정, ***김광록, ****안진희

*고려대 화학과 *한국화학연구원 대사증후군치료제연구센터 **한국화학연구원 난치성질환치료제연구센터 ***한국화학연구원 신물질 연구단 ****한국화학연구원 대사성질환연구팀*

Recent advances in stem cell biology may provide new approaches for the treatment of a number of diseases as well as tissue/organ injuries, including cardiovascular disease, neurodegenerative disease, musculoskeletal disease, diabetes and spinal-cord injuries. Neuronal differentiation of stem cells can be a new therapeutic strategy to the treatment of neurodegenerative diseases such as Parkinson's and Alzheimer's diseases. Moreover, small molecules that can direct differentiation of stem cells, are useful tools to facilitate therapeutic applications. Mesenchymal stem cells (MSCs) are highly important and easily accessible adult stem cells which could be differentiated into many cell types including osteoblasts, adipocytes, fibroblasts, myocytes and neurons. The ability of MSCs to differentiate into neurons holds considerable promise because of their potential to thus serve as a possible unlimited source of stem cells to treat neurodegenerative diseases. Several reports have shown the neuronal induction from MSCs using growth factors, cytokines and small molecules. In this presentation, we wish to report synthesis and neuronal differentiation of N-hydroxybenzamide derivatives in mesenchymal stem cells

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Neuronal Differentiation in Mesenchymal Stem Cells Using A Synthetic Small Molecule

이재홍, 권성욱, *강승규, **정희정, ***안진희, ****김광록

*고려대 화학과 *한국화학연구원 대사증후군치료제연구센터 **한국화학연구원 난치성질환치료제연구센터 ***한국화학연구원 대사성질환연구팀 ****한국화학연구원 신물질 연구단*

Mesenchymal stem cells (MSCs) are highly important and easily accessible adult stem cells which could be differentiated into many cell types including osteoblasts, adipocytes, fibroblasts, myocytes and neurons. The ability of MSCs to differentiate into neurons holds considerable promise because of their potential to thus serve as a possible unlimited source of stem cells to treat neurodegenerative diseases. Several reports have shown the neuronal induction from MSCs using growth factors, cytokines and small molecules. In this presentation, we wish to report the synthesis of a new quinoxalinone based small molecule and its neuronal differentiation capacity. We have discovered a new small molecule to show neuronal differentiation of MSCs, which was confirmed by morphological change, neuronal marker expression as well as neuronal electrophysiological properties. Also, it showed excellent differentiation efficiency (>95%) by cell counting without cell cytotoxicity.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and Evaluation of new Stilbene Derivatives for Imaging Amyloid Plaques

홍명찬, *김윤경, **최재용, ***최태현, ****장영태, *****이교철

*한양대 응용화학과 *National University of Singapore **연세대 핵의학과 ***원자력의학원 국가방사선비상진료센터 ****싱가포르 국립대학 화학과 *****한국원자력의학원 방사성의약품연구팀*

Alzheimer's disease(AD), the most common form of dementia among the elderly, is progressive, degenerative disorder of the brain with a loss of memory, and congition. The hallmarks of AD are an extracelluar deposition of beat-amyloid in the form of neutritic plaques, an intraneuronal cytoplastmatic deposition of neurofibrillary tangles. PET imaging of AD has many aspects of significance for diagnostic and therapeutic development. Small molecules for detecting the beta-amyloid plaques and tangles have been well developed. Among them, stilbene derivatives are one of the most potential traces. We report herein the synthesis and evaluation of new stilbene derivatives.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Preparation of 1,5-Anhydro-2,3-dideoxy-2-([^{125,131}I]5-iodouracil-1-yl)-D-*arabino*-hexitol for potential imaging agent

홍명찬, *김정영, *김은정, **최태현, ***오창현, ****이학준

한양대 응용화학과, 한국원자력의학원 방사성의약품연구팀
**한국원자력의학원 방사성의약품연구팀 **원자력의학원 국가방사선비상진료센터*
****KIST 바이오소재연구센터 ****한양대 응용화학과*

The sugar-modified nucleosides have led to the development of some nucleoside analogues with antiviral and antitumor properties as previously reported. In common, all compounds tend tobe phosphorylated by celluar or viral enzymes in order to exert their biological activity. In this studry, we try to develop 1,5-Anhydro-2,3-dideoxy-2-([^{125,131}I]5-iodouracil-1-yl)-D-*arabino*-hexitol(ADIDA) based on a six-membered carbohydrate moiety as potential imaging agent for tumor model

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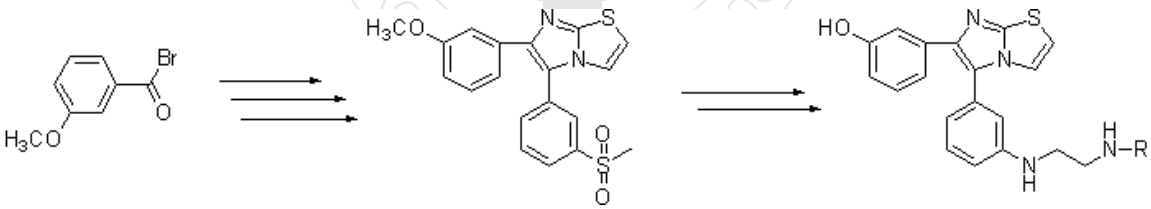
Synthesis and antiproliferative active of imidazo[2,1-*b*][1,3]thiazole derivatives for melanoma(Ⅱ)

박진헌, *심태보, *유경호, *조정혁, **이용섭, ***오창현

*경희대 기초약학과 *KIST 생체과학연구본부 **경희대 약학과 ***KIST 바이오소재연구센터*

Melanoma is the most aggressive form of skin cancer and is the fastest growing cancer in the UnitedStates. In this study, the synthesis of a new series of imidazo[2,1-b][1,3]thiazole scaffold is described.Their in vitro antiproliferative activities against human melanoma cell line A375 were tested and theeffect of substituents on the phenyl ring was investigated.



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Synthesis and Biological Evaluation of Oxazole and Isoxazole Derivatives as T-type Calcium Channel Blockers

김윤정, *최기항, **배애님, ***추현아, **조용서, ****임혜원

*고려대 화학 *고려대 화학과 **KIST 생체과학연구본부 ***KIST 생체과학연구부 ****KIST 의과학연구센터*

T-type calcium channels are low voltage-activated (LVA) calcium channels and located in muscle, glial cell, neurons and SA node. It has been reported that T-type calcium channel blocker could be used for the treatment of epilepsy, obesity and neuropathic pain. Mibefradil (Posicor^{R}), the first marketed selective T-type calcium channel blocker, was withdrawn due to toxicity from drug-drug interaction. Therefore, there have been many efforts to develop T-type calcium channel blockers with new scaffolds and no side effect. As part of discovering novel T-type calcium channel blockers, we designed oxazole and isoxazole derivatives and synthesized total 71 compounds. The synthesized compounds were biologically evaluated against T-type calcium channel. The detailed design, synthesis and biological evaluation of oxazole and isoxazole derivatives as T-type calcium channel blockers will be presented.

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Halenaquinone derivatives from tropical marine sponge *Xestospongia* sp.

김창권, *이연주, **신희재, ***이희승

*한양대 응용화학과 *한국해양연구원 해양바이오센터 **한국해양연구원 천연물연구실 ***한국해양연구원 해양천연물연구실*

Tropical marine sponges are fertile sources of secondary metabolites with novel molecular architectures. A variety of pentacyclic quinone and hydroquinone compounds has been isolated from marine sponge *Xetospongia* sp. These secondary metabolites have exhibited useful biological activities such as cardiotonicity, cytotoxicity, and enzyme inhibition. During our research for bioactive substances from tropical marine organisms, we isolated halenaquinolsulfate, xestoquinolsulfate, halenaquinone, tetrahydrohalenaquinone A, B, adociaquinone B, and xestosaprol from *Xestospongia* sp. collected from Chuuk, Federated State of Micronesia. The structures of these halenaquinone derivatives were elucidated on the basis of the spectral methods. Bioactivity of these metabolites will be presented.

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Synthesis and their biological activity of prenylated quinone compounds

최지은, 이석준, 오상태

관동대 의과대학 기초과학교실

Because more than 70% of the Earth's surface is covered by oceans, many marine plants are used for food, a source of minerals, dietary fiber, nutrition, and medicine. Numerous marine natural products and their unique constituents have been found to be useful for pharmacological studies to treat various diseases. Diverse quinones and chromanes with prenyl units originated from marine sources show various biological activities such as cytotoxicity against cancer cells, vasodilatation effect on basilar artery, cholinesterase inhibition effect for Alzheimer's disease, lipid peroxidation inhibitory effect, and antioxidation effect. Recently, we efficiently synthesized several prenylated quinone compounds and tested biological activities. In this presentation, we will show the results.

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Synthesis and their Vasodilation effect of natural Farnesyl acetones

전유진, 이석준, 오상태, 조성식

관동대 의과대학 기초과학교실

A variety of natural products has become an important tool for both the drug discovery process and biomedical studies. In particular, because more than 70% of the Earth's surface is covered by oceans, we can obtain many marine natural products which have a potentials to utilize for biomedical application. In order to make a potential chemical library for drug development, we are synthesizing several kinds of marine natural products and testing their biological effect by several screening systems. Recently, in the course of synthesizing marine natural product possessing vasodilatation effect, we discovered that some synthetic isomers showed a strong vaso-relaxation effect. In this presentation, we will show the synthesis of marine natural products and their biological usefulness.

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Preparation and Characterization of Inorganic Nanotube Composites for Colon-Specific Anticancer Drug Delivery

Farrukh R. Ahmed, K. E. Geckeler

광주과학기술원 신소재공학과, 나노바이오재료전자공학과

Inorganic nanotubes have found interest in several areas due to their specific application potential. Recently, especially halloysite, an inorganic clay material, has received increased attention for its application in drug delivery and nanobiotechnology due to its low cytotoxicity. In this study, halloysite nanotube-based composites have been prepared for simultaneous colon-specific delivery of 5-fluorouracil and folinic acid, the two most important drugs employed for the treatment of colorectal cancer. Three different composites were prepared by coating 5-fluorouracil-loaded nanotubes with folinic acid-conjugated chitosan. The different halloysite nanotube composites were characterized by FT-IR spectroscopy, XRD, TEM, and TGA.

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Synthesis and anticancer-activity of novel 1,6- and 3,6-disubstituted 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-7-one derivatives.

Vani N. Devegowda, *남길수, *배애님, *최경일

*University of Science and Technology *Korea Institute of Science and Technology*

A novel series of 1,6- and 3,6-disubstituted 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-7-ones were synthesized and evaluated on human cancer cell cytotoxicity such as prostate (DU-145), colon (HT-29 and HCT-116) and melanoma cancer (A375P) cell lines. Several compounds showed good anticancer activity in submicro-molar range concentrations. The key intermediate 6-substituted 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-7-one amines were readily synthesized in a large scale via facile three steps starting from commercially available primary amines. Further modifications were made on primary and secondary amine of pyrazol ring to obtain desired 4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-7-one derivatives. The most active compound KKJB1054 showed the GI50 value of 0.15 μM against HT-29.

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Synthesis and Biological Evaluation of Homopiperazine Derivatives as Potential T-type Calcium Channel Blockers

구수진, *송치만, *민선준, *이재균, *배애님, 한소엽, *장문호, *조용서

*이화여대 화학,나노과학부 *KIST 생체과학연구본부*

T-type calcium channel has been studied as one of the important drug targets for the treatment of hypertension, epilepsy and neuropathic pain. As an effort to develop potent and selective T-type calcium channel blockers, a library of homopiperazine derivatives was designed and synthesized in an efficient method. The in-vitro assays against α1G channel, a subtype of T-type calcium channels, and hERG channel were examined. In fact, we have found hit compounds showing not only high inhibitory effects on α1G channel but also low affinity toward hERG channel. On the basis of this result, we continue to study the structure-activity relationship (SAR) of such compounds to improve therapeutic properties.

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Facile synthesis of heterocyclic compounds as Nitric Oxide Synthase inhibitors.

표정인, *김현태, 김관수, **정찬성

*연세대 화학과 *연세대 생명공학과 **KIST 케모인포매틱스연구단*

Nitric Oxide (NO) is inclusively enticed to pathophysiological signal intertwined in a wide range of diseases such as cardiovascular, gastrointestinal, genitourinary, respiratory and nervous systems. It is synthesized from terminal nitrogen atom of arginine under the NADPH and dioxygen (O_2) dependent oxidation catalyzed by Nitric Oxide Synthases (NOSs). They have been classified a family of isoforms through the cell type or condition for endothelial NOS (eNOS), neuronal NOS (nNOS) and inducible or inflammatory NOS (iNOS). In this study, the useful synthesis and strategics based on the rigorous SAR and pharmacological tools within a wide variety of heterocyclic compounds will be achieved to get even more influential drug candidates on the selective inhibition of NOS isoforms.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and evaluation of potential inhibitors of Nitric oxide synthases(NOSs)

김현태, *표정인, 한균희, **정찬성

*연세대 생명공학과 *연세대 화학과 **KIST 케모인포매틱스연구단*

Nitric oxide (NO) is an important signaling molecule and involved in a number of physiological processes in mammalians. It is synthesized by nitric oxide synthases (NOSs) from L-arginine and molecular oxygen. Although NO mediates several physiological functions, its overproduction has been reported in a number of clinical disorders, including neurodegenerative disorders(parkinson's disease, alzheimer's disease). Three distinct NOS enzymes have been identified and characterized: neuronal (nNOS), endothelial (eNOS), and inducible (iNOS). NOSs are usually existed as dimer in their active form, required BH4((6R)-5,6,7,8-tetrahydrobiopterin) by cofactor. Our designated Pyrimidine derivatives synthesized by Vilsmeier-Haack reaction and cyclization. Block the BH4 binding site using our designated compounds, induce instabilization of NOSs, As a result, NO is expected to reduce

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Design, Synthesis and Biological Evaluation of Piperidine and Piperazine Derivatives as T-type Calcium Channel Blockers

최연희, *송치만, **민선준, ***이재균, **배애님, 백두종, **장문호, **조용서

*상명대 화학과 *KIST 케모인포매틱스연구단 **KIST 생체과학연구본부 ***KIST 응용과학연구부*

T-type calcium channels are identified as potential drug targets for the treatment of various diseases such as cardiovascular diseases, epilepsy, cancer and neuropathic pain. To seek new therapeutic candidates as T-type calcium channel blockers, we constructed a library of piperidine and piperazine derivatives, which originated from hit compounds based on in-silco virtual screening method. We have synthesized 84 new compounds and rapidly measured their in-vitro inhibitory activities against a1G/a1H channels using FDSS, high throughput screening (HTS) instrument. The compounds with high efficacies were further studied for evaluation of the selectivity against hERG channel, which was executed by means of manual patch–clamp. As a result, we have discovered highly potent and selective hit compounds against T-type calcium channel and continue studying the in-vivo activity of them using animal model.

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Discovery of a potential T-Type Calcium Channel blocker for the treatment of Neuropathic Pain

AHMED ABDUL WAHEED, *송치만, *민선준, **이재균, *배애님, *장문호, *조용서

*과학기술연합대학원대 *KIST 생체과학연구본부 **KIST 응용과학연구부*

T-type calcium channels may play a role in the expression of the neuropathic state. The data support the view that selective T-type calcium channel blockers may have significant potential in the treatment of neuropathic pain.In this study, based on the virtual screening we have synthesized compound libraries consisting of piperidine derivatives. On biological evaluation for T-type Calcium Channel blocking activity, some of the compounds have shown potency comparable to that of mibefradil (a T-type calcium channel blocker by Roche)

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Synthesis and SAR of (piperazin-1-yl-phenyl)-arylsulfonamides: a novel series of atypical antipsychtic agents

김소영, *박철민, **성철민, ***박노상, ****박우규, 하덕찬

*고려대 화학과 *한국화학연구원 의약화학 연구센터 **한국화학연구원 생명화학연구단 ***한국화학연구원 화학물질연구부 중추신경연구실 ****한국화학연구원 약리활성연구센터*

Serotonin receptors are known to be related with central nervous system (CNS) disorders. 5-HT_{2C} receptor antagonists are postulated to be potential drugs for the treatment of anxiety, depression, and other psychiatric disorders. 5-HT_6 receptor antagonists are known to be effective for treatment of cognitive diseases and schizophrenia. Thus, dual 5-HT_{2C} and 5-HT_6 receptor antagonists would be important for synergetically modulating schizophrenia, depression, and anxiety which are induced from Alzheimer's disease. This presentation will discuss the synthesis and SAR of (piperazin-1-yl-phenyl)-arylsulfonamides which show high binding affinities for both 5-HT_{2C} and 5-HT_6 receptors. Naphthalene-2-sulfonic acid isopropyl-[3-4-methyl-piperazin-1-yl]-phenyl]-amide exhibited high binding affinity towards both 5-HT_{2C} and 5-HT_6 receptors and considerable antagonistic activity for both receptors.

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Synthesis and Antitubercular Activity of a Beta-Lactam Triazole Library

황재민, *김성곤, **이일영, ***윤창수, ****박태호, *****Pradeep Kumar, *****Clifton E. Barry III, ******오태권, ******조상래, *******김필호

*한국화학연구원 난치성치료제연구센터 *경기대 화학과 **한국화학연구원 감영증치료물질연구팀 ***한국화학연구원 신물질연구단 난치성질환치료제연구센터 ****한국화학연구원 화학물질연구단 *****Tuberculosis Research Section, National Institute of Allergy and Infectious Diseases, NIH, Bethesda, Maryland, USA ******연세대 의과대학 *******한국화학연구원 감염증치료제연구센터*

Recently, it has been shown that a combination of carbapenem and clavulanate could effectively kill both replicating and non-replicating Mycobacterium tuberculosis (Mtb). Shortening the current long TB treatment regimen could be achieved by killing non-replicating Mtb effectively. In this context, since L,D-transpeptiase from Mtb (mtLDT) plays a significant role in the survival of non-replicating Mtb, it has been reported that mtLDT could be a reasonable TB drug target. Our studies centered around discovery of new beta-lactams as L,D-transpeptidase inhibitors, which eventually could lead to killing Mtb. We have designed and synthesized a novel beta-lactam library using click chemistry. We will present antitubercular activity of the generated library.

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Solid-phase synthesis of novel 7,8-functionalized pyrazolo[1,5-α] [1,3,5]-2,4-dithioxotriazine derivatives via cyclization reactions of dithiocarboxy resin bound pyrazoles

김정근, *이태임, **공영대, 하덕찬

*고려대 화학과 *한국화학연구원 대사증후군치료제연구센터 **동국대 화학과*

combinatorial synthesis has developed within a few years from a laboratory curiosity to a method that is taken seriously in drug research. Solid-Phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of our high-throughput synthesis program for drug discovery, we are trying to explore the potential of resin-bound dithiocarbazate as a versatile intermediates for generation of drug-like 7,8-functionalized Pyrazolo[1,5-α] [1,3,5]-2,4-dithioxotriazine derivatives. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of 7,8-functionalized Pyrazolo[1,5-α] [1,3,5]-2,4-dithioxotriazine from our previously reported resin-bound 5-amino-1-(substituted thiocarbamoyl)pyrazole derivatives. The progress of reactions could be monitored as solid-bound intermediates by ATR-FTIR spectroscopy. The final compounds were obtained in good yields and high purities

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Synthesis of F-18 labeled N-substituted Ciprofloxacin derivatives for the Imaging of bacterial infection with PET.

김동욱

전북대 의학과

A series of N-substituted piperazinyl quinolones derivatives were synthesized and evaluated for antibacterial activity against some Gram-negative. The antibacterial data reveled that N-substituted Ciprofloxacin derivatives had strong and better activity against tested Gram-negative organism than the reference quinolones such as Ciprofloxacin. In addition, to define structure-activity relationship of Ciprofloxacin at N-4 position of piperazin ring were prepared and tested. We described a new F-18 labeled N-substituted Ciprofloxacin derivatives. F-18 Fluoropropyl Ciprofloxacin was produced easily and highly efficient step using tertiary alcohol as a reaction media for nucleophilic fluorination. The reaction of fluoride ion with the corresponding Mesylate precursor. These data suggest that F-18 Fluoropropyl Ciprofloxacin shows favorable properties as PET tracer to image of bacterial infection.

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Study on the trans-2-enoyl-ACP reductase (FabI) inhibitor as a new antibiotics

차현주, *신계정, **최용석

*고려대 생명공학과 *KIST 생체과학연구본부 **고려대 생명과학대학*

Trans-2-enoyl-ACP reductase (FabI) catalyzes the final reduction step in bacteria fatty acid biosynthesis (FAS) cycle. FabI is known as the new antibiotic target and showed a hopeful inhibition effects. We have synthesized novel aryl and heteroaromatic amide derivatives for the treatment of resistant bacteria.

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Synthesis and biological activities of derivatives with diverse scaffolds as T-type calcium channel blockers

나윤수, *지완근, **박정은, *양정은, ***노은주, 전철호

*연세대 화학과 *고려대 화학과 **서강대 화학과 ***KIST 생체과학연구부*

A series of compounds were suggested and prepared as T-type calcium channel blocker from virtual screening. Based on scaffold structure, diverse derivatives were prepared and their inhibitory activities on T-type calcium channel were assayed using in vitro screening system FDSS 6000 for 1G and 1H calcium channel. They showed structure activity relationships and for the compounds with higher inhibition than 40% in FDSS assay system, the IC50 was measured by patch clamp method. If they showed IC50 lower than 2 M, the degree of hERG channel inhibition was assayed by auto patch to avoid cardiac toxicity. The criteria for further assay were IC50 (hERG/ 1G) ratio greater than 10.

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Synthesis and Biological evaluation of 3,5-diaminoindazole derivatives as an anti-cancer agent

홍지은, 이상효, 이진호

계명대 화학과

The cyclin-dependent kinases (CDKs) are serine-threonine protein kinases with roles in the control of the eukaryotic cell cycle and transcriptional regulation. Because of their critical role in the regulation of the cell cycle and the observed expression/activity pattern in most human cancers, considerable effort has been focused on the development of small molecule CDK inhibitors as potential therapeutic agents. Our previous efforts to discover novel CDK inhibitors led to the identification of the 3,5-diaminoindazole that was investigated as an anti-cancer agent. To improve physical properties of lead compounds, modifications of substituent at 5-position were performed. Cellular activities of newly synthesized compounds were evaluated with 5 human cancer cell lines. Also, the aqueous solubilities of compounds were studied.

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3,5-Diaminoindazoles inhibitors of cyclin dependent kinases

박종원, 노준호, 이진호

계명대 화학과

Cyclin-dependent kinases are members of a family of serine-threonine protein kinases responsible for regulation of the eukaryotic cell cycle. Cell proliferation is regulated by different CDKs coupled with a corresponding cyclin partner. Cancer is known as a disease of aberrant cellular proliferation and most cancer cells exhibit deregulation of CDKs. As a result, CDK inhibitors have been intensively pursued as potential anti-cancer agents. Our previous efforts to discover novel CDK inhibitors led to the identification of the 3,5-diaminoindazole. Indazoles with 1λ-isothiazolidine-1,1-dione substituent at 5-position were highly potent for both CDKs and cell proliferation. The modifications of substituents at 3 and 5 position were performed to improve physical and biological properties of lead compounds. Cellular activities of newly synthesized compouds were evaluated with 5 human cancer cell lines. In addition, the aqueous solubilities of compounds were studied.

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Construction of Thiazolo[4,5-b]pyridine Library using Friedländer reaction

이두현, 이태호, *공영대

*한국화학연구원 대사증후군치료제연구센터 *동국대 화학과*

The combinatorial synthesis of small organic molecules in either the solution-phase or on solid support has had a significant impact in the area of drug discovery. Previously, we reported a facile and rapid solid-phase synthetic methodology for constructing a small molecule library based on thiazole and thiazole-fused scaffolds. As a part of an ongoing drug discovery program, we have been exploring the potential of resin-bound thiazole derivatives as versatile intermediates for generation of drug-like heterocyclic compound libraries. Herein, we would like to present the construction of 2,5,7-trisubstituted thiazolo[4,5-b]pyridine derivatives using Friedländer reaction under microwave irradiation. The target compounds were achieved in traceless manner with various amine nucleophiles in good overall yields.

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Synthesis and Evaluation of 4-(4-phenoxy-4-phenylbutyl)piperazines for T-type Ca^{2+} channel blockers

김익수, 이숙자, *이주현, **금교창, ***강순방, ***김유승

*한국외국어대 화학과 *고려대 화학과*
***KIST 케모인포메틱스연구센터 ***KIST 생화학물질연구센터*

T-type Ca^{2+} channels are a type of voltage-dependent calcium channel and widely expressed in neurons. T-type Ca^{2+} channels have attracted much attention since they are able to be novel therapeutic targets such as hypertensions, absence epilepsy, neuropathic pains, sleep disorder, and obesity. It is recently reported that T-type Ca^{2+} channel show subtype-specific and region-specific role in the pain pathway. In order to develop T-type Ca^{2+} channel blockers with higher potency and selectivity we have prepared a series of new 4-(4-phenoxy-4-phenylbutyl)piperazine derivatives by using Mitsunobu reaction and N-alkylation protocol. Their inhibitory activities on T-type Ca^{2+} channel were evaluated by in vitro assay with α1G and α1H clones using FDSS screening system. Their activity, subtype selectivity, and structure-activity relationship (SAR) on T-type Ca^{2+} channels will be presented.

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Fluorine-18 Labeling of Isoquinoline Analogue

김희정, 김동연, *김인종, **박정훈, **김상욱, **허민구, *최상무, **양승대, 유국현

*동국대 화학과 *한국원자력연구소 방사선공업환경연구부*
***한국원자력연구원 방사선공업환경연구부*

Inhibitors of poly(ADP-ribose) polymerase-1 (PARP-1), an enzyme involved in a DNA repair and programmed cell death, play a crucial role in the treatment of breast cancer in monotherapy as well as in combination with chemotherapeutic agents and radiation. Recently, PARP-1 inhibitors have revealed the ability to reduce a VEGF-induced proliferation. Therefore, PARP-1 inhibitors may be considered as an attractive therapy. We selected the target compound as 1,5-isoquinolinediol known as PARP-1 inhibitor. 5-[18F]fluoroisoquinolin-1-ol was synthesized to investigate its potential for a cancer imaging agent for PET. Modified Balz-Schiemann method was used for the [^{2}F]fluoride labelling of the isoquinoline compound. The radiochemical yield of 5-[^{2}F]fluoroisoquinolin-1-ol was about 15% and the radiochemical purity was above 95%.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

A Novel Class of DAXX nuclear export inhibitors;Synthesis and biological evaluations of benzothiophene derivatives

이서현, 서지희, 이진아, 김낙정, 이규양

한국화학연구원 대사증후군치료제연구센터

DAXX is a Fas-binding proapoptotic protein that is a component of the death-inducing signaling complex in Fas-mediated apoptosis.During ischemic stress, Daxx translocates from the nucleus to the cytoplasm.The cytoplasmic presence of Daxx is essential for cell death upon ischemic insult.As part our efforts to find new scaffolds of DAXX nuclear export inhibitors as effective anti-ischemic agents, we have designed and synthesized a series of benzothiophene derivatives.Synthesized compounds were biologically evaluated using in vitro H9c2 cell Pharmacological activities correlated with their structures will be presented.

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Synthesis and Antitubercular Activity of Nitroimidazoles

이상호, *김수현, **윤민한, ***이일영, ****윤창수, *****박태호, ******조상래, ******오태권, *******김필호

*한국화학연구원 신약연구단 *경희대 기초약학과 **서강대 화학과 ***한국화학연구원 감영증치료물질연구팀 ****한국화학연구원 신물질연구단 난치성질환치료제연구센터 *****한국화학연구원 화학물질연구단 ******연세대 의과대학 *******한국화학연구원 감염증치료제연구센터*

Recent antitubercular drug discovery effort focuses on finding out new chemical entities, which could shorten the lengthy tuberculosis (TB) treatment regimens: 6-9 months for drug susceptible TB and 18-24 months for multi-drug resistant TB (MDR-TB). It has been shown that killing persistent or non-replicating Mycobacterium tuberculosis (Mtb) could play a significant role to shorten TB chemotherapy. Nitroimidazoles such as PA-824 and OPC-67683 are currently in clinical phase II development as a promising new class of therapeutics for TB. These clinical candidates have activities against both replicating and non-replicating Mtb so that they could lead to a shorter chemotherapy period. In an effort to discover new and more potent antitubercular nitroimidazoles, we have designed and synthesized a novel class of nitroimidazole analogs. Synthesis and antitubercular activity of nitroimidazoles will be presented.

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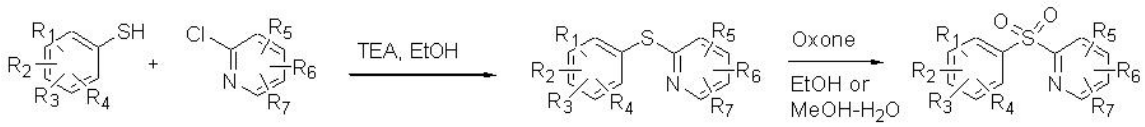
Synthesis and quorum sensing activity of biaryl-sulfide and biaryl-sulfone derivatives.

구영원, 임동렬, 박재관, 이윤학, *최상호, *김승민

*세종대 화학과 *서울대 농생명공학부*

Synthesis of various biaryl-sulfide and -sulfone derivatives was performed using classical nucleophilic aromatic substitution reaction. Among hundreds of new compounds prepared, several aryl-pyridyl sulfone analogs were identified as quorum sensing inhibitors of Vibrio vulnificus. The binding mode of our inhibitor with a putative receptor, LuxP, was proposed.



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Simultaneous Encapsulation of Anticancer and Imaging Agents by Apoferritin

최성호, K. E. Geckeler

광주과학기술원 나노바이오재료전자공학과, 신소재공학과, 의료시스템공학연구소

A novel nanocarrier for anticancer and imaging agents designed for simultaneous cancer diagnostics and therapeutics was prepared using the protein apoferritin. Thus, 5-fluorouracil as an anticancer agent and nile blue chloride as a NIR fluorescence imaging agent were simultaneously encapsulated. The central cavity, the multi-channel structure, and the chemical properties of apoferritin contribute to the specific targeted delivery for ferritin-binding sites or aiding the endocytosis in neoplastic cells. The bifunctional encapsulating nanocarriers were characterized by UV/visible, fluorescence, and circular dichroism spectroscopy as well as by native and sodium dodecyl sulfate poly(acrylamide) gel electrophoresis.

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Supramolecular Complexation of Single-Walled Carbon Nanotubes with the Green Fluorescent Protein

최성호, K. E. Geckeler

광주과학기술원 나노바이오재료전자공학과, 신소재공학과, 의료시스템공학연구소

A supramolecular complex of single-walled carbon nanotubes (SWNT) and the green fluorescent protein (GFP) was prepared for the first time in an aqueous solution using a controlled sonication procedure. The dispersion of the SWNT-GFP complex exhibited a strong near-infrared absorbance induced from the well-debundled and individualized SWNTs and maintained the excellent fluorescent property typical for the GFP. By circular dichroism spectroscopic analysis it was possible to confirm the secondary structure of the GFP. Furthermore, the dispersion of the SWNT-GFP complex was subjected to cell viability tests including cellular uptake and internalization experiments with mammalian and prokaryotic cells.

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Synthesis and Characterization of New Keggin-ion Pillared Gadolinium Hydroxynitrates

이승수, 윤호섭, 강준건

아주대 화학과

Gadolinium hydroxynitrate, $Gd_2(OH)_5(NO_3)\cdot xH_2O$, is a layered host whose interlayer nitrate ions can be exchangeable. We have prepared some new Keggin-ion pillared gadolinium hydroxynitrates via two different synthetic routes. At first, $PMo_{12}O_{40}^{3-}$ and $SiMo_{12}O_{40}^{4-}$ ions have been refluxed in the aqueous solution at 80 oC for 7 days. In another route, the same reactions carried out in the hydrothermal kit at 130°C for 5 days. Products were characterized using XRD, TG-DSC, and FT-IR analysis. Well-ordered (00l) reflections and increase of basal spacings in the XRD patterns prove intercalation of Keggin ions. In the IR spectra, the products show a new band around 700 cm^{-1}, which assigned as the bond between the host and Keggin ions. TG-DSC results indicate the higher thermal stability of the products was related to the presence of Keggin ions in the host layer. Different synthetic routes do not make any noticeable difference in the physical properties of the products.

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Thermal Properties of Gadolinium Hydroxynitrates and its Keggin-ion Pillared Complexes

이승수, 윤호섭, 강준건

아주대 화학과

The thermal properties of gadolinium hydroxynitrates and its Keggin-ion pillared complexes, $Gd_2(OH)_5(Z^{n-})_{1/n}\cdot xH_2O$($Z^{n-}$= $PMo_{12}O_{40}^{3-}$ and $SiMo_{12}O_{40}^{4-}$), have been investigated by TG-DSC and XRD analysis. TG-DSC data show three step mass losses for gadolinium hydroxynitrates: dehydration(RT~200 ℃), dehydroxylation(200~350℃) and transformation into Gd_2O_3 with losing NO_2, O_2 and H_2O(350~600℃). In case of Keggin-ion pillared complexes, dehydration and dehydroxylation occur with similar patterns to the host between RT and 350℃. In contrast to the host material, the Keggin-ion pillared complexes did not show no weight change in the wide temperature range(350~700℃) except a sharp exthothermic peak due to the phase transition of Keggin unit on DSC thermogram. The pillared samples, heat-treated respectively up to 200, 300, and 400℃, still represent well-defined XRD patterns. These means the Keggin uint between the host slabs could be maintained up to the high temperature region.

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Surface modifications of organic-inorganic hybrid film by Molecular Layer Deposition: An effective method to improve the strength of PDMS Stamp

남재우, 황재권, 성명모

한양대 화학과

Molecular Layer Deposition(MLD) has been utilized for the surface engineering. We chose the surface modification of Al_2O_3 and 1H, 1H, 2H, 2H - perfluorooctyltrichlorosilane(FTS) as an example to demonstrate the concept of MLD-based approach. The Samples were characterized by Contact Angle Analysis(CAA), Scanning Electron Microscopy(SEM), X-Ray Photoelectron Spectroscopy(XPS), Atomic Force Microscopy(AFM) and stamping test of surface modificated PDMS stamp using MLD. The results show that surface modificated PDMS stamp has better properties than PDMS stamp(not surface modificated).

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Low-Temperature Atomic Layer Deposition of Copper Metal Thin Films: Self-Limiting Surface Reaction of Copper Dimethylamino-2-propoxide with Diethylzinc

남재우, 이병훈, 성명모

한양대 화학과

Copper thin films were grown on Si (100) substrates by atomic layer deposition (ALD) using $[Cu(OCH(Me)CH_2NMe_2)_2]$ and Et_2Zn as precursors. The Cu metal is formed by treating the Cu precursor adsorbed on the Si with Et2Zn. The thickness, chemical composition, crystalline structure, and morphology of the deposited films were investigated by secondary electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and atomic force microscopy (AFM). The results show that Cu ALD using $[Cu(OCH(Me)CH_2NMe_2)_2]$ and Et_2Zn as precursors is self-controlled at temperatures of 100 - 120C. The copper film was grown with a preferred orientation toward the [111] direction.

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Characterization of LiBr-LiCl-LiF Eutectic as Molten Salt Electrolyte in Thermal Battery Applications

이아람, 박윤봉

충남대 화학과

Molten salt thermal batteries are activated by raising their temperature to above the melting point of the salt constituting the electrolyte. Lithium halide-based mixtures were mainly used as electrolytes for their low melting points(compared to sodium halide mixtures), low vapor pressure, and their relatively high ionic conductivities. Among them, LiBr-LiCl-LiF electrolyte has been selected and new processing procedure for the electrolyte has been developed. Its performance in Li-Si/FeS_2 single sells was tested and compared to the one with conventional LiBr-LiCl-LiF electrolyte. The discharging tests of the single cells showed as least 20% increase in its discharging capacity compared to the conventional electrolyte of the same kind. In this paper we will report its processing procedure and characterization results using discharging test, X-ray diffraction, thermogravimetric analysis, and differential thermal analysis.

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Synthesis and Characterization of Magnesium Oxide Nanoparticles and its application to Thermal Battery Applications

이아람, 권지희, 김병기, 박윤봉

충남대 화학과

Magnesium oxide (MgO) powders have been extensively used as binders in the separator of thermal batteries to immobilize the electrolyte by means of the capillary forces at high temperature. Therefore the control of pore size distribution and the surface areas of MgO particles are very important to minimize the deformation and electrolyte-leakage behavior of separator during the operation of thermal batteries. Another important factor to be considered is the amount of MgO used in the separator fabrication. By reducing the amount of MgO used in the separator the thermal battery performance can be improved due to reduced internal resistivity of the separator. In this work we have prepared MgO nanopaticles with large surface areas and controlled particle sizes, which are then used for separator fabrication. To evaluate the performance of the separator prepared discharging tests are done in Li-Si/FeS_2 single cells and compared with the ones with commercial MgO.

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Fabrication of nanostructured ZnO/metal chalcogenide multilayered thin film

김종영, *장경주

*요업기술원 이천분원 *한국세라믹기술원 이천분원*

Multilayered nanostructure of ZnO wire/rod and metal chalcogenide was fabricated by electrochemical and wet solution process. Wire/Rod-shaped ZnO semiconductor was deposited by potentiostatic electrodeposition, and metal chalcogenide such as cadmium sulfide, copper indium selenide were deposited by electrochemical deposition and chemical bath deposition. The photochemical property of the multilayered device was investigated by IV analysis using solar simulator.

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RTGG Synthesis of IZO thermoelectric materials using shape-controlled precursor

김종영, 장경주

한국세라믹기술원 이천분원

IZO-type thermoelectric materials was synthesized by RTGG method using plate-shaped Zn-precursors. The precursors were prepared by hydrothermal and wet chemical synthesis. Texture-controlled thermoelectric oxide was fabricated by tape casting technique using shape-controlled precursors.

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High Performance Thin Film Transitor with Nitrogen-doped ZnO as an Active Layer Grown at Low Temperature by Atomic Layer Deposition

조상호, 성명모

한양대 화학과

Many research groups have studied on oxide semiconductors as active channel materials for transparent TFTs. Especially, ZnO is considered as a promising candidate of oxide semiconductors because of absence of environmental concerns, and moderate mobility. In addition, TFTs with the ZnO thin films show high field effect mobility comparing to a-Si (>1cm^2/Vs) and better transparency because of the wide bandgap. However, carrier concentration in ZnO is so high (>10^{18}cm^{-3}) that ZnO thin films are very conductive even without applied gate voltage, which leads to degradation of the performance such as poor on/off current ratio which leads to problems in switching modulation.Causes of excessive carrier concentration in ZnO thin films are considered to be due to zinc interstitials, and oxygen vacancies. Many research groups tried to reduce those defects, controlling the deposition conditions such as oxygen pressure ratio in sputtering and pulsed laser deposition. In addition, they studied on doping systems to develop high field effect mobility ZnO, adopting Ⅲ-Ⅴ elements such as Ga and In.In this study, we studied nitrogen-doped ZnO (ZnO:N) thin films using ALD method. We investigated the change of microstucture and electrical properties of the thin films by using X-ray diffraction, scanning electron microscope, X-ray photoemission spectroscope. We present ZnO:N thin films deposited at low temperature (less than 100℃) for high performance thin film transistors. We could obtain the high performance TFTs on the flexible plastic substrate at low temperature using the ALD method: greater than 30cm^2/Vs of field effect mobility, >10^8 of on-off current ratio, 0.5V/decade of swing slope, and less than 1V of threshold voltage.

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Vapor-Phase Fabrication of Organic-Inorganic Hybrid Polymer Films Using Alkyl Metal and Bifunctional Monomers

조상호, 성명모

한양대 화학과

Inorganic films can be deposited with sequential dosing of multifunctional precursors and self-limiting surface chemistry process known as atomic layer deposition (ALD). Organic film can also be grown by similar method, named molecular layer deposition (MLD). Instead of multifunctional precursors in ALD, bifunctional monomers are used in MLD. These two film deposition method share good properties for high quality multicomponent superlattices such as precise control of film thickness, highly conformal layering, large-scale uniformity, sharp interfaces, etc. By combining ALD and MLD, organic-inorganic hybrid polymer films can be fabricated in vacuum condition. New class of organic-inorganic hybrid polymer films grown by sequential surface reaction of inorganic precursors and bifunctional organic monomers overcome the weakness of organic polymer films grown by bifunctional monomers only, thermal unstability. Moreover, these new hybrid films are expected to have combined properties of organic and inorganic materials and to improve the performance or to lead new useful properties.

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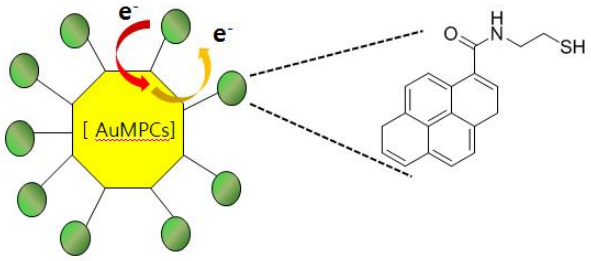
Electrochemical and optical characterization of pyrene functionalized gold nanoparticles

김성혜, 이동일

연세대 화학과

Understanding photoinduced electron and energy transfer processes in nanoparticle assemblies is of critical importance in their use in sensors, solar energy conversion and photocatalysis. In spite of many research efforts on fluorophore-functionalized gold nanoparticles, quantitative analysis of the fluorophore-nanoparticle interactions is still limited. We present synthesis and characterization of structurally and energetically well-defined Au25 monolayer-protected clusters (MPCs) functionalized with pyrene. Two methods were employed to produce pyrene-Au25 assemblies. In the first method, we functionalized hexanethiolate protected Au25 MPCs with pyrene-SH (N-(2-mercaptoethyl)-3,8-dihydropyrene-1-caroxamide) by the ligand exchange reaction. In the second method, glutathione protected Au25 MPCs were amide coupled with pyrene-NHS (pyrrolidin-1-yl pyrene-4-carboxylate). Pyrene loading on Au25 was varied by controlling the reaction condition and quantified by a combination of NMR and UV/Vis absorption spectroscopy. Electrochemical voltammetry shows a significant decrease in the HOMO-LUMO gap of Au25 from 1.6 eV to 1.3 eV with pyrene functionalization. In addition, pyrene fluorescence is drastically quenched upon binding to Au25. The origin of these effects is considered to be the electron transfer process between pyrene and Au25.



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Self-Assembly of CdTe Nanoparticles into Twisted Ribbons

이광원, 김기섭

충주대 화공생물공학과

The optical and electrical properties of nanoparticles (NPs) and nanowires (NWs) have been extensively studied for use in electronics, sensors, and photonics. Recently, one of the most active areas of research in nanoscience is to develop novel structures of nanomaterials such as nanohelices (NHs), nanosheets (NSs), and hollow nanocrystalls, which open up the possibility of a new generation of advanced materials. CdTe NP dispersions were prepared according to the method reported in the literature and the ratio of TGA to CD2+ was selected as 1.0.6 1.095g of Cd(ClO4)2 6H2O was dissolved in 200 mL of pure water, and TGA was added into the solution at a molar ratio of 1.0 against Cd2+.The pH values of the solution were adjusted to 11.4 by the dropwise addition of 1M NaOH solution.The solution was deaerated by N2 bubbling for 60 min.Under stirring, H2Te gas was passed through the solution with a nitrogen flow for 60 min. The precursors were converted to CdTe nanocrystals by refluxing at approximately 100 ℃ for 50 min. The dispersions with a maximum luminescence 542 nm were obtained. The luminescent color under UV light was green. The CdTe quantum dots (QDs) were precipitated by addition of methanol and then redissolved in pure water at PH 9.0. The dispersion was then exposed to ambient light (intensity 8.62mW) and aged.

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New Blue Emitting Indenopyrazine Derivatives for OLEDs : Improving the EL Properties Through Substitution Effects by Using Terphenyl Side Group

박영일, 석창훈, *이지훈, 박종욱

*가톨릭대 화학과 *충주대 나노고분자공학과*

Organic light-emitting diodes (OLED) are receiving the spotlight as next generation flat screen display among optoelectronic fields based on π-conjugated organic molecule, and many studies are recently being conducted on them. For realization of full color in such OLEDs, red, green and blue-emitting materials with excellent performance are necessary. However, blue emitting material accompanies serious problems of low efficiency and shorter lifetime compared to red or green emitting material due to difficulty in hole and electron injection with larger band gap. In our previous research paper, utilization of 6,12-Dihydro-diindeno[1,2-b;1',2'-e]pyrazine (indenopyrazine) as a new emitting core structure was reported for the first time. However, indenopyrazine itself has flat structure and shows frequent stacking of molecules, easily bringing unwanted bathocrhomic shift and reduction of luminescence efficiency as a blue emitting material. Accordingly, a systematic study on molecular structure that can effectively prevent intermolecular interactions is needed for the material to be used as a highly efficient and pure blue emitting material.

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Synthesis and Characterization of Amine-Terminated Monolayer-Protected Gold Clusters.

이현진, *Mary sajin devadas, 이동일

*연세대 화학과 *Michigan university, kalamazoo, Michigan 49008,U.S.A*

Alkanethiolate monolayer-protected gold clusters (gold MPCs) exhibit size-dependent chemical, electronic, and optical properties. For the utilization of these properties in nanoelectronics, biological-sensing, and optics, it is necessary to functionalize gold MPCs with specific functional groups such as chromophores and redox active species. To this end, we have synthesized various amine-terminated MPCs; aminothiophenol, cysteamine and L-cysteine, by a modified Brust's synthetics method. Aminothiophenol ligand is employed to prepare conjugated linker MPCs. Cysteamine and L-cysteine ligands are used to prepare organic and aqueous solvent soluble MPCs, respectively, with short ligand length. Optical absorption and emission properties of these amine-terminated MPCs are characterized by UV-vis absorption spectrometry and fluorescence spectrometry, respectively. The size of MPCs is determined by transmission electron microscopy. The effects of amino ligands on the size and optical properties of gold MPCs will be discussed. The functionalization of amine-terminated gold MPCs with pyrene by a coupling reaction will be presented.

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Synthesis of porous TiO_2 nano-cups by using electrospray

박성열, 김용신

한양대 응용화학

In this work, we prepared a composite solution of dissolving poly(methyl methacrylate) (PMMA) and titanium tetraisopropoxide (TTIP) in nitromethane. The solution was electrosprayed from the metal needle, typically applied to ~ 10kV, to a grounded collector. Under optimized conditions, the formed PMMA/TiO_2 composite was observed by SEM to have a cup-like nanostructure with porosity, being transformed to porous TiO_2 nano-cups by sequent calcination at 550°C. The detailed nano-cup structure such as a cup size and porosity was found to be controlled by the strength in electrical field and relative concentration between PMMA and TTIP. This simple methodology can provides a lot of opportunities to synthesis inorganic nanoparticles with non-spherical geometry with the aid of the template nanostructures formed by specific polymer under electrospray process.

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Synthesis of a silicoaluminophosphate molecular sieve from dry gels: Phase-selectivity

전종원, Nazmul Abedin Khan, 정성화

경북대 화학과

Silicoaluminophosphate (SAPO) molecular sieves with AFI and CHA structures have been synthesized from a reaction mixture containing triethylamine (TEA) as a template or structure-directing agent. The syntheses were carried out at 180 - 200 oC for several days both from dry gels (dry gel conversion) and homogeneous gels (conventional electric heating). From similar reaction mixtures, SAPO-5 (AFI structure) and SAPO-34 (CHA structure) molecular sieves are phase-selectively obtained from dry gel conversion and conventional electric heating, respectively. The phase-selectivity may be explained by the slow crystallization of the dry gel conversion due to low water or TEA concentration under the reaction conditions. This phase-selective synthesis with dry gel conversion may lead to a new method for the synthesis of relatively unstable molecular sieves such as VFI or VPI-5.Keyword: microporous materials; chemical synthesis; dry gel

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Facile syntheses of metal–organic framework Cu3(BTC)2(H2O)3 under ultrasound

Nazmul Abedin Khan, 정성화

경북대 화학과

Cu-BTC [Cu3(BTC)2(H2O)3, BTC=1,3,5-benzenetricarboxylate], one of the most well-known metal-organic framework materials (MOF), has been synthesized under atmospheric pressure and room temperature by using ultrasound. The Cu-BTC can be obtained in 1 min in the presence of DMF (N, N-dimethylformamide), suggesting the possibility of continuous production of Cu-BTC. Moreover, the morphology and phase depend on the concentration of DMF; Cu-BTC cannot be obtained at room temperature in the absence of DMF and aggregated Cu-BTC (with low surface area) is produced in the presence of high concentration of DMF. It seems that the deprotonation of benzenetricarboxylic acid by base (such as DMF) is inevitable for the room temperature syntheses. It is also found that the surface area and pore volume are higher for the Cu-BTC (without aggregation) synthesized by the present method compared with the materials synthesized by conventional electric heating and microwave heating at high temperature of 120 - 140 oC. Keyword: Metal-organic frameworks (MOF); rapid synthesis; ultrasound; Cu-BTC; morphology

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Facile purification of porous metal terephthalates with ultrasonic treatment in the presence of amides

Enamul Haque, 정성화

경북대 화학과

A facile purification method of metal-organic frameworks (MOFs), especially the ones containing insoluble 1,4-benzenedicarboxylic acid (terephthalic acid) in the pore, has been suggested. The purification method is composed of treating the MOF with amides such as N, N-dimethylformide, especially under ultrasound. The purification is completed in 1 h at 70 oC as has been confirmed by XRD, nitrogen adsorption, FTIR and TGA, etc. The purification method is simple, one-step, fast and energy-efficient. The MOFs purified by the proposed method show high surface area and micropore volume, showing the efficiency of the method. The suggested purification method will lead to a new way to activate (for example, to remove carboxylic acids) MOFs that are especially unstable above around 100 oC. Additionally, the method may be used to transform a non-porous MOF-type material into a porous MOF structure.Keyword: Metal-organic frameworks, Microporous materials, Purification, Ultrasound, Amides

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The Characterization of Borohydride-Stablized Nanosilvers in Laponite Sol Using ^{1}H NMR: Its Ligand Exchange Reactions with MUA and TOP

서재석, 손동민, 이한나, 김지광, 김유혁

단국대 첨단과학대학 화학과

The borohydride-protected nanosilvers in laponite sol show that the silver particles are aggregated in the manner of forming short chains and dumbbell shape. The borohydride on nanosilver can be exchanged with 11-mercaptoundecanoic acid (MUA) and trioctylphosphine. Transmission electron microscopyand UV-vis spectroscopy data show that the number of aggregated silver nanoparticles is decreased upon addition of aforementioned ligands due to the formation of silver MPCs (monolayer-protected clusters). Adsorption of MUA and trioctylphosphine on nanosilver is confirmed through the observation of broad proton resonances of MPCs in ^{1}H NMR spectra.

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Hydrothermal Synthesis and Characterization of Ag@SiO_2 Core-Shell Embedded in Silica Particles

손동민, 강병규, 서재석, 이한나, 김지광, 김유혁

단국대 첨단과학대학 화학과

Hydrothermal synthetic method has been demonstrated for the synthesis of Ag@SiO_2 core-shell embedded in silica particles with silver diameters in the range of 20~80 nm, and thickness of silica shell about 20 nm. The first step of this synthetic method involved the formation of Ag nanoparticles by reducing $AgNO_3$ with hydrazine in the presence of NaOH stabilized active silicic acid, which is generated by ion-exchange method from water glass. Hydrothermal treatment of Ag nanoparticles at 180^0C gives well-defined Ag@SiO_2 core-shell in aggregated silica particles. The concentration of active silicic acid affects the morphology of Ag particles. The formation of Ag nanoparticles and Ag@SiO_2 core-shell is confirmed by UV-visible absorption spectra, TEM and EDS data.

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Synthesis, Photoluminescence and Thermal Properties of Laponite-(X,Ce)(X = Eu, Tb) Phosphors

이한나, 서재석, *박승혁, 김지광, 김유혁

*단국대 첨단과학대학 화학과 *고려대 화학과*

In order to give emission functionality for laponite the laponite-(X,Ce)(X = Eu, Tb) phosphors were prepared by calcination of cryogels which were prepared through Na ion exchange reaction with Eu and Tb ions. Thermal stability and emission properties of new laponite phosphors were investigated by X-ray diffractormeter and UV/VUV spectrofluorometer. The phosphors were stable around up to 600°C and new crystalline phases were observed at 650°C. Red and green emissions of phosphors under UV/VUV excitation were also identified at 300°C and 500°C as emission peaks of Eu^{3+} and Tb^{3+},respectively.

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Dispersion Stability of Protein-Wrapped Single-Walled Carbon Nanotubes and Their Cytotoxicity in vitro

이연주, 문영주, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*

Carbon nanotubes feature a poor solubility and low dispersability in aqueous and organic liquids because of their aggregation tendency. This leads to difficulties in their incorporation into the biological interphase and enhances the cell toxicity. Therefore, it is crucial to investigate and optimize the dispersion properties of carbon nanotubes. In this study, aggregated carbon nanotubes were dispersed in different media containing proteins such as cell culture media to study the dispersion stability of protein-wrapped carbon nanotubes and their cytotoxicity in vitro. The products were characterized by transmission electron and scanning electron microscopy as well as by Raman spectroscopy. In addition, the interactions between the products and the media were investigated by Zeta potential measurements and UV-vis-NIR spectroscopy. Also, in vitro cytotoxicity tests on culture mouse embryonic fibroblast cells were performed to determine the cell proliferation.

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Synthesis of DNT Derivatives for Chemical Sensor System

이웅희, 장현준, *김석찬, 유연규

*국민대 생명나노화학과 *국민대 화학과*

TNT 와 DNT 는 대표적인 이다. DNT 의 승화로 인해 발생하는 기체 DNT 를 검출하여 위험을 미연에 방지할 수 있는 Biosensor 를 만들기 위해, DNT 유도체인 4-(2,4-dinitrophenyl)butan-1-amine 를 합성하였다. 4-(2,4-dinitrophenyl)butan-1-amine 을 Biotine 나 SAMs 물질과 결합시켜 immobilize 하고, M13 phage 를 이용하여 DNT 에 특이적으로 결합하는 단백질을 찾아 Biosensor 를 만들고자 한다.

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Two-dimensional arrays of gold nanoparticles fabricated on aminofunctional surfaces micropatterned based on vacuum ultraviolet lithography

J.H. Yang, Y.J. Kim, T. Ichii, K. Murase, H. Sugimura

Department of Materials Science and Engineering, Kyoto University

Functionalization of quartz surfaces has been attracted much attention in last few years in order to enhance their excellent optical properties. In particular, immobilization of gold nanoparticles (AuNPs) onto quartz is of considerable interest in view of optoelectronic applications attained with plasmonic properties of the AuNPs. Here, we demonstrate the regular arrangement of AuNPs in a linear fashion by controlling function and microstructure of a quartz surface through the formation of a 3-aminopropyltriethoxysilane self-assembled monolayer (APS-SAM) and the subsequent vacuum ultraviolet (VUV) lithography. AuNPs were spatially arranged on the area covered with APS-SAM. X-ray photoelectron spectra of the samples revealed that AuNPs were certainly immobilized on their surfaces. Features of area-selectively immobilized AnNPs onto the VUV-patterned APS-SAMs were confirmed via atomic force microscope images. The selective immobilization of AuNPs originated from the attractive electrostatic interaction between the AuNPs and amino groups terminating the APS-SAM surface. On the contrary, there was the repulsive interaction with the AuNPs on the naked quartz surface where the APS-SAM had been removed by VUV-lithography. Consequently, the AuNPs were accurately aligned on the aminofucntional micropatterns. The spatial resolution less than 1 μm has been successfully acheived on this area-selective AuNP arrangement.

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Surface modification of cyclo-olefin polymer in atmospheric pressure vacuum ultraviolet light

Y.J. Kim, H. Sugimura, K. Murase, *Y. Taniguchi, *Y. Taguchi

*Kyoto University *Alps Electric*

In recent years, cyclo-olefin polymer (COP) resins have been used in a variety of applications owing to their excellent properties and low cost, and the market for cop resins is growing every year. For improving adhesivity, dyeability, and wettability, extensive researches in order to develop practical and economical surface modification methods of COP have been carried out by many groups. In this study, the surface of COP was treated with vacuum ultraviolet (VUV) light at 172 nm in wavelength to improve the wettability and adhesion properties. We report how different the chemical nature of COP surfaces irradiated with the VUV light is, dependent on the VUV-irradiation atmosphere. The extent of oxygenation was evaluated by XPS and FTIR-ATR spectra, and it was shown that the surface properties, hydrophilicity, and functionalization were crucially dependent on the VUV irradiation atmosphere. Roles of oxygen, nitrogen and water molecules in the VUV-irradiation environment have been elucidated.

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Investigation of various Polysulfone Polymer Electrolyte Membranes (PEM) for Direct Methanol Fuel Cells(DMFC)

길승철, 이원목

세종대 화학과

DMFC 는 메탄올을 직접 연료로 사용하여 장치가 간단하며, 연료 저장의 효율성 등으로 이동용 공급 전원으로서 큰 관심을 받고 있다. Polysulfone 은 높은 유리전이 온도를 가지고 있으며, 열적, 기계적 안정성이 우수하므로 Nafion 대체 PEM 으로 가능성이 높다. 본 연구에서는 Polysulfone 을 DMFC PEM 에 적용하기 위해 단량체(Dichlorodiphenylsulfone)를 설폰화 시킨 후, Bisphenol A 와의 축합중합반응을 통해 합성한 후, 만들어진 Polysufone 에 반응성 말단기를 도입, In-situ crosslinked membrane 을 제조하였으며, 또한 고분산성 무기 Nano particle 을 이용한 composite membrane 들을 제작 하여 그 물성을 측정하였다.

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Importance of unbound ligand elimination in the physicochemical property and cytotoxicity assay of surface conjugated nanoparticles

박경미, 문대원, 송남웅

한국표준과학연구원 나노바이오융합연구단

The effects on biological systems with exposure to nanoparticles (NPs) are important to be understood since they are closely related with the environment, health and safety (EHS) issues of the nanotech industrial products which have been recently expanded in high growth rate. The interaction behaviors of NPs with living bodies are governed by the characteristics of NPs, e.g. size, shape, composition, surface charge, and hydrophobicity/hydrophilicity. As a part of studies on the property specific NP interaction with biological systems, we have investigated the physicochemical properties and cytotoxicities of Au NPs having the same core but different surface ligands. Au NPs conjugated with four different types of molecules, which were citrate, O-[2-(3-Mercaptopropionylamino)ethyl]-O'-methyl-PEG (HS-$CH_2C(O)NH$-PEG-OMe) and mercaptoundecane triethyleneglycolcarboxylic acid (HS-(CH_2)11-EG_3-OCH_2-COO^-) or mercaptoundecane triethyleneglycolamine (HS-$(CH_2)_{11}$-EG_3-$N(CH_3)^{3+}$), were prepared respectively to provide Au NPs having the same properties except the surface characteristics. Au NPs were synthesized from the reduction of Au cations. Then the surface ligand was exchanged and the excess unbound molecules were removed by using dialysis or centrifuge method. Although the dialysis method is frequently used for purification of large compounds in solution, unbound ligand molecules used in this study could not be fully removed. The existence of unbound ligand molecules highly deteriorated the results of characteristic analysis of Au NPs. The observed physicochemical properties in physiological condition and cytotoxicity of Au NPs in the existence or absence of unbound molecules will be presented and the importance of free ligand removal will be discussed.

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Synthesis of Aligned Few-walled Carbon Nanotubes on Conductive Substrates

김병우

고려대 신소재공학부

We report a robust synthesis of densely aligned few-walled carbon nanotubes (CNTs) on conductive substrates that are industrially useful, such as carbon fibers and carbon papers, employing water-assisted chemical vapor deposition (CVD). The CNTs were tightly bound and electrically connected to the substrates, as confirmed by ultrasonication and cyclic voltammetry (CV), respectively. High quality CNTs synthesized on conductive substrates may find applications in fuel cells, lithium-ion batteries, and field emitters.

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Electrodeposition and characterization of CuSe thin films

손영석, *김참, *김종태, *한윤수, 윤태관, 배재영

*계명대 화학과 *대구경북과학기술연구원 나노바이오연구부*

The CuSe thin films have been deposited on FTO glass by the electrochemical deposition method. The deposition parameters, such as deposition potential, deposition time, bath temperature and annealing temperature were optimized. The structure, morphology, absorbance and composition of the films were analysed by using X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-vis differential reflectance spectra (UVDRS) and electron probe micro analysis (EPMA). Increasing the bath temperature was improved the crystallinity of CuSe compound.

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The powders of spinel-type alumiates at low temperature by the combustion technique

하태양, 김성진, *정진안, **김유영

*전주대 나노신소재공학과 *전주대 화학과 **전주대 화학신소재학과*

The powders of spinel-type MAl_2O_4 (M^{2+} = Mg, Co, Ni) were synthesized at 210 oC applying the (metal nitrate – malonic acid –ammonium hydroxide – ammonium nitrate) system. The optimum conditions to prepare the powders were determined: the amount of concentrated ammonia water and the initial decomposition temperature. The MAl_2O_4precursors were prepared evaporating the initial solutions in the electrical furnace fixed at 80 oC under the 25 torr vacuum. The initial solution was one to dissolve all of the starting materials. When the prepared precursor was decomposed at 210 oC, the powder to include the maximum contents of MAl_2O_4 crystallites was prepared. The chemical compositions of the precursor were as followed. The molar ratios of M^{2+} ion, malonic acid, ammonia and ammonia nitrate to the Al^{3+} ion were 0.5, 1.40, 2.56 and 2.00, respectively. 0.2 mole of the Al^{3+} ion was used. The characteristics of the powders obtained were examined by X-ray diffraction, optical microscopy, Fourier transformation infrared spectroscopy and Brunauer-Emmett-Teller technique.

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Preparation of Antimony doped $SnO_2$and its heterojunction with TiO_2 for the formation of visible light photocatalyst.

Sher Bahadur Rawal, 김용주, **ashok chakraborty**, 이완인

인하대 화학과

Antimony-doped tin oxide ($Sb_xSn_{1-x}O_2$,x=0.1) was prepared by coprecipitation of $SnCl_4.5H_2O$ & $SbCl_3$ with post annealing & characterized by XRD, TEM, SEM & EDX. $Sb_xSn_{1-x}O_2/TiO_2$, a heterojunction structure between antimony doped tin oxide (ATO) and TiO_2, was prepared by covering the surface of the 50-100 nm-sized ATO particles with ~7nm sized TiO_2 by sol-gel method. Under visible light irradiation ($\lambda \geq 420$ nm), $Sb_xSn_{1-x}O_2/TiO_2$ showed a notably high photocatalytic activity in removal of gaseous 2-propanol and evolution of CO_2. It was found that ATO($Sb_xSn_{1-x}O_2$) shows a profound absorption over the visible range in comparison to pure SnO_2 and its valence band (VB) is located lower than that of TiO_2. The high photocatalytic efficiency of the $Sb_xSn_{1-x}O_2/TiO_2$ under visible light irradiation was therefore deduced to be caused by the hole transfer between the VB of $Sb_xSn_{1-x}O_2$ and TiO_2.

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Synthesis and silica coating of Cu_2S nanoparticles

양희승, 유리, 김유진

한국세라믹기술원 에너지반도체센터

The Cu_2S nano-particles have attracted widely at attention because Cu_2S is known to be a photovoltaic materials in a hetero-structure of Cu_2S/CdS. In order to use the Cu_2S nanoparticles into applications, the Cu_2S must possess thermal and chemical stability at high temperature. Heating Cu_2S in air will ultimately produce Cu_xO beyond a critical temperature. In this work, we proposed core-shell type multi-layer system with silica for high thermal stability. Firstly, the Cu_2S particles can be synthesized with various shapes such as dots, rods and wires. The various type Cu_2S nanoparticles were coated with silica using Tetraethylorthosilicate (TEOS) in basic solution. The prepared silica coated nanoparticles were characterized by X-ray powder diffraction (XRD), transmission electron microscopy (TEM) and thermo gravimetric analysis (TGA). In addition, thermal stability of silica coated nanoparticles was studied by high temperature x-ray diffraction.

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Study on Single-Walled Carbon Nanotube-Based Ink and its Application for Flexible Thin Film Transistor Materials

최석주, *정수경, *이연주, **K. E. Geckeler

*광주과학기술원 나노바이오재료전자공학과 *광주과학기술원 신소재공학과*
***광주과학기술원 신소재공학과, 나노바이오재료전자공학과*

Research on carbon nanotube-based thin films has been of remarkable interest to understand their fundamental properties and potential applications in the fabrication of electronic devices, e.g., for flexible displays with plastic substrates based on low temperature processes. In this study, a novel ink formulation based on carbon nanotubes and a conducting polymer was designed and prepared in order to apply the ink-jet printing process for the fabrication of flexible thin-film transistors with the achievement of optimum performance and reliability of the printing system. The novel ink was characterized by UV-vis spectroscopy, SEM, TEM as well as viscosity and surface tension measurements. The UV-vis spectroscopic characterization showed that the carbon nanotubes were well dispersed in the ink.and it also fulfilled the essential requirements for the processing during ink-jet printing.

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A Simple Method for the Synthesis and Shape Manipulation of Gold Nanostructures

Thathan Premkumar, K. E. Geckeler

광주과학기술원 신소재공학과, 나노바이오재료전자공학과

An easy and inexpensive shape-selective synthesis method of gold nanoparticles through the reaction of an aqueous solution of a gold salt, the potassium tetrachloroaurate(III), with a detergent at room temperature was developed. We demonstrate that, by altering the reaction conditions such as concentration of the reactants and temperature, the shape of the gold nanostructures can be manipulated. The approach introduced here does not require any harsh and/or toxic reducing agents and also no manipulative skills. The as-prepared gold nanoparticles were characterized by UV-vis-NIR absorption spectroscopy, transmission electron microscopy, and atomic force microscopy. This method is facile and employs gentle reaction conditions in contrast to the conventional techniques reported using polymers, other reactants, and/or harsh reductants.

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UV-curable silver inks and paste for electronic devices

조성연, 김정수, 양해정, *구상만

*한양대 화학공학과 *한양대 화학공학*

UV-curable Ag inks and pastes have been investigated intensively because they can be widely applied in bus/address electrode patterns for plasma displays (PDP) and polymer thin film transistor (TFT), circuit patterns for 3-D micro electromechanical systems (MEMS) and radio frequency identification (RFID), and grid patterns for photovoltaic cells. In this study, we prepared Ag complex ink (Ag-CI), Ag particle ink (Ag-PI), and their pastes from Ag-neodecanoate (Ag-ND). Ag-film for conductivity measurement was fabricated by spin coating method using Ag inks on polyimide substrate. The patterns using Ag-ND paste were obtained on a glass substrate by the screen printing method. The properties of Ag films were characterized by SEM, XRD, and 4-point probe analysis. SEM images of cured films indicated that Ag-CI and Ag-PI on polyimide film got agglomerated and grain growth to larger silver particles after UV-irradiation. XRD pattern of cured Ag-CI film showed diffraction peaks at 2Θ of 38, 44, 64, 77° indicating the face-centered cubic (FCC) structure (JCPDS 04-0783) of typical silver. The increase in irradiation time and the decrease in irradiation height made the peak of XRD patterns sharper showing better crystalinity of silver nanoparticles formed. After UV-irradiation at 10cm of height, sheet resistances of Ag films using Ag-CI, -PI, and pattern with Ag-paste were 0.094 Ω/□, 0.358 Ω/□ and 371 mΩ/□, respectively. In conclusion, UV-curable Ag inks and pastes developed in this study would be a good alternative for electronic devices with the low sintering temperature and can be widely used to flexible display technology.

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Synthesis of various metal nanoparticle using MWCNT-Polyaniline

박창현, 김영준, *송재희

*충남대 화학과 *순천대 화학과*

MWCNT-Polyaniline-emeraldine salt(ES) and MWCNT-Polyaniline-emeraldine base(EB) were synthesized through the polymerization of surface modified MWCNT and aniline monomer. Gold and palladium nanoparticles were produced by MWCNT-PANI-EB as a reducing agent. As a result, several types of MWCNT-PANI-metal nanoparticle composites were generated, and have been characterized by UV-Visible and FE-TEM.

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A New Platform for DNA Delivery based on Gold Nanoparticles

유수윤, 장홍제, 김영관, 민달희

KAIST 화학과

Gold nanoparticles are inorganic nanoparticles which possess characteristic electrical, optical, and thermal properties. Gold nanoparticles have great potentials for cellular delivery in therapeutic applications as well as biosensor, and in vivo imaging. Gene therapy based on oligonucleotides (DNAzyme, siRNA, and DNA etc.) has faced the challenge in achieving the successful delivery system which can be one of powerful strategy to treat various diseases. Gold nanoparticles are tunable materials showing the shape- and size- dependent properties and these structurally fabricated nanostructures can further improve their unique properties.In this report, a class of gold nanoparticles were synthesized and used as novel carriers for mammalian cell transfection and the cytotoxicity of these particles was tested. We believe that the geometry and biocompatibility of the gold nanoparticles make this nanomaterial suitable for DNA/RNA transfection carrier.

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A Reverse Gene Transfection Cell Chip based on Gold Nanorods

장홍제, 유수윤, 김영관, 민달희

KAIST 화학과

Recently, the fabrication of gene transfection arrays for cell-based high throughput screening is one of the important goals in biotechnology from the viewpoints of both basic science and medical research. However, the practical application of the conventional reverse transfection arrays based on cationic polymer and lipoplex is limited due to relatively low transfection efficiency and toxicity of the polymers and lipids. To solve this problem, there were several approaches based on microspike structured substrate and electroporation mediated transfection. These approaches still carry biocompatibility and cellular toxicity issues. In this study, we employed gold nanorod as a transfection mediator because a gold nanorod efficiently converts light energy to heat energy. This local hyperthermia generated by gold nanorods could transiently and locally make cell membranes more susceptible for cellular uptake of extracellular materials presumably due to membrane perforation, which in turn can improve transfection efficiency. At the same time, this platform enables spatio-temporal control over gene transfection on a cell chip using an external stimulus, which is light.For fabrication of gene transfection arrays, gold nanorods were immobilized on the SiO2/Si substrate functionalized with thiol terminated silanes. Then, plasmid DNAs were adsorbed on the immobilized gold nanorods. HeLa cells were plated on the fabricated transfection chip and the chip was exposed to near IR light corresponding to longitudinal Plasmon band of gold nanorods for controlled and efficient transfection of loaded gene into adhered cells. To the best of our knowledge, this gold nanorod based reverse transfection chip is the first example of controlled and efficient reverse transfection chip. We believe this novel approach could be a useful tool for researches in cell biology and medicine.

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Hybrid Thin Films Composed of Reduced Graphene Oxide and Other Nanomaterials

김영관, 장홍제, *나희경, 민달희

*KAIST 화학과 *한국화학연구원 의약화학연구센터*

Graphene is recently considered as a promising candidate for fabrication of electronic devices and biosensors. Therefore, many approaches have been tried to synthesize highly crystallized graphene by peeling off, epitaxial growth and chemical vapor deposition method. However, these methods are not scalable. For mass production, chemical oxidation and reduction of graphite is a scalable and cost effective method. Nevertheless, this method still requires cumbersome post transfer process and showed relatively poor conductivity for fabrication of thin films. In this work, we describe a novel self-assembly of aminated multi-walled carbon nanotube and direct growth of gold nanostructure on reduced graphene oxide (RGO) surface for the construction of hybrid thin films as a transparent electrode and enhanced Raman scattering platform. To the best of our knowledge, this work is the first example of construction of large area and highly transparent hybrid thin films consisted of RGO and aminated MWNT or gold nanomaterials on transparent substrates. We believe this self-assembly and direct growth approaches will be a convenient tool to fabricate hybrid thin films composed of RGO and other important nanomaterials for various applications.

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Nano-propping effect of residual silicas on reversible lithium storage over highly ordered mesoporous SnO_2 materials

손정국, 황성희, 문기영, 김명실, *이윤연, 김지만

*성균관대 화학과 *성균관대 나노과학기술협동학부*

Highly ordered mesoporous SnO_2 materials with residual silica species were successfully synthesized from a mesoporous silica template (SBA-15) via nano-replication and simple etching processes. A tin precursor, $SnCl_2$•$2H_2O$, was infiltrated spontaneously within the mesopores of the silica templates by melting the precursor at 353 K without using a solvent. After the heat-treatment of composite materials at 973 K under static air conditions, the controlled removal of silica templates using NaOH or HF solutions with different concentrations results in the successful preparation of mesoporous SnO_2 materials, where the amounts of residual silica species are in the range 0.9–17.4 wt%. The residual silica species induce a nano-propping effect enabling the mesoporous SnO_2 material (containing 6.0 wt% of silica species) to remain stable up to 973 K without any significant structural collapse. More importantly, the optimum amount of residual silica species (3.9–6.0 wt%) results in a dramatic reduction in capacity fading after prolonged charging–discharging cycles in Li-ion battery. The mesoporous SnO_2 material with 3.9 wt% of silica species still exhibits a large capacity (about 600 mAh g^{-1}) after the 30th cycle, which is probably because the residual silica species act as a physical barrier to suppress the aggregation of Sn clusters formed in the mesoporous SnO_2 materials during the reversible lithium storage.

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The preparation of S-doped TiO_2 nanotube arrays for photolysis of water under UV and visible light

신연미, 이성훈

서울대 화학부

Self-organized hole-array materials formed by electrochemical anodization of various valve metals have been a great deal of interest due to unique geometrical structures, facile fabrication process, economic feasibility, and a wide range of applications in the field of nanoscience. Among them, titanium oxide (TiO_2) nanotube arrays are used as a photoanode in the photolysis of water, due to the excellent properties such as high aspect ratio, the proper band gap position, and photo-stability. However, the limitation in the application of TiO_2 nanotube arrays as a photoanode in the split of water is the large band gap. That is, TiO_2 is only photoresponsive to a UV region. To expand photocatalytic activity to visible light, doping of transition metal ions or C, N, B, S into TiO_2 is necessary.Here, we report sulfur-doped TiO_2 nanotube arrays using self-organized regular TiO_2 nanotube arrays formed through a two-step anodizing process with an electropolished Ti. The incorporation of S ions into TiO_2 was confirmed by X-ray photoelectron spectroscopy (XPS). The S-doped TiO_2 nanotube arrays showed higher photocurrent density than undoped TiO_2 nanotube arrays under a simulated AM 1.5 illumination.

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Synthesis of Ordered Mesoporous Carbon Materials for Very Stable Pt Nano-particle

김진회, 윤정아, 박은주, 김지만

성균관대 화학과

Polymer electrolyte membrane fuel cell (PEMFC) and direct methanol fuel cell (DMFC) are considered as next-generation power sources of vehicles, small power plants and portable electronic devices due to their many advantages including high energy density, green emissions and ambient operating conditions. However, there are many problems remained for commercialization of PEMFC and DMFC system. Especially, the main problem is low electro-catalytic of the cathode reaction. The kinetics and efficiency of the reaction is strongly depended on catalyst size and dispersion property. And sintering of Pt nano-particles also occurred in fuel cell operation condition.In the present studies, new types of nanoporous carbon materials such as activated carbon, carbon nanotube (CNT) and graphitic porous carbon are used as catalyst support materials for fuel cell catalyst to enhance the electro-catalytic activity and fuel cell efficiency. Especially, ordered mesoporous carbon (OMC) is prominent support material due to the high surface area, large regular mesopores and easy control of morphology. However, to further improve the OMC as a carbon support, the control of properties such as conductivity, pore size and surface structure is still challenging. In this study, we discuss about the synthesis of surface modified nanoporous carbon material and their properties on the catalyst stability for enhanced performance of DMFC cathode reaction.

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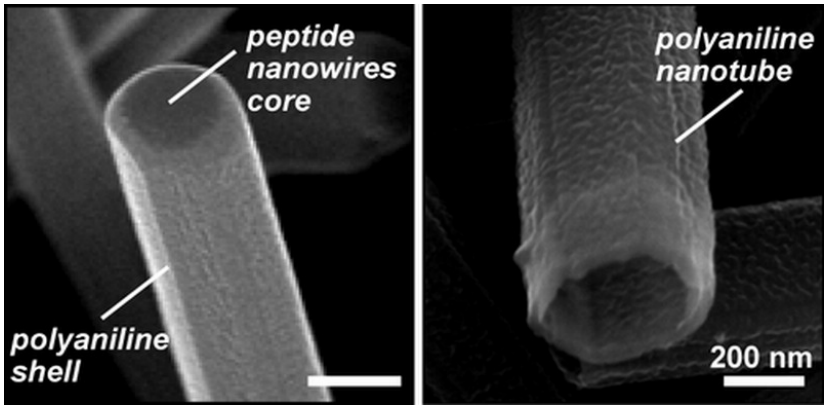
Fabrication of one-dimensional polyaniline nanostructures by peptide self-assembly

유정기, 박찬범

KAIST 신소재공학과

We report the fabrication of one-dimensional nanostructures of conjugated polymers such as polyaniline (PANI) nanowires and nanotubes, which find their applications in gas-sensing and electronics, by using peptide-self assembled nanowires (PNWs) as a template. Peptide-based self-assembled nanomaterials have drawn much attention because of their molecular recognition capability and functional flexibility. Here we used diphenylalanine (Phe-Phe or FF) as a building block, which is one of best-known self-assembling short peptides, for the growth of PNWs. PNW template was prepared by high-temperature self-assembly of FF in the presence of aniline vapor. We found that PANI readily and uniformly coated PNWs, resulting in the formation of PNW/PANI core/shell nanowires. The formation of PANI shell on PNW was confirmed by multiple analytical tools such as electron microscopy, Fourier-transform infrared (FT-IR) spectroscopy, and cyclic voltammetry. Our results show that PANI grows preferentially along the side-wall of PNWs by specific interaction between PNWs and PANI during the polymerization process. The thickness of PANI coating on PNW could be controlled by varying the reaction time and the number of PANI coatings. On the basis of the results, we could also fabricate hollow PANI nanotubes by selectively removing PNW core from PNW/PANI nanowires. The present study demonstrates that self-assembled peptide nanostructures can be used as a versatile template for the synthesis of functional nanomaterials.



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Characterization of LiF-LiBr-KBr Eutectic as Molten Salt Electrolyte in Thermal Battery Applications

김병기, 박윤봉

충남대 화학과

Molten salt thermal batteries are activated by raising their temperature to above the melting point of the salt constituting the electrolyte. Lithium halide-based mixtures were mainly used as electrolytes for their low melting points, low vapor pressure and their relatively high ionic conductivities. However, LiF-LiBr-KBr eutectic (0.67/45.38/53.5 wt%) has even lower melting point at 324℃. The melting points of electrolytes are very important in determining the effective operating temperature window and operation time for their use of thermal battery applications. In this work we have prepared LiF-LiBr-KBr electrolyte and measured its performance in Li-Si/FeS_2 single cells. Even though LiF-LiBr-KBr eutectic is known to have relatively lower ionic conductivity than lithium halide-based mixtures, lower melting points provide longer battery operation time. In this paper discharging tests of the single cells with LiF-LiBr-KBr electrolyte will be given in detail and its performance will be compared with lithium halide-based mixtures.

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Bio-Inspired Fabrication of Superhydrophobic Surfaces through Peptide Self-Assembly

이준석, *유정기, *박찬범

*KAIST 신소재공학 *KAIST 신소재공학과*

A vertically aligned peptide nanowire film, prepared by the self-assembly of diphenylalanine upon exposure to fluorinated aniline vapor at high temperature, exhibits a superhydrophobic property due to its nanoscale roughness and low surface free energy. We fabricated a self-cleaning, superhydrophobic surface by hierarchically re-organizing peptide nanowires into a hill-and-valley-like structure using capillary force induced by solvent-evaporation. Our approach provides an alternative way of nanofabrication for superhydrophobic materials, which should broaden the spectrum of applications for peptide self-assembly.

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Debundling and individual dispersion of single-walled carbon nanotubes using a neutral pH water soluble chitosan derivative

Najeeb.C.K, 이재혁, 남광현, 창징보, 김재호

아주대 분자과학기술학과

Individual carbon nanotubes dispersed in a biocompatible media are of particular interest for many biomedical and nanomedicine applications. Various biomolecules and biopolymers such as DNA, proteins, poly L–lysine, starch, gelatin, steroid biosurfactants, and chitosan have shown capability for the effective dispersion of carbon nanotubes in water. Chitosan has demonstrated capacity for effective dispersion of single-walled carbon nanotubes (SWNTs) in acidic medium and it also showed tendency to preferentially disperse smaller diameter nanotubes. Herein, we present individual suspension of SWNTs using a chitosan derivative, N-acetylated chitosan, which is soluble in neutral pH water as dispersant obtained by functionalizing the amino groups of chitosan with acetic anhydride. The N-acetylated chitosan demonstrated very good dispersibility and exfoliation of nanotubes, and the characterizations of CNT dispersion by SEM, TEM and AFM imaging revealed that the diameter of nanotubes were in the range of 1.2 to 2.8 nm size.

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Transparent Thin Films of Red Emitting CdSe/ZnS Core/Shell Quantum Dots

오지혜, 김형근, *도영락

*국민대 화학과 *국민대 생명나노화학과*

We studied red emitting CdSe/ZnS Core/Shell quantum dots (QDs), which were synthesized through a colloidal chemical synthesis and a surface-passivation method overcoating on the core CdSe with a wide bandgap material, ZnS. Transparent thin films of red emitting QDs were spin-coated onto glass substrate using an organic polymer matrix-QDs solution. Scanning Electron Microscopy (SEM), UV-Visible spectroscopy and Photoluminescence (PL) were used to characterize the thickness and optical properties of the transparent thin films of red emitting QDs.

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장소: 대전컨벤션센터
발표코드: **Ⅱ39P272포**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 목 16:30~18:30

Optical properties of $Sr_xBa_xSi_xO_x$: Eu^{2+} Thin Film Phosphors fabricated by electron beam evaporation

문정호, *오지혜

*국민대 화학과 *국민대 생명나노화학과*

This study investigates yellow emitting Eu^{2+} doped $Sr_xBa_xSi_xO_x$ Thin Film Phosphors(TFPs). $Sr_xBa_xSi_xO_x$: Eu^{2+} TFPs studied for color-tunable white-light emitting diode. $Sr_xBa_xSi_xO_x$: Eu^{2+} TFPs deposited on Si 2x2cm^2 substrates by E-beam evaporator. The electron beam evaporation was carried out under the following conditions: a base pressure of 1.3 x 10^{-6} torr, a working pressure of 1.7 x 10^{-6} torr, substrate temperature of 200℃, rotation speed of 30rpm, deposition rate of 10 ㎚/sec. Then, the $Sr_xBa_xSi_xO_x$2+ TFPs deposited substrates were sintered at different temperatures in a range of 800 and 1200℃ for 2 hours in a 25%H_2+75%N_2 reduction atmosphere. They were characterized by means of Photoluminescence (PL), X-ray Diffraction (XRD) and Atomic force microscopy (AFM).

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The effects of the enhanced photoluminescence efficiency of sol-gel derived $Y_2O_3:Eu^{3+}$ thick film phosphors

오정록, *박재형, *박후근, *도영락

*국민대 화학과 *국민대 생명나노화학과*

We have investigated the effects of the enhanced photoluminescence efficiency of film phosphors(FPs). There are three main factors affecting the external PL brightness of a $Y_2O_3:Eu^{3+}$ film phosphor, the optimized internal efficiency, increased photon-solid interaction volume and enhanced extraction efficiency factors. The overall aim was to improve the PL brightness of FPs over commercial and sol-gel synthesized screened-powder phosphors. We have fabricated very bright film phosphor over screened powder phosphor (130%) by Pechini sol-gel method.

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Efficiency enhancement and color tuning of deep-blue microcavity OLEDs using dielectric Bragg mirrors

김형근, *도영락

*국민대 화학과 *국민대 생명나노화학과*

We fabricated deep-blue microcavity organic light emitting diodes (OLEDs) with SiO_2/TiO_2 stacks as dielectric Bragg mirrors. We used Bragg mirrors of different center wavelengths. The structure of the OLEDs was glass substrate/Bragg mirrors/ITO/2TNATA/NPB/TAT/Alq3/LiF/Al. In that case, cavity-length is from Bragg mirrors to LiF layer. The TAT [9,10-bis(3',5'-diphenylphenyl)-10-(3''',5'''-diphenylbiphenyl-4''-yl)anthracene] was used as blue emission materials. Colors of microcavity OLEDs were easily tuned by changing thickness of organic layers and center wavelengths of Bragg mirrors. Efficiency of OLEDs was enhanced by Bragg mirrors.

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Optical properties of flux contained Y_2O_3:Er thin-film phosphor on sapphire

박재형, 도영락

국민대 생명나노화학과

Flux($LiCO_3$) contained Y_2O_3:Er thin-film phosphors have been grown on a sapphire substrate using a Pechini-type Sol-gel process by employing Yttrium nitrate, Erbium nitrate, and citric acid as precursor materials. Y_2O_3:Er thin-films were annealed at various temperatures between 1000~1400℃ for two hours in an air atmosphere after deposition. To enhance optical properties of Y_2O_3:Er thin-film phosphors, we studied various preparation conditions, such as annealing temperature and flux concentration. The optical properties of flux contained Y_2O_3:Er thin-film phosphors were discussed and characterized by scanning electron microscopy(SEM), X-ray diffraction(XRD), atomic force microscopy(AFM), and photoluminescence(PL).

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Enhancement of sensitivity of ZnO UV Sensor by single-walled carbon nanotubes

창징보, 이재혁, Najeeb.C.K, 남광현, 김재호

아주대 분자과학기술학과

Heterojunctions with various compositions and interfaces create built-in electric fields that deplete or accumulate electrons and holes within the nanostructure, which have already demonstrated distinctive performances in nanodevice applications for optoelectronic technologies like light-emitting diodes, photovoltaics, and optical sensors. [1,2]. There has been great interest in UV sensor based on Single walled carbon nanotube (SWNT)-zinc oxide (ZnO) heterojunctions because SWNTs can enhance UV photoresponse owning to high electron mobility. The SWNT-ZnO heterojunction film was fabricated by two step processes: first, a SWNT Langmuir-Blodgett (LB) film was deposited on an anodic aluminum oxide (AAO) template; and then, ZnO film was made by vacuum filtration of ZnO nanowire solution. The UV sensor based on combination of SWNT-ZnO demonstrated fast photoresponse. We also observed highly efficient photovoltaic effects in the SWNT-ZnO junctions when the device was illuminated by UV radiation. Furthermore, the mechanism of UV sensitivity enhancement and photovoltaic effects was assumed to result from the high electron mobility in the SWNT-ZnO heterojunctions.

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Novel Metal Catalysts Supported on Magnetic Silica Spheres

강동현, 이윤지, 김서영, 엄민식, 정미선, 이규련, 이종인, 허남회

서강대 화학과

We report the synthesis of novel metal (M) catalysts supported on highly uniform superparamagnetic mesoporous silica spheres (SMSs), M-CoFe2O4@SiO2, with submicron scale that are composed of core/shell type silicas and spinel CoFe2O4 ferrites and describe their catalytic activities. The metal nanoparticles (NPs) were immobilized on the oxide surface using a bi-functional linker molecule. The resulting supported catalysts were completely characterized by a combination of techniques such as XRD, ICP-MS, SEM, and TEM. High resolution SEM images of the M-CoFe2O4@SiO2 SMS show that the metal NPs are ranged from 3 to 7 nm, which are evenly distributed on the oxide surface and some of them are closely contacted with large CoFe2O4 NPs. We have conducted various hydrogenation reactions with the supported catalysts, showing very unusual products that have never been obtained from the same reactions with simple metal NPs. Moreover, they are very stable towards leaching of the metal surface and are easily recovered by a magnet, thus showing good potential as recyclable catalysts.

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Organic-inorganic Nano-hybrid Semiconducting thin films for Flexible Electronic Devices

조상호, 김수환, 성명모

한양대 화학과

We report a high-performance and air-stable flexible semiconductor which can be substituted for n-type organic semiconductors. We combined crystalline inorganic nanolayers with organic layers, leading to organic-inorganic nanohybrid n-type semiconductors. The inorganic layer constitutes an extended framework bonded by powerful covalent or ionic interactions to furnish high carrier mobility and good thermal and mechanical stability. The organic layer adds mechanical flexibility to the inorganic framework. Molecular layer doposition combined with atomic layer deposition was applied to fabricate a new n-type organic–inorganic nanohybrid semiconductor on flexible plastic substrates with accurate control of film thickness, large-scale uniformity, excellent conformality, good reproducibility, multilayer processing capability, sharp interfaces, and excellent film qualities at low temperature. The prepared nanohybrid thin films exhibited good thermal and mechanical stability, good flexibility, and excellent field effect mobility (>7 cm^2/Vs) under low voltage operation (3 V). Furthermore, we also demonstrate the performance of p-n junction diodes prepared with the SAOLs-ZnO nanohybrid superlattice and pentacene.

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Performance Enhancement of Semiconducting Device by Engineering Layout of SWNT Langmuir-Blodgett Film

남광현, 이재혁, 창징보, Najeeb.C.K, 김재호

아주대 분자과학기술학과

Single-walled carbon nanotube (SWNT)-based devices with dominantly semiconducting property were achieved by engineering the layout of SWNT channel. Highly packed and unidirectionally aligned SWNT film was fabricated by Langmuir-Blodgett technique and used for engineering layouts with and without patterns by soft lithography. As comparing electrical conductivity properties, the patterned device showed superior semiconducting property due to limiting lateral crosstalk of electron transport between SWNTs. This method has potential for improving applicability of SWNT-based devices owing to control over metallic and semiconducting properties in devices.

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Carbazole-based Organogelator Featuring Gelation-Induced Enhanced Emission

김은하

서울대 공과대학 재료공학부

In recent years, functional organogels made from low-molecular-mass organic gelators (LMOGs) with π-conjugated molecular structures are attracting considerable interest due to their unique 1-D nano-/microstructures which promise for their optoelectronic applications such as field-effect transistors (FETs), light-emitting diodes (LEDs), lasers and sensors. In this work, we report a new carbazole-based organogelator incorporating π-conjugated aromatic units with multiple $-CF_3$ substituents. Attributed to the outstanding self-assembling tendency and high crystallinity of this organogelator, 1-D nanostructures were easily produced either by solvent-exchange, re-crystallization, or by slow evaporation of solvent. SEM and optical microscopic images of xerogel showed the formation of highly fluorescent fibrous network structures. Crystallographic analysis of the fine single crystal revealed that the antiparallel molecular stacking induced by asymmetric $-CF_3$ substituent resulted in the strong cofacial π-π stacking between carbazole units which are considered beneficial as an ideal system of the charge transport channel. Most uniquely, unlike most organic fluorescent materials, our novel organogelator is non-fluorescent in solution state but highly fluorescent in the gel or crystalline powder state, showing aggregation-induced enhanced emission (AIEE)[1-3]. Reference1.An, B. K.; Kwon, S. K.; Jung, S. D.; Park, S. Y. J. Am. Chem. Soc. 2002, 124, 144102.An, B. K.; Lee, D. S.; Lee, J. S.; Park, Y. S.; Song, H. S.; Park, S. Y. J. Am. Chem. Soc. 2004, 126, 102323.An, B. K.; Gihm, S. H.; Chung, J. W.; Park, C. R.; Kwon, S. K.; Park, S. Y. J. Am. Chem. Soc. 2009, 131, 3950

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Influence and characterization of carbon coating on TiO_2 surface as working electrode for dye sensitized solar cell

박유림, 류광선

울산대 화학과

Despite the initial success of the 11.1% solar conversion efficiency in dye sensitized solar cell (DSSC), the efforts to further improve their performance have yielded little progress. TiO_2 was the most widely used photocatalyst because of its good activity, chemical stability, commercial availability, and inexpensiveness. However, only a small UV fraction of solar light (3–5%) could be utilized because of the wide band gap of TiO_2. Therefore, it was urgent to develop a particular photocatalyst sensitive to sunlight. We studied the influence and characteristics of carbon coating on TiO_2 surface as working electrode for DSSC. Characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Brunauer-Emmet-Teller(BET) measurements, as well as the photovoltaic performance of the incident photon-to-current conversion efficiency (IPCE) as a function of wavelength was measured.

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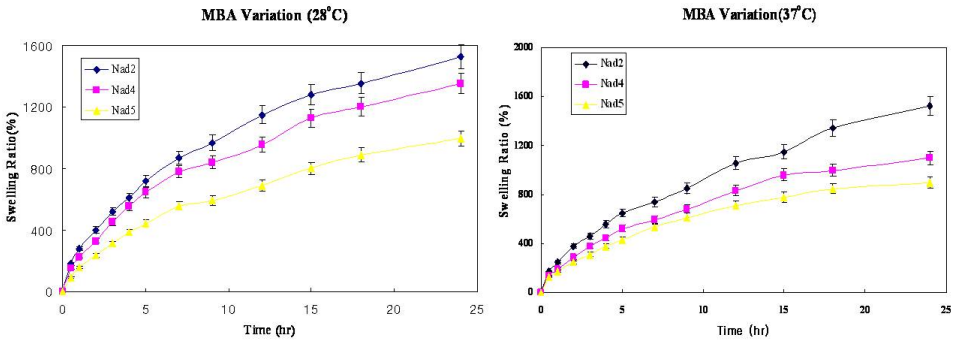
Synthesis of Ketorolac Tromethamine Loaded-Poly(*N'*-Isopropylacrylamide-*co*-Acryloyl Phenylalanine) Hydrogels and Its *In Vitro* Release Studies

김용현, Vadde Ramesh Babu, 이용일

창원대 화학과

Thermosensitive hydrogels composed with acryloyl phenylalanine (APA) and *N'*-isopropylacrylamide (NIPA) and crosslinked by *N,N*-methylene bisacrylamide (MBA) are synthesized using free radical polymerization. Ketorolac tromethamine (KT), an anti-inflammatory and analgesic agent, was successfully encapsulated into hydrogels. Various formulations were prepared by varying the amount of NIPAm and APA, MBA and amount of drug. The KT loaded gels were characterized by X- ray diffraction (x-RD) and differential scanning calorimetric (DSC) studies were performed to understand the crystalline nature of the drug after encapsulation into hydrogels. Encapsulation efficiency was found to be in the range of 20 to 74 % measured using UV-vis method at 324 nm. The swelling studies were indicated a dependence of extent of crosslinking, monomer ratio and drug content in the hydrogels. The swelling studies are also carried at two different temperature i.e., below and above of the LCST (32 ^{0}C). These studies clearly confirm the dependence of temperature on swelling studies. Figure 1. % Swelling of hydrogels in buffer solution.



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Facile Synthesis of Mesoporous Aluminum Oxides Using an Aqueous $NaAlO_2$ Solution

나정현, 김정수, 김용현, *구상만

*한양대 화학공학과 *한양대 화학공학*

Aluminum hydroxides have been investigated for scientific and industrial application such as catalysts, sorbents, ceramics, and supporting materials. Various synthetic methods for mesoporous aluminum oxides have been reported in the literature including the template-based synthesis, emulsion process, and hydrothermal process. We have studied the preparation of mesoporous materials using a template-free solution route from a sodium aluminate ($NaAlO_2$) precursor. Aluminum oxides with various internal and external structures could be prepared by controlling reaction conditions such as reactant concentrations, reaction temperature/time, and dropping rate. First, amorphous spherical particles were prepared at 12℃ when the dropping rate was 0.57mL/sec. These amorphous particles could be converted to γ-Al_2O_3 spherical particles with the calcination at 900℃. The BET surface areas were 64 m^2g^{-1} for as-prepared particles and 96.6 m^2g^{-1} for calcined ones. Secondly, urchin-shaped AlOOH hollow particles were obtained when the reaction temperature was raised to 60℃. This materials could be transferred to γ-Al_2O_3 particles after the calcination at 700℃. The BET surface areas were found to be 192 m^2g^{-1} for as-prepared particles and 266 m^2g^{-1} for calcined ones. The pore size was 6.2 nm for as-prepared, 3.7 nm and 7.6 nm for calcined particles.

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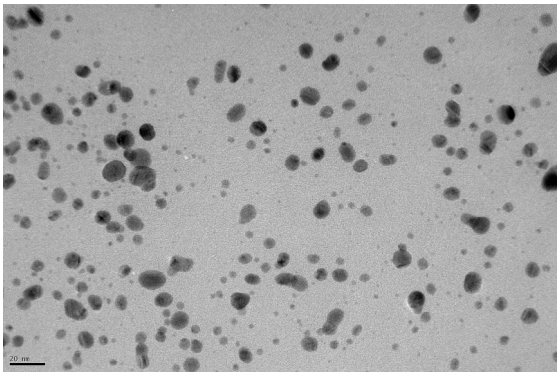
Synthesis of Novel Poly(Acrylamide-*co*-Acryloyl Phenylalanine) P(AAm-*co*-APA)-Silver Nanocomposite Hydrogels and Anti Bacterial Studies

차형래, Vadde Ramesh Babu, 김태영, 이용일

창원대 화학과

AAm and APA monomers with different molar ratios and certain amount of crosslinker, MBA were dissolved in distilled water at room temperature (APA dissolved in equimolar ratios of NaOH). Then the initiator KPS were added to allow the copolymerization for 4 h at room temperature. Thereafter, the hydrogel prepared was taken out and immersed in distilled water for 3 days at room temperature. During this period, the distilled water was refreshed every several hours in order to leach out the residue. The hydrogel was evaluated for its swelling studies. The hydrogels were characterized by UV-Visible spectroscopy (UV-Vis), X-ray diffraction (XRD), scanning electron microscope (SEM), thermal gravimetrical analysis (TGA) and transmission electron microscopy (TEM). Scanning electron microscopy studies confirms the formation of agglomerated silver nanoparticles. Thermal analysis clearly suggested the wide difference between pristine hydrogel and silver nanocomposite hydrogel. Narrow distribution of silver nanoparticles in hydrogel has been conformed by TEM analysis. Figure. TEM image of silver nanoparticles



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CdSe–Polypyrrole Composite Nanorods: Synthesis, Characterization

강원석, 남광현, 이종화, 김재호

아주대 분자과학기술학과

Inorganic semiconductor materials of nano-dimension have drawn much attention in recent years because of their size-tunable optoelectronic properties arising from the quantum confinement effect. These materials, however, cannot be applied alone under most circumstances and need to be incorporated with other materials, often polymers, to acquire necessary processability and protection. Embedding of inorganic semiconductor materials inside conducting polymers has become one of the popular methods for formulation of nanocomposites because they often exhibit improved chemical, physical and electrical properties, and hence can be used in a broader range of applications such as nonvolatile electronic memory, independently addressable remotely triggerable switches and gates , spinnable bioactive coatings, and sensing devices. This paper describes the template assisted synthesis of new variations of CdSe-Polypyrrole composite nanorods. To fabricate CdSe-Polypyrrole composite nanorods, 5 nm CdSe particles were dispersed in monomeric pyrrole solution and ECD was performed. By adjusting the time, rate of electrode position and the concentration of CdSe particles, the dimension and composition of the composite nanorods were able to precisely control. The transmission electron microscopy and fluorescence microscopic measurements showed that CdSe particles were homogeneously dispersed in the composite nanorods with diameters and length of 200 ~ 320 nm and 15 μm respectively. The I-V measurement showed that CdSe-Polypyrrole composite nanorods are very resistive in the dark and showed pronounced photoconductivity even under low intensity visible light. This structure can be used in the applications of UV-visible sensors.

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Study on CMPO (carbamoylphosphate) Derivative Hybrid Ordered Mesoporous Silicates for Selective Removal of Fission Products

권법진, 박승일, 유국현, 정현

동국대 화학과

To remove fission product (FP) elements from high level liquid waste, carbamoylphosphate (CMPO) silane grafted mesoporous silicates were synthesized by simple hydrolysis and condensation reaction. The carbamoylphosphosphonate silane [CMPO analogue; 2-(diphenylphosphoryl)-N-(3-(triethoxysilyl)-propyl)acetamide] modified mesoporous silicates were prepared via a post-synthesis grafting method. The guest CMPO analogue was synthesized by direct coupling reaction of 2-(diphenylphosphoryl) acetic acid and 3-(triethoxysilyl)propan-1-amine. Various mesoporous silicates such as MCM-41, SBA-15, or amorphous silica nanoparticles were adopted as host materials. The resulting surface modified mesoporous materials were characterized with respect to their structural integrity, surface area, and pore size and the concentration of the CMPO silane species. The effects of type of host materials, pore size and surface area on the sorption of FP elements were investigated by using simulated HLW [Zr(Ⅳ), Mo(Ⅵ), Pd(Ⅱ), Cs(Ⅰ) and Sr(Ⅱ)]. To describe the sorption patterns, mathematical modeling was also discussed in detail.

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Synthesis of Highly Luminescent Green and Red III-V Quantum Dots

정주현, 이성훈

서울대 화학부

We present highly luminescent green and red InP@ZnSeS core@shell structured quantum dots(QDs). InP cores are coated with ZnSeS shells by a subsequent injection of Zn precursor (Zn-oleate) and then Se and S precursors (S and Se powder dissolved in tri-n-octylphosphine (TOP)) into the same solution. ZnSe has a suitable band gap (2.7 eV @RT, bulk) and a band position and relieve a lattice mismatch between InP (lattice constant 5.87 Å) and ZnS (5.42 Å) layers. Lattice constants of InP, ZnSe, and ZnS are 5.87, 5.67, and 5.42 Å, respectively. ZnSe and ZnS have 3% and 8% lattice mismatch relative to InP, respectively. QDs are characterized by UV-Vis. absorption spectroscopy, photoluminescence spectroscopy, and transmission electron microscopy. Through the moderate control of the reaction conditions (reaction temperature, concentration, and ratio of reaction precursors), we are able to produce highly luminescence InP@ZnSeS quantum dots.

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Solid-Phase Self-Assembly and Fibrillation of Prion Peptide

구숙희, 박찬범

KAIST 신소재공학과

The conformational change of cellular prion protein (PrP^{C}) to its infectious isoform (PrP^{Sc}) is a hallmark of prion diseases. We have developed a novel solid surface-based system for efficient prion fibrillation in vitro by immobilizing prion peptides onto a chemically activated solid surface. The self-assembly of prion peptides into fibrils was more highly accelerated on the solid surface than in solution after 72 h of incubation at 37 °C. According to our observation using ex situ atomic force microscopy, fibrils were over 200 nm long and 5-8 nm in diameter. Amyloid-like properties of fibrils self-assembled on the solid surface were confirmed by multiple analyses with circular dichroism and amyloid specific dyes such as Congo red and thioflavin T. The fibril formation of prion peptides was substantially affected by the incubation temperature, and preformed fibrils disassembled after additional heat treatment at 100 °C. The solid surface-based prion fibrillation system developed in the present work may become a useful tool for the in vitro study of prion aggregation. The adoption of this system will allow the efficient investigation of environmental factors and inhibitor screening.

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Pt_3Co Nanoparticles with Different Co and Pt Distributions by Polyol Processes with and without Sonication and Their Magnetic and Electrocatalytic Properties

이양희, 권영욱

성균관대 화학과

We report on the use of ultrasound irradiation during the polyol synthesis of Pt_3Co nanoparticles to induce a different elemental distribution within the nanoparticles from those starting from $Pt(acac)_2$ and $Co(acac)_2$ as the metal sources. We found that the sonication facilitates the conversion of $Co(acac)_2$ with a high vapor pressure to Co^0, which was not possible by the conventional polyol process without sonication. On the contrary, the sonication suppresses the conversion of $Pt(acac)_2$ with a low vapor pressure slightly. Therefore, the reaction with sonication produced Pt_3Co nanoparticles with Co-rich cores and Pt-rich shells whereas the reaction without sonication produces nanoparticles with Pt-cores and Co-rich shells. These different elemental distributions affect the magnetic properties and the electrochemical properties of Pt_3Co nanoparticles. Especially, the sonochemically synthesized Pt_3Co nanoparticles show 1.5 times enhanced oxygen reduction reaction than the other Pt_3Co nanoparticles.

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Synthesis and Crystal Structure of a New Pentanary Thiophosphate, $Li_2AlSr_2(PO_4)_3$

박소정, *곽현정, *김성철, *김승주, **윤호섭

*아주대 응용화학 *아주대 에너지시스템학부 **아주대 화학과*

A new highly promising cathode material for lithium-ion batteries, $Li_2AlSr_2(PO_4)_3$ is prepared and the crystal structure of the compound has been determined by single crystal X-ray techniques. This compound crystallize in the space group P21/n of the monoclinic system with four formula unite in a cell of dimensions, a=4.9446(2)Å, b=22.0876(7)Å, c=8.6318(3)Å, and β=91.466(1), V=942.52Å. The structure of the compound is comprised of Al-centered octahedra and P-centered tetrahedra. These polyhedra are sharing O atoms to form a layer perpendicular to the b-axis. Sr^{2+} and PO_4^{3-} ions reside between the layers to stabilize the structure through electrostatic interaction. A bond-valance calculation indicates that the classical charge valence of the compound should be described as $[Li^+]_2[Al^{3+}][Sr^{2+}]_2[PO_4^{3-}]_3$.

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Thermal stability study of Silica Coated Iron Oxide Nano Pigments

유리, 양희승, 김유진, *피재환

*한국세라믹기술원 에너지반도체센터 *요업기술원 이천분원 산업도자실*

The iron oxide have been investigated in past years due to their remarkable electron, magnetic, optics properties. The iron oxide is a promising materials as a pigment because iron oxides were non-toxic elements and easily controllable coloration depend on their shape and size. However, nano size pigment were easily aggregated and loss the coloration owing to growing nanosize to microsize. In the work, we study the silica effect on thermal stability of iron oxide nanoparticles. The silica coating α-Fe_2O_3 nano particles, displaying consistent properties up to a heating temperature of 1000℃ were synthesized, nearly no color change which indicates that the silica coating actually minimizes the aggregation and oxidation of the nano particles. Thermal stability effect of silica coating were characterized by high temperature x-ray diffraction (XRD) and CIE $L^*a^*b^*$ colorimeter.

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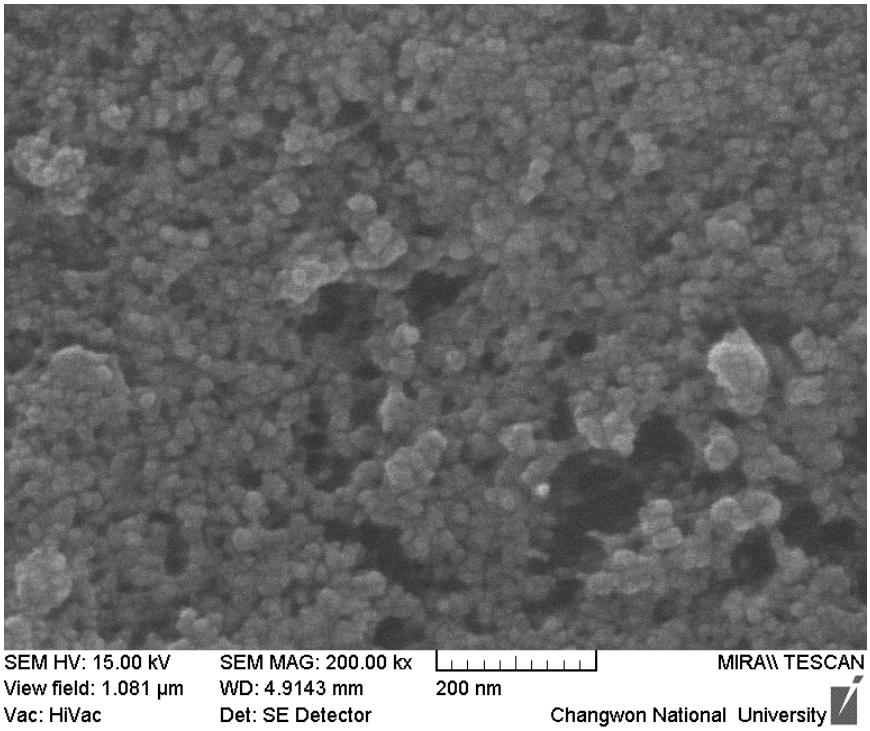
Fabrication of silver nanoparticles in semi-interpenetrating polymeric hydrogel and its facile studies on E. Coli

Vadde Ramesh Babu, 이용일

창원대 화학과

Semi-interpenetrating polymer network [semi-IPN] hydrogels composed with combination of carbohydrate polymers, chitosan, sodium alginate with 2-hydroxyethyl methacrylate. The semi-IPN hydrogels are successfully synthesised by free radical polymerization and loaded silver nitrate. Silver nanopaticles were formed by reduction of silver nitrate with sodium borohydrate under room temperature. The formed silver nanoparticles were well characterized using UV-visible spectroscopy, thermo gravimetrical analysis, x-ray diffractrometry studies, scanning electron microscopy and transmission electron microscopy studies. The silver nanoparticles are tested on E.coli bacteria for anti bacterial studies. Thermal and x-ray driffraction analysis conformed the formation of silver nanoparticles in semi-IPN hydrogel. SEM images clearly suggest the formation of group of silver nanoparticles with size range of 10-20 nm. The sizes of silver nanoparticles are confirmed by transmission electron microscopy results. The silver nanoparticles shown very good antibacterial activity on E.coli, thus it reveals that the silver nanoparticles are acting as good antibiotics. Fig.1. SEM image of silver nanoparticles in hydrogel



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Thermal variation of structure and energy band gap for hydrated antimony oxides

김성철, 김지혜, 김승주

아주대 에너지시스템학부

The hydrated antimony pentoxide nanoparticles were synthesized by oxidizing antimony trioxide in aqueous solution. After heat treatment at various temperatures, the change in composition and crystal structure of hydrated antimony oxides were monitored by means of powder X-ray diffraction and thermogravimetric method. All the analyzed compounds crystallize pyrochlore structure in the cubic symmetry with space group *Fd*-3*m* (no. 227). The room temperature phase is formulated as Sb_2O_5-$4H_2O$ in which H_3O^+ ions are fully occupied at *16d* site. The dehydration and reduction process successively proceed on heating the hydrated antimony oxide; Sb_2O_5-$4H_2O$ → Sb_2O_5-$2H_2O$ → $Sb_2O_{4.33}$ → Sb_2O_4. Cell parameter decreases as the temperature increase from 200℃ to 400℃: i.e. a = 10.35Å for 200℃, a = 10.10Å for 400℃. At high temperature above 400℃, it increases again to 10.30Å at 600℃. The energy band gap estimated from UV-Vis diffuse reflectance data decreases in the temperature range of 200℃ ~ 450℃ and increases again above 450℃.

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Photocatalytic and Electrochemical Properties of the SnO_2-Pillared Titanate Nanohybrids Depending on Their Porous Structure

고지은, *하형욱, *김인영, **황성주, 정현

*동국대 화학과 *이화여대 나노과학부 **이화여대 화학·나노과학과*

SnO_2 pillared titanate nanohybrids were synthesized by restacking reaction of exfoliated layered titanate sheets with the nanosized SnO_2 sol particles. The host two dimensional colloidal nano-sheets could be obtained by intercalating tetrabutylammonium cation into the layered protonic titanate by successive exfoliating process. The SnO_2 nanosol solution was prepared by simple sol-gel reaction of $SnCl_4 \cdot 5H_2O$. Nanohybrid materials were prepared by flocculation between negatively charged titanate nanosheets and positively charged SnO_2 nanosol particles. Finally, micro and mesoporous hybrid materials were obtained by thermal treatments at various temperatures. Depending on the temperature, the pore size of final products could be controlled from micropore to mesopore size range. The pillar and porous structure characterizations on final porous nanohybrid have been carried out, along with the test of their photocatalytic and electrochemical property.

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Synthesis and photoluminescence properties of Ga_2O_3 and doped Ga_2O_3 nanowires

김경래, 강위경

숭실대 화학과

Monoclinic gallium oxide (Ga_2O_3) is chemically and thermally stable compound with an optical band gap of 4.9eV. Ga_2O_3 one-dimensional (1D) nanostructure (nanowires, nanobelts and nanorods) are fabricated through thermal evaporation method. Ga_2O_3 nanowires are synthesized using milled gallium oxide powder and graphite powder at 1100℃ in Ar atmosphere on Au-coated silicon as the substrate. The shape of the 1D structure are controlled by the thickness of the sputtered gold layer. The growth process are proposed on the basis of vapor-liquid-solid (VLS) crystal growth mechanisms. Ga_2O_3 nanowires have diameters ranging several hundreds of nanometers and lengths ranging from several to several tens micrometers. The morphology and structure of the nanowires are characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), photoluminescence spectroscopy (PL). The influence of doping on these properties has also been studied. Pure and doped Ga_2O_3 nanowires have been proved to be reproducible. Photoluminescence measurement shows that the nanowires have blue emission and ultraviolet emission.

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Binary Amine-Phosphine Passivation of Surface Traps in CdSe Nanocrystals

임성준, 김원정, 신승구

포항공과대 화학과

Surface traps of CdSe nanocrystals were effectively passivated by combining both primary amine and tertiary phosphine ligands. CdSe nanocrystals with zinc-blende structure were prepared using a non-coordinating solvent system containing only stearate in 1-octadecene. The effects of propylamine and tributylphosphine on the optical properties of nanocrystals in chloroform were studied. Absorption and emission spectra and fluorescence lifetimes of nanocrystal solutions were measured at room temperature by varying the amounts of ligands. Stearate-covered CdSe nanocrystals showed only 3% quantum efficiency with a multi-exponential fluorescence decay. Addition of propylamine induced blue shifts in both absorption and emission spectra but no distinct variation in fluorescence decay with respect to the stearate-covered nanocrystals. Meanwhile, addition of tributylphosphine produced a significant reduction in fluorescence lifetime but little spectral shift in the optical spectra. However, addition of both propylamine and tributylphosphine yielded bright nanocrystals of ~50% quantum efficiency with a nearly single-exponential fluorescence decay. These results indicate that both electron and hole traps on the nanocrystal surface has been effectively passivated by a binary amine-phosphine organic layer.

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Crystal structure and electrical properties of $Mo_{1-x}Ta_xSe_2$

최선의, 정재훈, 김승주

아주대 에너지시스템학부

Molybdenum diselenide is attracting a great deal of attention because of its significant thermoelectrical and antifriction characteristics. However the low conductivity of $MoSe_2$ is the main obstacle of being used widely in the pure form. To make the electrical conductivity of $MoSe_2$ increased molybdenum is tially substitiuted by tantalum. In this study, a series of solid solution $Mo_{1-x}Ta_xSe_2$ were prepared and characterized. $MoSe_2$ has hexagonal 2-H type structure, while $TaSe_2$ has hexagonal 3-R type structure. The electrical/thermal conductivity of these compounds will be discussed in view of crystal structure.

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Facile Fabrication of Au Nanodot Patterns from Soft Lithographic Patterning of Polymer/Precursor Composite Thin Films

박민우, 정운룡

연세대 신소재공학과

Gold nanoparticles have been massively studied due to their easy synthesis and surface modification with various chemical methods, excellent localized surface plasmon resonance (LSPR) which can be used in biomedical areas. Recently, many researches for LSPR biosensors which consist of gold nanoparticle patterns have been performed but the conventional lithography requires high cost and complicated process. To solve this problem, we fabricated isolated gold nanodot patterns by means of capillary force lithography (CFL). The key to the success was control hydrophilicity of PEO/HAuCl4 composite by adjusting molar ratio between PEO and HAuCl4. This work will present the feasibility of various patterns and possible applications for sensing units.

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The various property of metal doped SnO2 nanofiber gas sensor through electrospinnig.

김규태, 정운룡

연세대 신소재공학과

SnO2 is an n-type semiconductor oxide with wide band gap energy and is always applied as gas sensing material to detect combustible, toxic and pollutant gases because of high sensitivity, simple design and low cost. Metal oxide fiber(SnO2) are fabricated by electrospinning, and this semiconductor fiber are sintered on furnace at 450℃ for crystallization. Transition metals such as, palladium, platinium nanoparticles are doped on the surface of tin oxide (SnO2) nanofiber for gas sensors. Semiconducting metal oxide nanofibers doped with metal nanoparticles are applied for highly sensitive and selective gas sensors due to their porous structure. (large surface-to-volume ratio) The sensitivity and selectivity of these fibers are measured with 1wt%, 3wt% Pd and 1wt%, 3wt% Pt doped SnO2. Prepared nanofiber is characterized by X-ray diffraction (XRD), Scanning electron microscope, and High resolution trans-electron microscopy (HRTEM).

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Three-Dimensional Analysis of Zigzagged TiO_2 and CdO One-Dimensional Nanostructures Using Electron Tomography

김한성, 명윤, 지경환, 조용재, 박정희, *안재평

*고려대 소재화학과 *KIST 산업화지원센터*

One-dimensional (1D) nanostructures have attracted considerable attention due to their potential use as building blocks for assembling active and integrated nanosystems. Recently, interest in zigzagged nanostructures has been steadily increasing, owing to their attractive morphology and properties. Electron tomography and high-resolution transmission electron microscopy were used to characterize the unique 3-dimensional structures of zigzagged TiO_2 nanobelts and CdO nanowires. The TiO_2 nanobelts adopt a twinning structure that consists of isosceles triangular slice segments terminated by [100], [01-1], and [-101] directions with the axial [010] direction. The zigzagged CdO nanowires consisted of linked rhombohedrons having the side edges matched to the and direction, and the [111] axial direction. These results would open a new field for investigating the nanostructures with high spatial resolution that could impact on the understanding of the growth mechanism and the application of nanodevices in many fields, where the crystal structure plays an important role on the final properties.

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Controlled Astaxanthin Nanosome Release with Nanoporous Silicified Phospholipids coated BN Powder

최홍경, *장정호

*고려대 화공생명공학과 *한국세라믹기술원 바이오융합팀*

This work demonstrates the controlled release of astaxanthin nanosome with synthesized nanoporous silicified phospholipids coated boron nitride powder for cosmetic application. The materials were obtained by silicification of tetraethylorthosilicate (TEOS) with the hydrophilic region of phospholipids and the process involves the incorporation of a chemically active phospholipids within the porous silica matrix. The asta nanosome as a functional materials was adapted and their controlled release profile was achieved as a function of time.

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Effective adsorption / elimination of ethidium bromide by mesoporous silica particles

안치영, *장정호

*고려대 신소재공학과 *한국세라믹기술원 바이오융합팀*

This work describes the innovative development of ethidium bromide (EtBr) elimination using the molecularly self-assembled mesoporous silicas. The mesoporous silicas were prepared by sol-gel method. This mesoporous silicas have the large pores and high surface areas. The adsorption of EtBr was achieved as a function of the amount of used mesoporous silicas. EtBr molecules on mesoporous silicas were easily eliminated by acid. The characterization was achieved by spectroscopic methods.

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Multimodal porous structure of magnetic mesoporous silicas by thermal hydrogenation process

이지호, *장정호, 박상언

*인하대 화학과 *한국세라믹기술원 바이오융합팀*

Multimodal porous structure of magnetic mesoporous silicas was synthesized by thermal hydrogenation process. The materials were obtained by the incorporation of iron(II) chloride tetrahydride into the inner pores of ordered mesoporous silicas as a magnetic precursor, and hydrogenation catalyst, and then achieved thermal hydrogenation with various temperature from 400 to 1,000 ℃. The results exhibited the magnetic property and pore sizes were closely related with hydrogenation time and temperature. The characterization for multimodal porous structure of magnetic mesoporous silica were achieved by various state-of-the-art techniques, such as SAXS, WAXS, FE-SEM, TEM, FT-IR, SQUID and nitrogen sorption. We confirmed multimodal porous structure of magnetic mesoporous silicas has superparamagnetic property and various pore size (10 nm to 100 nm) in accordance with temperature in thermal hydrogenation process.

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Nano-structured Films as a Novel Substrate for Cell culture

김효섭, 송영아, 김재호

아주대 분자과학기술학과

We fabricated a large area of monolayer silica nano-particle array on glass substrates for the cell growth by the Langmuir-Blodgett technique. A thin film of 300 nm sized mono-dispersed silica particles was constructed on the water interface and transferred onto a glass substrate. Chondrocytes were cultured on nano-structured substrates and bare glass for 8 days, respectively. The characterizations of chondrocytes on nano-structured substrate were conducted on 3rd and 6th day using confocal laser microscopy and with MTT assay for 8 days. The chondrocytes cultured on nano-structured substrate showed podia like spike and their size was larger than that formed on bare glass. The metabolic activity of chondrocytes on nano-structured substrate was lower than that on bare glass at early-stage, but it was recovered after 4 days.

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Preparation of silicified hollow magnetic nanospheres using lecithins and ferric ions and their characterization for biomedical applications

정연환, 장정호

한국세라믹기술원 바이오융합팀

Magnetic nanospheres have been studied to utilize in the field of the stroke therapy and cancer therapy, brain swelling, MRI contrast agents, hyperthermia, detoxification of blood, and as a carrier for drug and gene delivery due to the magnetic property of materials. We present the new hollow magnetic nanosphere preparation method for biomedical application such as drug storage. We have made liposomes using lecithin and ferric ions and then silicified the liposomes. The silicified liposomes were magnetized with flowing hydrogen gas at 800 oC. The characterization of hollow magnetic silica liposomes was carried out with FT-IR, TEM, TGA, XRD, and VSM analysis.

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Synthesis of Controllable Different Shapes TiO_2 Nanoparticlesby a Hydrothermal Method

이종탁, 변홍복, 윤태관, 배재영

계명대 화학과

TiO_2 nanoparticles with different shapes were synthesized by a hydrothermal method using surfactant. P123, F68 and ethylene glycol are used as a surfactant and controlled pH using ammonium hydroxide. The samples were characterized by TG-DTA, XRD, N2-sorption, SEM, and DRS techniques. The shape of TiO_2nanoparicles were rod, needle and cubic. Because surfactants make hydrogen bond with different TiO_2 facets, shapes of TiO_2 nanoparticles are controlled. The photodegradation of congo red in water has been investigated over different shapes TiO_2. TiO_2 with variable shapes were higher photocatalytic effect than anatase TiO_2 with a spherical shape.

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Synthesis of Nitrogen-Doped Graphite Outerlayers on the Vertically-Aligned Silicon Nanowire Array, and Their Application in Field Emission Display and Lithium Ion Battery

조용재, 서영석, 명윤, 김한성, 박정희, *조재필

*고려대 소재화학과 *울산과학기술대 에너지공학부*

Vertically-aligned silicon nanowire arrays on a large area of silicon substrates, with a desired diameter, length, and crystallographic orientation were synthesized by a facile metal-nanoparticle-assisted catalytic etching technique. The graphite and nitrogen-doped graphite layers were subsequently deposited on the silicon nanowire array using a pyrolysis of acetylene, and acetylene/ammonia mixture, respectively. The thickness of the outerlayers was controlled in the range 5-20 nm, and the nitrogen concentration was controlled up to 10 at. % by increasing the NH3 flow rate. X-ray photoelectron spectroscopy reveals that the pyridine-like structures becomes dominant as the nitrogen concentration increases. Field emission from the core-shell nanocables exhibits a large enhancement of current density with the graphite outerlayers, strongly correlated with the electronic structure revealed by X-ray photoelectron spectroscopy. The turn-on field producing a current density of 0.1 A/cm2 is 3.3 V/ m, and the emission current reaches 1.5 mA/cm2 at an applied voltage of 11.0 V/m. These core-shell nanocables have high charge storage capacity (~1000 mAh/g) for lithium ion battery.

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Study of commercial TiO_2 nanoparticle size effect on the performnce of dye sensitzed solar cells by SLIM-PCV measurement.

김정민, 구광호, 김용주, 임구일, 이완인, 최영식

인하대 화학과

The technique of stepped light-induced transient measurements of photocurrent and voltage (SLIM-PCV) was used for the measurement of electron diffusion coefficient (D_e) and electron lifetime (τ) for the dye - sensitized solar cells (DSSC) fabricated from several TiO_2 nanoparticles indifferent sizes. Stepped light-induced transient measurements method, the power of a CW (continuous wave) laser irradiating to the DSSCs was decreased abruptly by ~3% with a function generator, and tempoaral variations of the transient photocurrents and photovoltages measured, from which the D_e and τ values were extracted. Because this study used commertial TiO_2 phastes, solar cell were show same stability. Determined D_e and τ were measured by SLIM-PCV to investigate the particle size effect. It has been found that the $D_e$increases and τ increases with the increase of particle size. This increase was related to the decrease of grain boundaries that was efficient transport of electrons. This study suggests that the optimized TiO_2particle size is required for the efficient transport of electrons in DSSC.

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Controlled Growth of Pt Nanostructures on Graphene and Their Enhanced Performance as Electrocatalysts in Fuel Cells

양혜민, *이하진, *최원산, **전일철

*전북대 나노과학기술학과 *한국기초과학지원연구원 전주센터 **전북대 화학과*

Synthesis of platinum nanostructures with controlled size and shape is one of the most important goals in developing highly active Pt catalysts for many industrial applications, including fine chemical synthesis, gas sensing, hydrogen production, and fuel cell. Among them, it is widely recognized that the biggest concern in fuel cells is to improve the performance of the Pt on the cathode. To do so, many efforts have been focused on the synthesis of Pt nanostructures with great catalytic performance. Despite the progress made in the past, production of Pt catalyst with great catalytic performance and utilization efficiency is still costly and far from being trivial. It remains a grand challenge to synthesize Pt nanostructures with high surface areas via a surfactant-free, mild chemical route. For high performance, flattened supporting layers with high conductivity are also required to reduce contact resistance. Here we report a simple room temperature aqueous phase synthesis of cube-shaped Pt nanostructures on the graphene, and study their catalytic activity for the methanol oxidation reaction (MOR) in fuel cells.

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Nitrogen-Doped Nanostructured TiO_2 for Photovoltaic Devices

변홍복, 이종탁, 윤태관, 배재영

계명대 화학과

A highly efficient photovoltaic devices were fabricated using nanostructured nitrogen-doped TiO_2 powders. The properties of the nitrogen-doped TiO_2 powders and photovoltaic devices were investigated. The samples were characterized by XRD, N_2-sorption, IPCE, SEM, and DRS techniques. The UV-vis spectrum of nitrogen-doped TiO_2 powders showed a visible light absorption in the wavelength range from 400 nm to 580 nm. An enhancement of the IPCE in the range of 400~550 nm and 580~750 nm was observed. An 8% overall conversion efficiency has been achieved. The conversion efficiency was improved by nitrogen doping.

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Appearance of superlattice structure in the gas-phase cation substitution reaction from the CdS to Cu1.8S Nanowires

성태광, 김한성, 명윤, 박정희

고려대 소재화학과

As inspired by the discovery of carbon nanotubes, the current nanotechnology research is driving toward the development of diverse 1-dimensional nanostructures as well-defined building blocks to fabricate nanoscale electronic and optoelectronic devices. It is expected that the success of semiconductor integrated nanoscale circuits would be largely hinged upon the capability of heteronanostructure formation through carefully controlled doping and interfacing. In particular, the longitudinally modulated heterostuctures such as the nanowire heterojunctions and superlattices have been synthesized by a large number of research groups. Indeed, they have already demonstrated a great potential in the nanodevice applications such as light-emitting diode. In the present work, we first observed unique superlattice structure of wurtzite CdS and cubic Cu1.8S nanowires from the conversion reaction of the CdS nanowires into the Cu1.8S nanowires. The superlattice CdS nanowires consist uniformly of two (or four) layered segments along the [0001] growth directions. The complete substitution of Cd elements produced the superlattice Cu1.8S nanowires grown along the [110] direction. They have a structure along the [111] directions, with uniformly of six layered segments. These superlattice structures irreversibly evolved into the single-crystalline structures, after irradiating the electron beam of transmission electron microscopy.

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Supramolecule recognition on single-walled carbon nanotubes

남보라, *박상규, *강성호, **이하진

*전북대 바이오나노시스템공학과 *전북대 화학과 **한국기초과학지원연구원 전주센터*

Single-walled carbon nanotubes (SWNTs) are molecular wires that exhibit interesting structural, mechanical, electrical, and electromechanical properties[1]. In spite of that, the advances of their technological applications including electronic devices and chemical/bio-sensors have been interrupted because of their low solubility in solvents. Chemical modification of SWCNTs and physical adsorption of organic molecules or polymers on SWCNT surfaces are useful strategies to improve the solubility of SWCNT in solvents. Herein we report the solubilization of SWCNTs in aqueous media based on the π-π interaction between pyrene moiety and SWCNTs and investigate macrocycle molecule, cucurbit[n]uril (CB[*n*], *n* = *6* and *7*) recognition on SWCNT surface. CB[*n*] is the fancy name given to the pumpkin-shaped macrocycle molecule obtained from the condensation reaction between glycoluril and formaldehyde. CB[*7*] and CB[*6*] homologues have high affinity with viologen moiety and easily make their host-guest complexes. We designed and synthesized viologen derivative linked with pyrene moiety (py-vg) to investigate supramolecular interaction between CB[*n*] and viologen moiety on SWCNT surface. SWCNTs have been easily dispersed in aqueous solution of the py-vg via noncovalent π-π interaction between pyrene groups of py-vg and SWCNTs sidewall. The viologen moieties functionalized on SWCNT surface form their complexes with CB[*7*] and CB[*6*] by supramolecular host-guest reaction in aqueous media with different reactivity which monitored by spectroscopic methods such as UV-vis, fluorescence and ^{1}H-NMR instruments. We expect the supramolecular interaction on SWCNT surface *via* host-guest reaction is technologically critical to control the dispersion property of SWCNTs in aqueous systems

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Treatment of Anionic Surfactant on Polyelectrolyte Multilayers (PEMs) for Renewing the Structures and Properties of PEMs

MD. ARIFUR RAHIM, *최원산, *이하진, **전일철

*전북대 나노기술학과 *한국기초과학지원연구원 전주센터 **전북대 화학과*

We report on unusual behavior of polyelectrolyte multilayer (PEM) films induced by electrostatic interaction between anionic surfactant and PEMs. The charged sodium dodecyl sulfate (SDS) destabilizes the outer layer of the PEMs and in consequence outer polyelectrolytes (PEs) are desorbed from PEMs, which leads to the decrease in thickness of PEMs. Furthermore, the desorption rate and amount of PEs from the PEM films could be controlled by varying the surfactants, ending layers, and reaction times. It is able to retune the surface morphology and film thickness of PEMs even after build up of PEMs, which means that controlled desorption of PEs can be an effective tool to renew the structures and properties of PEMs. We expect that the essence of this interesting phenomenon might reveal some structural and morphological aspects of PEMs upon interaction between the surfactants and PEs. Our goal is to renew the structures and properties of PEM films using controlled desorption of PEs induced by electrostatic interaction between ionic surfactants and PEMs.

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Single-walled Carbon Nanotube based Biosensor by Metal Work Function Modulation

이재혁, 남광현, 창징보, Najeeb.C.K, 김재호

아주대 분자과학기술학과

Single-walled carbon nanotubes have been studied due to their potential applications in various fields. In electrical biosensors, the carbon nanotube biosensor has shown higher sensitivity and great promise in non-labeling detection systems, and nano-scale devices. There have been many attempts to fabricate highly sensitive sensor devices sine the electrical properties and surfae modification of SWNT became known. In this work, we have fabricated highly sensitive network SWNT devices, which have successfully detected specific adsorptions of streptavidin at 1 pM concentrations.

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Measurements of Photocurrent and Voltage using Commercial TiO_2 nanoparticles in Dye-Sensitized Solar Cells : SLIM-PCV and PLIM-PCV.

구광호, 김정민, 김용주, 임구일, 이완인, 최영식

인하대 화학과

The technique of SLIM-PCV(stepped light-induced transient mearsurements of photocurrents and photovoltages) and PLIM-PCV(pulsed light-induced transient measurements of photocurrents and photovoltages) were applied to measure diffusion coefficients (D_e) and lifetimes (τ) of electrons in dye-sensitized solar cells (DSSCs). SLIM-PCV method used to investigate a current transient induced by a stepwise change of the laser light intensity by function generator. PLIM-PCV method used to investigate a current transient induced by small-intensity laser pulse superimposed on bias light. solar cells were irradiated by a short pulse laser from the platinum electrode side.We used the P25 and P90 for commercial TiO_2 nanoparticles .This study suggests that the optimized measurement method is require for the measurement of electron diffusion coefficients (D_e) and lifetimes (τ) of electrons.

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High sensitivity detection of hIgG/anti-hIgG using periodic nanostructured Au film based SPR chip

송영아, 김효섭, 이종화, 김재호

아주대 분자과학기술학과

Surface Plasmon Resonance (SPR) has attracted considerable attention owing to their promising application as non-labeling biomolecular detection[1]. Recently, for sensitivity enhancement in the SPR detection, attempts of using surface plasmon have been performed after fabrications of nanostructures instead of using flat films. In this study, to make habitually associated Au nanostructures on SPR sensor chip, 2-dimensional crystalline colloidal film was fabricated and used as a template for constructing Au nanostructures on surface of SPR chip[2]. After Au nanostructures deposited on the chip either by thermal evaporation or sputtering process, the colloidal film was removed.In order to make well-ordered Au nanostructures on SPR sensor chip, thin films of hexagonally close packed (hcp) silica nanoparticles with average sizes of 300 ± 7 nm or 150 ± 4 nm were deposited on a glass substrate by the Langmuir Blodgett (LB) technique and used as the template. It is reported that LB technique takes advantage of high reproducibility, large area films formation, mass production capability at low cost. After Au deposited into the voids of silica particle hcp film, the nanostructures were obtained by the removal of colloidal film, as shown in figure 1. The size and close packing of silica colloids on the substrate were measured by scanning electron microscope (SEM). Also, we obtained periodic triangular pyramidal Au nanostructures on Au SPR chip as shown figure 2. In addition, the protein-protein interaction was observed using anti-hIgG and hIgG to evaluate application of SPR chip. In our future work, we will study the effect of the size of Au nanostructure on SPR sensitivity enhancement by controlling the size of silica nanoparticles used for the template fabrication.

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Synthesis of Bowl-Shaped Polymer Hollow Particles and Their Application in Encapsulation

이수진, *최원산, *이하진, 한재량

*전북대 화학과 *한국기초과학지원연구원 전주센터*

Colloidal particles with hollow interiors play important roles in the fields of drug deliveries, microencapsulations, cosmetics, inks, and pigments. A variety of materials that include polymers, ceramics, composites and metals has been widely used for preparing such particles. Among them, polymers are considered as promising materials for above applications due to the flexible properties and easy chemical modification. For polymers, methods such as emulsion polymerization, phase separation, crosslinking of micelles and self-assembly have also been demonstrated for generating hollow structures. The development of novel synthetic methods for the preparation of polymer hollow particles is highly desirable with much potential for future applications and fundamental studies. Here we report a simple synthesis of bowl-shaped polymer hollow particles prepared by means of thermal annealing after synthesis of metal nanoparticles on polymer structures. We guess that small particles could be encapsulated into the inside of bowl-type particles through controlled thermal annealing.

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Metal Ions Doped Mesoporous TiO2 Particle for Dye Sensitized Solar Cell

김성수, 김명실, *이윤연, 윤정아, 김지만

*성균관대 화학과 *성균관대 나노과학기술협동학부*

Dye-sensitized solar cell (DSSC) is regarded as a regenerative low-cost alternative to conventional devices. A lot of semiconducting metal oxides such as SnO2, ZnO, Nb2O5, CeO2, TiO2 has been widely utilized for DSSC electrode. Recently, various forms of nanocrystalline TiO2 have been extensively investigated as a potential material for DSSC. In addition to this, a great deal of attention has been focused on developing new sensitizers, new electrolyte, and new semiconductor electrode materials. For DSSC, the TiO2 material should have extremely high surface area so that the dye can be sufficiently adsorbed, resulting in the generation of a high photocurrent. However, TiO2 electrode only response to UV light due to their wide band gap (3.2 eV for anatase) is still remained problem. In this study, metal ions doped Mesoporous TiO2 was synthesized by nanocasting method using mesoporous silica as the structure directing template. Metal ions doped mesoporous TiO2 has not only a high surface area, but also uniform nanoparticles and nanochanels that can be easily accessed by the electrolyte for I3- ion transport.

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Ambipolar organic light-emitting field-effect transistors based on bilayer heterojunction

서훈석, 안민준, **Zhang Ying**, 최종호

고려대 화학과

We report air-stable organic light-emitting field-effect transistors (OLEFETs) based on a sequential deposited films of N,N'-ditridecylperylene-3,4,9,10-tetracarboxylic diimide (P13) as a electron-transport material and tetracene as a hole-transport material using the neutral cluster beam deposition (NCBD) method. The surface morphology and structures for the untreated and thermally treated P13/tetracene films were examined by atomic force microscopy (AFM), X-ray diffraction (XRD), and laser scanning confocal microscopy (LSCM). The device characteristics of bilayer heterojunction structure show features of ambipolar operation. According to the charged coupled device (CCD) images, the light intensity is controlled by both the drain-source voltage (V_{DS}) and the gate-source voltage (V_{GS}).

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IrO_2 Nanoparticles for Dye-Sensitized Water Oxidation Catalyst

윤용태, 강용철, 김영일

부경대 화학과

Iridium oxide is a useful catalyst for water oxidation. IrO_2 nanoparticles were formed by thermal hydrolysis of $IrCl_6^{2-}$ without any stabilizer. Temperature was controlled at 60, 90, 200 ℃ respectively. Hydrolysis rate was proportional to the temperature. Synthesized temperature didn't affect the size of IrO_2 nanoparticles. Using XPS, XRD and UV-Vis spectroscopy, synthesized nanoparticles were studied. Water oxidation ability was affected by some factors like synthesized time, temperaure. As synthesized time and temperature increased water oxidation ability decreased. Also buffer solutions affect water oxidation. Catalytic effect of IrO_2 nanoparticles were investigated in $Ru(bpy)_3^{2+}$ as a sensitizer and persulfate as a elecron acceptor.

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Terahertz Absorption and Emission from Vertically-Aligned Silicon Nanowire and Silicon-Carbon Core-Shell Nanocable Array

서영석, 정경복, 조용재, 명윤, 김한성, 박정희

고려대 소재화학과

We synthesized vertically-aligned p-type and n-type silicon nanowire arrays on a large area of silicon substrates, with a desired diameter, length, and crystallographic orientation, using by a metal-nanoparticle-assisted catalytic etching technique. The length was controlled from 500 nm and 3 μm. We observed the terahertz (THz) emission from these Si nanowires (NWs) excited by a 100 fs pulse of 810 nm radiation from a Ti:Sapphire laser system, and compared it with that of a Si film. The frequency spectrum (0-4 THz) of the THz emission from the Si NWs is red shifted by 0.2 THz. This red shift is though to originate from the anisotropic nanowire geometry, which causes a decrease of the longitudinal plasmon oscillation frequency. The graphite layers were subsequently deposited on the silicon nanowire array using a pyrolysis of acetylene. We observed that the graphite deposition enhances significantly the THz absorption, owing to their increased conductivity.

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Various CdS and ZnSe Hybrid Nanotube/Nanowire Arrays for Photoelectrochemical Water Splitting

손용재

고려대 소재화학과

High-density TiO2 nanotube arrays were synthesized using electroanodizing method, and the CuO nanowire array was synthesized using thermal oxidation of Cu foils. Their diameter was controlled using the growth condition. The CdS and ZnSe layers were uniformly deposited on the pre-grown TiO2 nanotubes (anatase) and CuO nanowires, using vapor transport method. The thickness of the CdS shell was uniformly controlled to be 50 nm. The CdS shell layers consisted of a number of single-crystalline domains whose wurtzite [001] direction aligned along the wire axis. The thicker CdS outerlayer results in a higher value of photoconversion efficiency. As the thickness of CdS shell in the nancables increases, a hydrogen generation rate reaches to 2.5 mmol/h under 100 mW/cm2 visible light irradiation. To best of our knowledge, this hydrogen generation rate is the highest for a NW based photocatalytic or photoelectrochemical cell.

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Solvothermal synthesis of single-crystalline PbS nanowires using steric effect of octylamine ligand

송윤미, *장소영, *김한성, *박정희

*고려대 소재화학과 태양에너지소재 *고려대 소재화학과*

Colloidal single-crystalline PbS nanowires (NWs) were synthesized with well-controlled shape and growth direction through the novel use of the steric effect of the capping ligands. Octylamine was used as coordinating co-ligands in the non-coordinating solvent, 1-octadecene (ODE). They can act as “sufficient” protection ligands, which can control the shape of the mono-dispersed NCs. The PbS NCs exhibit a remarkable shape evolution from dots to NWs when the amines are added. They consisted of rock-salt structure PbS nanocrystals uniformly grown in the [100] or [110] direction, controlled by the growth condition. We also fabricated field-effect transistors using single PbS NW, proving it to be intrinsically p-type semiconductor.

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Nanoparticle Route Synthesis of Mesoporous Zirconia Thin Films

고영선, 권영욱

성균관대 화학과

We synthesized mesoporous zirconia thin films by using a mixed solution in which zirconia nanoparticles were self-assembled with block copolymers. To synthesize non-silica mesoporous materials, we should control not only the self-assembly properties of block copolymers as templates, but also the condensation reactions of inorganic species. The self-assembly of block copolymers can be controlled quite easily through thermodynamics. In contrast, the behavior of inorganic species depends on kinetic factors, so that controlling the kinetics is more difficult and complex. Thus, we developed the synthesis of mesoporous zirconia in two steps: (1) the synthesis of zirconia nanopaticles and (2) the spin-coating technique with the solution mixed nanoparticles and block copolymers in ethanol. This method suppresses the condensation of inorganic species in an aging step of the synthesis of mesoporous zirconia. Therefore, we expect to synthesize mesoporous zirconia thin films more reproducibly because the mesostructures will be controlled only by the self-assembly of block copolymers.

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Platinum films with controlled morphologies and their effects on surface enhanced raman scattering

이은선, 권영욱

성균관대 화학과

We report the synthesis of Pt replica thin films with controlled morphologies that can support surface enhanced raman scattering (SERS). Mesostructured Pt films synthesized by two steps: First, mesoporous silica thin films with controlled morphologies were formed on Pt-coated Si wafer. The pore have a diameter of 8~9nm with 2~3nm gaps. Second, Pt metal was deposited into the pores of the templates by an electrochemical deposition method. After the electrochemical deposition, the silica template is removed by soaking the substrate(film) in 1wt% HF. In these process, films were mechanically robust and chemically stable. We performed electrochemical analyses on these Pt films to measure the exposed surface areas and studied the SERS effecto f nanostructured Pt films on rhodamine 6G.

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Dendritic Pt Nanoparticles with Enhanced Activity and Durability for PEMFC Catalyst

김청희

연세대 화공생명공학과

Shape-controlled platinum nanoparticles can offer enhanced catalytic properties. Especially, dendritic shape has attracted interests for electrocatalytic application due to its considerable advantages of high surface area. Here, we synthesized dendric Pt nanoparticles by reducing aqueous mixture of K_2PtCl_4 and TTAB with L-ascorbic acid. Various sizes of dendric Pt nanoparticles were synthesized by changing the reduction temperature. The dendritic Pt nanoparticles were tested for oxygen reduction reaction (ORR) and their activity and durability were evaluated. These results were compared with commercial Pt/C catalysts (E-tek) and showed that dendritic Pt nanoparticles are more active based on equivalent Pt mass for ORR. Particularly, durability of dendritic Pt nanoparticles is much better than Pt/C. We also investigated size effect of dendritic Pt nanoparticles for ORR activity and durability.

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Pore Size Extension of Mesoporous Silica Thin Films

이기림, 권영욱

성균관대 화학과

We report the controlled expansion of pore within mesoporous silica thin films using polypropylene glycol (PPG) as a swelling agent. Our method uses the tunable molar ratio of F127/PPG to induce the controlled swelling of the triblock copolymer surfactant templating agents. The swelling process eventually leads to the control of pore diameters and hexagonal or cubic spacing within the mesoporous silica thin films. X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) techniques were used to observed pore diameter, silica wall thickness, and structure of mesoporous thin films.

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Catecholamine Adhesive Reducing Agent (poly(dopamine)) for Gold Nanoparticle Synthesis on a Variety of Surfaces

홍선기, 이해신

KAIST 화학과

Gold nanoparticle 은 bulk 와는 다른 특이한 optical, electronic, magnetic, catalytic properties 로 인해 많은 관심을 받고 있다. 이러한 성질을 응용하기 위해 가장 중요한 기술은 gold nanoparticle 을 원하는 표면에 붙이는 것이다. 우리는 Adhesive Reducing Agent(ARA)를 이용하여 표면의 성질에 관계없이 쉽게 gold nanoparticle 을 attaching 하는 새로운 기술을 제안한다. 본 연구에서 사용한 adhesive reducing agent 는 surface-independent 하게 어떤 surface 에서든지 코팅 능력을 가지는 것으로 밝혀진 dopamine 이며, poly(dopamine)이 가지는 환원력을 이용하여 표면에서 직접 attaching 된 AuNP 를 생성한다. 이는 표면의 종류에 관계없이 gold nanoparticle 을 attaching 할 수 있는 간단하면서도 중요한 기술이며, 반응시간, 온도, salt 농도에 따라 particle 의 size, shape 을 조절할 수 있기 때문에 다양한 응용범위를 제시한다. Gold nanoparticles have been attracting much attention due to their interesting optical, electronic, magnetic, catalytic properties. For applications, the most challenging part is attaching the NPs on the surface with moderate dispersion. We propose a new method for attaching the NPs regardless of surface characteristics through introducing Adhesive Reducing Agent (ARA). The process of reducing gold source and attaching on the surface is completed at the same time with ARA. This method can control the size and shape of NPs by temperature, reaction time, salt concentration. Surface independent attaching of AuNPs is very important technique and it gives potential on various applications.

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Organic CMOS - like inverter circuits employing two heterojunction ambipolar P13 and DH6T field - effect transistor.

안민준, 서훈석, Zhang Ying, 최종호

고려대 화학과

We have demonstrated the fabrication and characterization of heterostructure OFETs based on N,N' - ditridecylperylene - 3,4,9,10 - tetracarboxylic diimide (P13) and α,ω - dihexylsexithiophene (DH6T) exhibited ambipolar transport with well balanced hole and electron mobilities of 2.22×10^{-2} cm^2/ Vs and 2.78×10^{-2} cm^2/ Vs. A complementary metal oxide semiconductor (CMOS) - like inverter was fabricated on a single substrate using two identical ambipolar OFETs with P13 and DH6T bilayer. The inverter showed a low hysteretic inversion of the input voltage (V_{IN}) .

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new approaches to the synthesis of Ⅰ-Ⅲ-Ⅵ semiconductor nanocrystals

유의덕, 이선숙, 정택모, 김창균

한국화학연구원 화학소재연구단

$CuInS_2$ and other Ⅰ-Ⅲ-Ⅵ semiconductor nanocrystals have actively been studied for their application in photovoltaic cell because their direct band gap energy of 1.45 eV (855 nm), allows $CuInS_2$ nanocrystal to emit from the visible to near-infrared region by tuning their size and to enhance an absorption coefficient. Furthermore, $CuInS_2$ nanocrystals are important in photovoltaic devices as an environmental-friendly material. Although $CuInS_2$ nanocrystals have many advantages, there have been barely investigated high quality of $CuInS_2$ such as Photoluminescence.Here we present the new approaches to the synthesis of $CuInS_2$ as a defect free semiconductor by implementing the secondary injection.

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Synthesis and Characterizations of The New Layered Oxysulfide, $BaNbPS_2O_4$

김경희, 나주란, *윤호섭

*아주대 에너지시스템학부 *아주대 화학과*

The new pentanary oxysulfide, $BaNbPS_2O_4$has been synthesized with the reactive halide flux and structurally characterized by single-crystal X-ray diffraction techniques. $BaNbPS_2O_4$ crystallizes in the space group P4/nmm of the tetragonal system with two formula unit in a cell of dimensions: a = 6.5104(8), c = 8.1215(14) Å, and V=344.23(8) $Å^3$. Each layer is comprised of Nb-centered octahedra and P-centered tetrahedra. Nb-centered octahedron, NbS_2O_4 is composed of two trans sulfur atoms and four oxygen atoms in the ab plane. These polyhedra are connected by sharing oxygen atoms to form two-dimensional anionic layers, $[NbPS_2O_4^{2-}]$ perpendicular to the c-axis. These layers are stabilized through ionic interactions with Ba^{2+} cations to complete the three-dimensional structure. The classical charge balance of the title compound can be described as $[Ba^{2+}][Nb^{5+}][P^{5+}][S^{2-}]_2[0^{2-}]_4$.

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Pentacene-Based Organic Thin Film Transistors Treated with Molecular Hedgehog Self-Assembled Monolayer

정상미, 박지웅

광주과학기술원 신소재공학과, 분자레벨집적화기초연구센터

We fabricated organic thin film transistors (OTFTs) with the twisted biaryl monolayers coated between the insulator and semiconductor layers. The biaryl monolayer surface, especially binaphthyl (BN) monolayer, is rough only on the molecular level and can be regarded as a field of molecular hedgehogs. Pentacene was thermally evaporated onto the silica substrates treated with or without the BN monolayer for comparison. The electrical properties of these devices were compared with those constructed on the bare silica surface. The field-effect mobility (μ) of the device with the BN monolayers appeared 50% higher than that of the non-treated devices. The morphology of the semiconductor layer was investigated using atomic force microscopy (AFM) and X-ray diffraction (XRD) method. AFM image showed that the pentacene layer on the BN monolayers consisted of larger and more interconnected grains than those on the silica surface. XRD spectra of the 50 nm thick pentacene film exhibited that the pentacene crystals on the BN monolayers consisted of mostly thin film phase (d001=~15.5Å) while those on the silica surface contained both the thin film phase (d001=~15.5Å) and bulk phase (d001=~14.5Å).

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Synthesis and Characterization of Poly (2-(acryloyloxy) ethyl cinnamate-co-polyhedral oligomeric silsesquioxane) Hybrid Nanocomposites

BHARANI KUMAR, 김윤경, 이용일

창원대 화학과

Polyhedral oligomeric silsesquioxane (POSS) is a class of inorganic compounds that has a well-defined structure with a silica-like core (Si_8O_{12}) surrounded by eight organic corner groups (functional or inert). The functional corner groups enable POSS to copolymerize with organic monomers, such as acrylates, styrenes,2,5 norbornenes, epoxy, siloxane, urethane, and so on. In present invention, we report the synthesis and characterization of a series of novel octavinyl-POSS-based poly (2-(acryloyloxy) ethyl cinnamate-co-polyhedral oligomeric silsesquioxane) hybrid nanocomposites with star-type structure as well as the properties and the applications.Keywords: Nanocomposite, hybrid materials, silsesquioxane.

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Fabrication of Langmuir-Blodgett films using Au-core/Silica-shell nanoparticles for surface plasmon resonance sensitivity enhancement

이종화

아주대 분자과학기술학과

In recent years, the Surface Plasmon Resonance (SPR) has been widely employed for biosensor applications owing to the capability of label - free detection of biomolecular interactions.[1] Many research efforts have been concentrated on the fabrication and structural optimization of nanostructures based SPR sensor chips for the enhancement of sensitivity. In this study to enhancement of SPR sensitivity, we fabricated 2-D hexagonally close packed Langmuir-Blodgett (LB) films of Au-core/ silica-shell nanoparticles on the Au coated glass substrate for the SPR sensor chip. The film fabrication by LB technique is suitable for mass production of nanostructured SPR sensor chip with high reproducibility. The inter-particle distances between Au colloid cores in the film was controlled by adjusting the thickness of silica-shell in the synthesis process. In this study, we synthesized uniform sized 20 nm Au-core and silica-shell nanoparticles with four different thicknesses of 40 nm, 70 nm, 120 nm and 180 nm by seed-growth method. Well-ordered 2D colloidal films by the LB method were fabricated with large area (7 μm x 5 μm). The SPR signals were sensitively affected by variation of the thickness of silica shell. An optimal thickness of silica shell was depended on the characteristics of probe on the chip and target in the sample. The Au-core/silica-shell film based SPR sensor chip demonstrated significant enhancement of SPR signal compared with a bare gold film.

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Poly(methyl methacrylate) dielectric material applied in ambipolar heterojuntion-based organic light-emitting field-effect transistors

Zhang Ying, 서훈석, 안민준, 최종호

고려대 화학과

The properties of bilayer heterojunction-based organic light-emitting field-effect transistors (OLEFETs) with poly(methyl methacrylate) (PMMA) as a dielectric layer have been investigated. A sequential deposited films of N,N'-ditridecylperylene-3,4,9,10-tetracarboxylic diimide (P13) as electron-transport material and tetracene as hole-transport material by using the neutral cluster beam deposition (NCBD) method. Based upon well-balanced ambipolarity, the air-stable OLEFETs have demonstrated good field-effect characteristics, stress-free operational stability and electroluminescence under ambient condition.

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Preparation and Properties of Luminescent Graphene/ Lanthanides(III) and its Incorporation into a Polyimide Matrix

오영희, 김장용, 김혜진, 이진봉, 강경남, *신구

*동의대 화학과 *세종대 화학과*

Novel photoluminescent graphene/lanthanide(III) nanostructured composites have been prepared from the graphene, pyridoin and lanthanium salts(Ln= Eu, Tb) in alcoholic solution. Morphology and the structures and properties of the composites have been examined. Those showed the same photoluminescence as the corresponding lanthanide complexes. Incorporation of the composites into a polyimide have been tried to improve strength of the polymer and to show luminescence.

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Large-Area Fabrication of Patterned ZnO-Nanowire Arrays Using Light Stamping Lithography

황재권, 당정미, 성명모

한양대 화학과

We demonstrate selective adsorption and alignment of ZnO nanowires on patterned poly (dimethylsiloxane) (PDMS) thin layers with aminopropylsiloxane self-assembled monolayers (SAMs). Light stamping lithography (LSL) was used to prepare patterned PDMS thin layers as neutral passivation regions on Si substrates. 3-Aminopropyltriethoxysilane-based SAMs were selectively formed only on regions exposing the silanol groups of the Si substrates. The patterned positively charged amino groups define and direct the selective adsorption of ZnO nanowires with negative surface charges in the protonic solvent. This procedure can be adopted in automated printing machines that generate patterned ZnO-nanowires arrays on large-area substrates. To demonstrate its usefulness, the LSL method was applied to prepare ZnO-nanowire transistor arrays on 4" Si wafers.

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A facile fabrication of polymer thin films on solid substrates

김민성, 정연태

부경대 화상정보공학부

Surface properties are important for determining the functions and uses of materials. So modification of materials with polymer thin films has emerged as an important method to control the physical and chemical properties of the surface layer. We report a simple and effective method to photochemically attach thin polymeric layers to solid surface without chemical derivatization of the substrate and/or the polymer. The system is based on a photoreactive poly(4-vinylpyridine) (P4VP) thin film which is formed on the SiO2 surface via spin coating. This substrate is then covered with another polymer film that is reacted with the benzyl radical moieties by UV irradiation. As a result of photochemical reaction, a thin layer of the later polymer is covalently bound to the surface of P4VP. Unbounded polymer is removed by sonication. The thickness of the attached film is a function of the irradiation time and the molecular weight of the polymer. Spatially defined polymer thin films can be fabricated by way of photolithography.

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Fabrication of functionalized ordered mesoporous carbon(OMC) using conducting polymer as cathode catalyst support for direct methanol fuel cells (DMFC)

윤정아, 김진회, 박은주, 김지만

성균관대 화학과

The mesoporous carbon is promising applications as catalyst support for DMFC. OMC materials have large surface area, good electrical conductivity for providing electrical pathway, uniform pore textures for facile diffusion of reactants and by-products. In spite of they have lots of merits, many researchers are try to control the property of support materials to enhance the catalyst activity such as oxygen reduction reaction(ORR). To enhance the activity, we tried to synthesize C-OMC materials using conducting polymer(CP) and selectively functionalize the outer surface of OMC particles with CP. Polyaniline(PANI) and polypyrrole(PPy) were selected as CPs, because they has high conductivity, thermal stability, readily synthesized from the monomer, and stable under ambient conditions. The C-OMC have been synthesized using mesoporous silica materials as templates and CP as carbon precursor. The CP based C-OMC was synthesized by in situ polymerization of conductive monomer into pores of the silica template containing oxidant. C-OMC is obtained after the carbonization and removing the silica template by dissolution in aqueous HF. Selectively covered OMC on the outer surface with CP was adsorbed on the surface of OMC after removing the mesoporous silica by polymerization of monomer with oxidant. The samples were systematically investigated using N2 adsorption, small and wide angle power X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Furier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), and conductivity mesured using the four-probe methode .

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Characterization of Quantum Dot-Conducting Polymer Hybrid Films and Their Application to Light-Emitting Diodes

배완기, *이성훈

*서울대 화학생물공학부 *서울대 화학부*

We report QD-conducting polymer hybrid films of extensive process capability, by grafting block copolymers containing a conducting polymer block and a thiol anchoring block (poly(para-methyl triphenylamine-b-cysteamine acrylamide, PTPA-b-CAA) to CdSe@ZnS QDs. The hybrid films have uniform QD distribution over various solution-based processes and possess hybridization capability with pattering techniques. We also demonstrate performances of QLEDs employing the hybrid films as the active layers, exhibiting moderate turn-on voltage (< 4 V), high external quantum efficiency (> 1.5 %), and high color-purity (FWHM ~ 30 nm). The approaches and results presented here represent significant progress toward the practical realization of QLEDs, and may also lead to reasonable platforms for optoelectronic devices, such as photodetectors or photovoltaic devices, based on the organic-inorganic hybridization.

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Inorganic Thin Film Transfer Printing Using Atomic Layer Deposition

김수환, 이병훈, 남재우, 성명모

한양대 화학과

We report a new approach to fabricate the periodic channel of metal oxide film by using the water-mediated TFTP combined with atomic layer deposition (ALD). In the patterning method, the Al_2O_3 film is deposited on FTS-based SAMs by using ALD at growth temperature of 100 C. The CF_3-terminated alkylsiloxane monolayer, which is coated on PDMS stamp, provides a weak adhesion between the deposited Al_2O_3 and stamp, and promotes the easy and complete release of Al_2O_3 film from the stamp. And also, the water layer serves as an adhesion layer to provide good conformal contact and form strong covalent bonding between the Al_2O_3 layer and Si substrate. Therefore, the transferred Al_2O_3 channel patterns chemically bound to the substrate surface and thus exhibit strong adhesion. We foresee that this approach could become a framework for fabricating nanochannels of various inorganic materials.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Patterning of Ag thin films with micro Transfer Molding

당정미, 곽은비, 성명모

한양대 화학과

We report a new metal particle transfer printing method using inkpad method. In this technique, an elastomeric stamp is prepared by casting against a master. A Ag particle pad is formed on the oxidized surface of the substrate by spin coating. The patterned PDMS contacts to the metal particle ink pad a few seconds. When the PDMS lifted up, the metal particle on the raised regions of the stamp is transferred to the oxide substrate and a metal pattern is formed. The Ag particle-coated prepatterned PDMS can make conformal contact with SiO2 substrate. The patterned Silver films have been investigated by atomic force microscopy (AFM), optical microscopy (OM) and scanning electron microscopy (SEM).

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Patterning of Aluminum Thin Film using Solvent assisted nano Transfer Printing

곽은비, 당정미, 성명모

한양대 화학과

We report a new metal transfer printing method that uses a water-mediated transfer process with contact inking stamps. Water-mediated nTP is based on the direct transfer of a metal thin film from a stamp to a substrate via a water-mediated surface bonding between the stamp and the substrate. In water-mediated transfer printing, the water layer serves as an adhesion layer to provide good conformal contact and form strong covalent bonding between the Al thin film and the Si substrate. The transferred Al patterns are chemically bound to the substrate surface and, thus, exhibit strong adhesion. The SAMs ensures efficient release of the Al pattern when the stamp is removed. When the PDMS lifted up, the metal on the raised regions of the stamp is transferred to the oxide substrate and a metal pattern is formed. The Al-coated patterned PDMS can make conformal contact with SiO2 substrate. The patterned Al films have been investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM).

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Preparation, Characterization, and Optical Properties of Gold Nanoshells Having Silica Core

배효선, 권법진, 정현

동국대 화학과

Metal nanoshells grown on the surface of dielectric core particles have been of great interest due to their potential applications as optical and electronic devices or biosensing and drug delivery systems. Among various metal nanoshell structures, gold nanoshell has been attractive not only because of it's tunable optical properties, but also it's inertness in biological system. Monodispered silica nanoparticles are obtained by the Stöber method as a dielectric core. 7.0 ml of ammonia water (25 %) was added to 100 ml of absolute ethanol. After 3 ml of TEOS (tetraethylorthosilicate) was added dropwise, the solution was stirred overnight. The obtained silica nanoparticles have a diameter of approximately 100 nm by TEM measurement. In order to obtain a nanoshell structure, the surface of silica nanoparticles are modified by aminopropyltrimethoxysilane (APTMS). 50 μl of APTMS was added to the silica suspension solution with vigorous stirring. Colloidal gold nanoparticles with diameter of 2-3 nm were prepared by Duff method. Finally, gold nanoshells were obtained by attachment of colloidal gold nanopartciles to APTMS functionalized silica core. The size, morphology, and elemetal composition of the products were characterized by FE-SEM, TEM, TG-DTA and FT-IR spectroscopy. The optical properties of the gold nanoshells were analyzed by UV-vis spectroscopy.

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Synthesis, Ion-exchange, and Colloids of $RE_2(OH)_5NO_3 \cdot nH_2O$ (RE = rare-earths)

이수연, 이경희, 변송호

경희대 화학과

Although the layered double hydroxides (LDHs) have attracted a great deal of interest because they have a number of attractive properties for diverse applications, it was not until very recently that the layered materials composed of pure cationic rare-earth hydroxide layers were reported. Such a series of compounds, called the layered rare-earth hydroxides (LRHs), has the general formula $RE_2(OH)_5X \cdot nH_2O$ where RE = rare-earths. In the present work, RE = Sm, Eu, and Gd members of this family were synthesized by using a hydrothermal reaction under a controlled pH condition. In contrast, a non-aqueous solvothermal procedure was applied to prepare RE = Nd and La members because it is difficult to synthesize these members in an aqueous system. A series of 1-alkanesulfonate, alkylsulfate, and organic carboxylate anions are easily intercalated into these layered rare-earth hydroxides by the ion-exchange reaction. Interestingly, the alkali-metal nitrates were partially intercalated in the interlayer gallery of the as-synthesized hydroxide from non-aqueous solvothermal reaction. The hydration of the alkali-metal salts intercalated LRHs resulted in the colloidal LRH suspensions in water.

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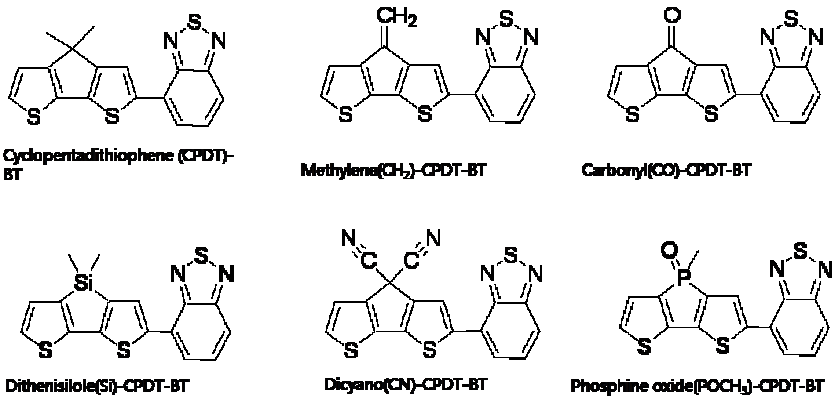
Newly designed polymer units for solar cell applications: a DFT study

구자민, *장윤희

광주과학기술원 신소재공학과, PIMS *광주과학기술원 신소재공학*

A great deal of effort in developing high-efficiency organic solar cells is focused on finding low band-gap polymers which can better harvest the solar spectrum. It is well known that alternating donor and acceptor units generally lowers the band gap of the polymer. In our previous study we studied on several donor-acceptor systems having a promising BT (benzothiadiazole) acceptor unit, among which CPDT-BT (cyclopentadithiophene-BT) showed the lowest band gap as well as the deepest HOMO/LUMO levels and was predicted to the highest solar cell efficiency. Based on these principles, in the current work, new donor-acceptor systems were designed to potentially have low band gaps by retaining the CPDT-BT backbone and deeper HOMO/LUMO levels than CPDT-BT by introducing withdrawing functional groups such as C=CH2, C=O, Si(CH3)2, C(CN)2, and P=O(CH3). The geometry, electronic structure, and the electronic transitions of these CPDT-BT derivatives were calculated with the density functional theory (DFT) and the time-dependent (TDDFT) calculations at the B3LYP/6-311G** level. Indeed, the calculation predicts that a carbonyl derivative of CPDT-BT (CO-CPDT-BT) can have higher solar cell efficiency than CPDT-BT, once its solubility problem is taken care of.



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Nanosheets of Layered Rare-Earth Hydroxides Dispersed in Toluene

유지호, 이병일, 변송호

경희대 화학과

Exfoliation or delamination of layered compounds into single layers provides an efficient route to the ultimate two-dimensional anisotropy and the inorganic macromolecules. The clay minerals such as montmorillonite, smectites, and the synthetic clay laponite are delaminated to generate the negatively charged nanosheets. In contrast, the layered double hydroxides (LDHs) produce positively charged nanosheets. The layered rare-earth hydroxides (LRHs) are structurally similar to the LDHs, overall layered structure consisting of alternating positively charged hydroxide and anion layers. In the present work, our efforts have been made toward the exfoliation of $RE_2(OH)_5NO_3{\cdot}nH_2O$ series (RE = rare-earths). As in the case of classical LDHs, the exfoliated nanosheets of LRHs have potential as a building block for the fabrication of a wide variety of functional nanostructured materials.LRHs were synthesized via a hydrothermal reaction. The ion-exchange reactions between NO_3^- and oleate ($C_{17}H_{33}COO^-$) anions in the interlayer space of LRHs were carried out. Exfoliation was accomplished by dispersing LRHs–Ole in toluene. To facilitate the exfoliation, the dispersion was ultrasonically treated in successive intervals of 10 min. Typical SAED patterns, which were taken from a randomly chosen particles in the colloidal solutions, exhibited clear spots, indicating their single-crystalline nature. The height profiles of the AFM images reveal two distinct thicknesses of ~ 4 nm and ~ 8 nm. By considering the ~ 4.6 nm basal spacing of LRH–Ole, such thicknesses suggest that the nanosheets exfoliated in the suspension mainly consist of one to two monolayers.

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Simple synthesis and characterization of monodisperse thioether-bridged organosilicas

김정호, *김민식, **Nitin Chaudhari, **kiran chaudhari, **김민우, **임신묵, **송민영, *유종성

*고려대 신소재 화학과 *고려대 신소재화학과 **고려대 소재화학과*

A noteworthy hybrid material involves inorganic–organic coordination compounds, in which the inorganic and organic groups can be easily connected by chemical links at molecular level, which exhibit combinative properties from organic and inorganic groups. However, the morphology of such materials is hard to control. Multifunctional container like nanomaterials with unique properties is always in demand due to their applications in fields like drug, gene and protein delivery and separation sciences. With organic groups bridged with in the framework, organosilicas symbolize one of the most exciting achievements in the field of nanostructure materials. The chemical and physical properties of the material can be changed dramatically by incorporating different organic groups in the framework which may help in facilitating access to guest molecules to the internal surfaces of these nanostructures. Bis(3-triethoxysilylpropyl) tetrasulfide (TESPTS) is one such organic silane with ethoxy and tetrasulfane groups (S4 ring) and its interactions with silica are well documented. Silica modified with TESPTS has been used to reinforce silica on rubber, as reaction between ethoxy groups and hydroxyl groups favour this reinforcement. It reacts both with the silanol groups present on the silica surface and also preferable sulphur transferring agent.We herein report, development of novel, differently functionalized monodispersed thioether-bridged organosilica, silica and carbon. Very uniform and monodisperse dense thioether-bridged organosilicas with diameter of ca. 350 nm were prepared based on Stöber method in ethanolic solution with water. We hereby present a synthetic procedure of monodisperse thioether-bridged organosilica spheres using sol-gel process.

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Fabrication of graphene

김주한

서울대 화학부

We have developed a controllable method to fabricate high-quality graphene sheets using a thermal plasma jet system. A carbon atomic beam was generated by injecting ethanol into Ar plasma continuously; the beam was then flowed through a carbon tube attached to the anode. Graphene sheets were made by an epitaxial growth when the carbon atomic beam having a proper energy collided with a graphite plate.

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Electrophoretic Synthesis of Porous Cobalt Oxide Films with Controllable Morphology and Crystal structure

송민선, *김태우, 황성주

*이화여대 화학·나노과학과 *이화여대 지능형 나노바이오소재 연구센터*

We have fabricated successfully porous cobalt oxide films with controllable morphology and crystal structure via an electrophoretic deposition of exfoliated CoO_2 nanosheets. Considering that the exfoliated CoO_2 nanosheets have negative surface charge enough to be applicable for the electrophoretic deposition, we selected this method to fabricate porous cobalt oxide film. The morphology and crystal structure of the deposited films could be controlled not only by tuning deposition time but also by changing electrolyte solvent. The electrochemical activity of the obtained films was confirmed by cyclic voltammetry, showing distinct reduction and oxidation peaks at specific potentials. This finding strongly suggests the applicability of the cobalt oxide films as electrodes for thin film Li^+ ion batteries and supercapacitors.

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Phase Transformation Routes to Mixed Metal Oxide and Metal Oxide-Graphene Nanocomposites Applicable for Li Intercalation Electrodes

우명아, 황성주

이화여대 화학·나노과학과

Through the phase transformation of hydrotalcite-type Zn-M-layered double hydroxide (Zn-M-LDH; M = Fe, Co) at elevated temperatures, we were successful in synthesizing mixed metal oxide nanocomposites applicable for Li intercalation electrode. According to powder X-ray diffraction and X-ray absorption spectroscopic analyses, the heat treatment for the pristine Zn-M-LDH leads to the formation of mixed metal oxide nanocomposites composed of spinel ZnM_2O_4 and wurzite ZnO phases. Also, we were able to synthesize novel metal oxide-graphene nanocomposites via the heat-treatment for the restacked nanohybrid of exfoliated Zn-M-LDH nanosheets and graphene nanosheets. The hybridization between Zn-M-LDH and graphene could be achieved by electrostatic interaction between two oppositely charged nanosheets. The obtained mixed metal oxide and metal oxide-graphene nanocomposites were applied as anode materials for lithium ion batteries. Their electrode performances will be discussed in detail, along with their structural and physicochemical properties.

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Reversible Oxidation-Reduction Process at Al/$La_{1-x}Sr_xMnO_3$ Interface: a Computational Study for Resistance Random Access Memory Applications

이노도, *장윤희

광주과학기술원 신소재공학과, PIMS *광주과학기술원 신소재공학*

Metal/$R_{1-x}A_xMnO_3$/Metal (Metal = Al and Ag; R = La and Pr; A = Ca and Sr) capacitor like structures are promising candidates for resistance random access memory (ReRAM) devices. The origin of the resistive switching phenomenon in such devices, however, is still controversial. The reversible oxidation and reduction of the metal electrode due to the oxygen migration between the perovskite oxide and the metal electrode is one of the hypotheses on the resistive switching mechanism. In order to validate this hypothesis, in our previous study, we studied on the component materials [Al, AlO_x, $LaMnO_3$, and $La_{1-x}Sr_xMnO_3$ (LSMO)] of a promising ReRAM device material (Al/LSMO). Based on the structures and properties of these materials, in the current study, we built up two models of the Al/LSMO interface (Model I with LaO-terminated LSMO and Model II with MnO_2-terminated LSMO) and carried out density functional theory quantum mechanics calculations on their structure, energy, and electronic properties (total and partial density of states as well as I-V characteristics). The calculated energy barrier as well as the change in the density of states during the oxidation-reduction process indicates that the hypothesis is plausible especially at the interface between Al and MnO_2-terminated LSMO (Model II). Calculations with the surface reconstruction taken into account are on the way.

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Synthesis of nanoporous TiO_2 spheres and its photocatalytic activity

한송이, 성상도, 김상모, 이충혁, 이완인

인하대 화학과

We synthesized nanoporous TiO_2 spheres of various size ranges from 200 nm to 800 nm by hydrothermal reaction. The size of TiO_2 spheres was controlled by adjusting the ratio of H_2O & methylamine. The photocatalytic activity of the prepared nanoporous TiO_2 was measured by monitoring the degradation of 2-propanol in gas phase under UV light irradiation. The photocatalytic efficiency was compared as a function of the size of TiO_2 nanosphere, and the obtained photocatalytic trend was discussed in this study.

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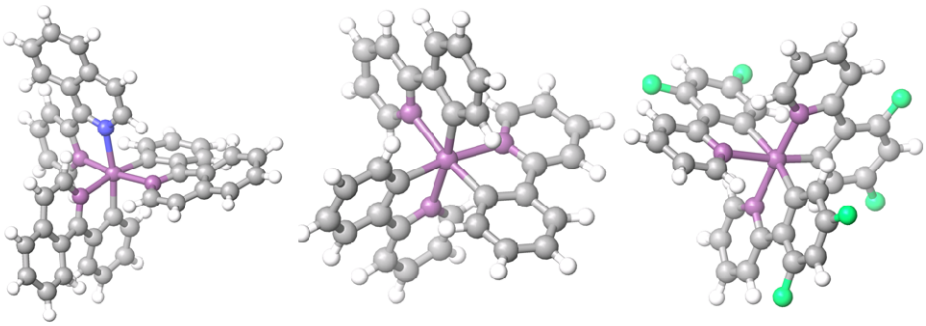
Red, Green, Blue Phosphorescent Iridium(Ⅲ) Complexes: a Time-Dependent DFT Study for Organic Light Emitting Diode Applications

유택희, 구자민, *장윤희

*광주과학기술원 신소재공학과, PIMS *광주과학기술원 신소재공학*

Phosphorescent Iridium(Ⅲ) complexes exhibiting both singlet and triplet excitations have high luminescence efficiency and have received a great attention as essential components of organic light emitting diode (OLED) devices. Various colors of light have been achieved by tuning the molecular structure of ligands in the complex. Ir(piq)3 [= tris(1-phenylisoquinoline) iridium(Ⅲ)], Ir(ppy)3 [= tris(2-phenylpyridine) iridium(Ⅲ)], and Flr(ppy)3 [= fac-tris{2-(4', 6'-difluorophenyl) pyridine-c', N} iridium(Ⅲ)] are representative examples of red, green, and blue phosphorescent materials widely used in OLED. In order to understand the relationship between the molecular structure and the phosphorescence properties of these complexes, we performed density functional theory (DFT) and time-dependent DFT (TDDFT) quantum mechanical calculations at the B3LYP/LACV3P** level. The calculated excitation energies were in good correlation with the color of the light emitted from these complexes, and we were able to understand the variation of excitation energies as a function of molecular structures in terms of the energy levels and orbital shapes of the frontier molecular orbitals (HOMO and LUMO levels).



Ir(piq)3 Ir(ppy)3 Flrppy3

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Electronic Structure of graphene, nitrogen-doped graphene, and their hybrid nanostructures.

김창현, 손용재, 박기영, 조용재, 김한성, 박정희

고려대 소재화학과

Graphene-a single layer of carbon atoms bonded into a two-dimensional hexagonal network-has been the subject of intense research since it was first isolated in free-standing form in 2004. Just as related forms of carbon such as fullerenes and nanotubes had previously been found to have many remarkable properties, so too did freestanding graphene. Among the most unexpected and promising of these were its thermodynamic stability, extremely high charge-carrier mobilities, and mechanical stiffness, the last of which distinguishes it from monoatomic metallic films. Doping is a common approach to tailor the electronic properties of the semiconductor materials, and thus nitrogen-doping would dramatically alter the electronic structure of grapheme. In the present work, we synthesized graphene and nitrogen-doped graphene using two different synthesis routes; chemical vapor deposition and solvothermal method. We employed X-ray photoelectron spectroscopy to reveal their electronic strictures depending on the nitrogen concentration. Furthermore, we synthesized various hybrid nanostructures with platinum and semiconductor nanocrystals, ands examine their electronic structures.

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Water Dispersible Nano-Graphite Hollow Spheres

박지은, *김성진

*이화여대 화학.나노과학과 *이화여대 화학과*

Here we report on the preparation and properties of a new carbon nanomaterial consisting of partially ordered graphite oxide layers. The graphitic multilayered nano hollows were synthesized by soft chemical route comprising hydrothermal glucose carbonization on the double shell Fe3O4@SiO2 templates. The oxidized graphitic nano hollows were found to possess remarkable properties including water solubility, photoluminescence and partial crystallinity. Owing to the their nano size, hollow structure, intrinsic optical properties and solubility, this material holds promise for biological and medical applications. The resulting nanocomposites were investigated by TEM, XRD, MAS 13C NMR, Raman, UV-vis-NIR and fluorescence spectroscopy.

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Size-controllable colloidal synthesis of thermoelectric material of Bi_2Se_3 nanocrystals

김희진, *이기중, 한미경, **김성진

*이화여대 화학나노과학부 *NMH school 12th **이화여대 화학과*

Many of bismuth chalcogenide materials have potential applications in thermoelectric devices. A simple route to the production of high-quality, monodispersive Bi_2Se_3 nanocrystallites is presented. Spherical Bi_2Se_3 nanoparticles with diameters of 5-100 nm have been successfully synthesized via a colloidal method. The reactions of bismuth acetate with the corresponding elemental chalcogen in 1-octadecence result in pure phases of the bismuth chalcogenide. In this method, the size of Bi_2Se_3 nanoparticles can be easily controlled by varying the synthetic parameters. The as-prepared nanoparticles were characterized by X-ray diffractometer (XRD), and transmission electron microscope (TEM/HRTEM) equipped with an energy-disperse X-ray spectrometer (EDS).

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발표종류: 포스터, 발표일시: 금 14:00~16:00

Pulsed Electrodeposition of Bi_2Te_3 Nanowires in AAO Template

김하영, 김성진

이화여대 화학과

We synthesized bismuth telluride (Bi_2Te_3) nanowires in the present of $Bi(NO_3)_3{\cdot}5H_2O$ and TeO_2 in 1.0 M HNO_3 using porous anodic alumina template by pulsed-potential electrodeposition method. The deposition potentials for Bi_2Te_3 nanowires were selected at about -200mV vs $Hg/HgCl_2$ (sat. KCl) and a pulsed-potential was used in a region of the CV where there is no current between reduction and oxidation potentials of the compound. The Bi:Te ratio of the wires was controlled by applied voltage and relaxation time. Samples were analyzed by PXRD, SEM and TEM. Uniformed size and high-density of Bi_2Te_3 nanowires were obtained and their thermoelectric properties are under investigation.

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Synthesis and Characterization of Metal Nanoparticles Decorated Tin Dioxide Nanowires

김솔, 김성진

이화여대 화학과

The controlled thermal evaporation growth (TEG) allows the achievement of wide band-gap rutile metal oxide(SnO_2) semiconductor nanowires with uniform composition and structural perfection. The growth morphologies are investigated via TEM, WXRD analysis and their optoelectronic properties relative to the oxygen-defect metal oxide(SnO_2) rutile nanostructures are discussed. Proven usefulness of this process for IV-VI(SnO_2) semiconducting compounds is presently extended to the morphological control of other nanosized wide band-gap semiconductors. Single-crystalline SnO_2 nanowires were further modified with various metal nanoparticles through self-assemblies. Poly(vinylpyrrolidone) as a stabilizer plays a key role in loading metal nanoparticles onto the surfaces of SnO_2 nanowires.

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Blue Light Emitting Materials Based on Anthracene Derivatives for OLEDs

ZHANGSHUANG, *CHENJUN, *조청화, **권순기, ***김윤희

*경상대 고분자 *경상대 고분자공학과 **경상대 나노신소재공학부 ***경상대 화학과*

The blue emitter materials were synthesized based on anthracene by the Suzuki coupling reaction. The thermal, optical and electronic properties of the materials were investigated by thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), UV-vis absorption, photoluminescence spectroscopy, cyclic voltammetry. The absorption maximum spectra of the materials were observed around 364, 382, 403 nm in solution state and 372, 395, 416 nm in film state. The PL maximum spectra of the materials were observed at about 453~462 nm in solution state and 460~484 nm in film state, respectively. The materials showed thermal stability of decomposition temperature at about 370 oC. And all these materials will be used in the fabrication of organic light emitting diodes (OLEDs).

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New Soluble OTFT Materials Based on cyclohexyl-alkyl Substituted Oligothiophene

CHENJUN, *ZHANGSHUANG, 박종원, **권순기, ***김윤희

*경상대 고분자공학과 *경상대 고분자 **경상대 나노신소재공학부 ***경상대 화학과*

Various cyclohexyl-alkyl substituted oligomeric semiconductors based on oligothiophene have been synthesized using Stille coupling. These materials exhibit increased solubility over their unsubstituted and hexyl-substituted counterparts . The cyclohexyl-alkyl group adds steric bulkiness at the periphery of the molecule that provides for improved solubility without having a detrimental effect on the molecular packing in the thin film phase. The thermal, optical and electronic properties of these oligomers has been investigated using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), UV-vis absorption, cyclic voltammetry. With the series of materials, a correlation between the size of the endgroup with respect to the size of the inner semiconducting core of the molecule is found to be an important factor in orienting the molecules in the thin film phase. The oligomers were showed highly thermal stability of decomposition temperature over 300 oC.

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Synthesis and Chatacterization of High Performance Semiconductors for OTFT

이동희, *김윤희, **권순기

*경상대 고분자공학과 *경상대 화학과 **경상대 나노신소재공학부*

This is one of the most promising small molecules for solution-processible organic semiconductors. The monomers were prepared with highly yields the key step of which is the acid-induced intramolecular cyclization reaction of aromatic methyl sulfoxides and the monomer is confirmed by elemental analysis, 1H NMR, UV absorption, photoluminescence (PL), and cyclic voltammetry (CV). The monomer showed a field effect mobility value as high and greater mobility.

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Preparation and Characterization of Mesoporous Mixed Oxide Materials by Hybridization of Highly Crystalline Colloidal SnO_2 Nanoparticles and Exfoliated Molybdenum Trioxide Nanosheets

심은하, 고지은, 정현

동국대 화학과

To fabricate a porous mixed oxide structures, the exfoliated layered molybdenum oxide sheets in aqueous solution was reassembled in the presence of surface modified SnO_2 nanoparticles. Two-dimensional nanosheets of orthorhombic molybdenum oxide were prepared by using ion exchange lithiation in the presence of an external oxidizing agent. Highly crystalline colloidal SnO_2 nanoparticles were obtained by thermal decomposition reaction of tin 2-ethylhexanoate in diphenyl ether and *n*-dodecylamine as surface capping agents. In order to obtain hybrid mesoporous structure, the hydrophobic SnO_2 nanoparticles were transformed into hydrophilic ones by simple ion exchange reaction with bipolar surfactant allowing dispersion of SnO_2 nanoparticles in water. The obtained SnO_2 nanoparticles have a diameter of around 3nm with unique size. Finally, the mesoporous mixed oxide materials were obtained by electrostatic reassembling route between negatively charged molybdenum oxide nanosheets and positively charged water soluble SnO_2 nanoparticles. X-ray diffraction (XRD), N_2-adsoption-desoption isotherms, inductively coupled plasma, Fourier transform infrared (FTIR) spectroscopy and thermal analysis were carried out to study the hybridizing process and the porous structure of hybrid mesoporous mixed oxide.

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Syntheses and Properties of Novel Metal-free Phthalocyanines derived from sterically hindered Phenols

이우성, 육심범, 김재필

서울대 재료공학부

Although phthalocyanines have continuously been the subjects of research due to their wide application, low solubility of phthalocyanines limited their applications. In this study, novel metal-free phthalocyanines containing alkyl and alkoxy substituted phenols have been designed and synthesized to enhance solubility. Phthalocyanines possess alkyl and alkoxy substituted phenols are forced by steric hinderance and non-planar conformation by steric hinderance greatly improved solubility of phthalocyanines in many organic solvents, especially in PGMEA commonly used in electronics industry. In addition , synthesized phthalocyanines have been characterized by UV-vis spectrometer , TGA and DSC methods.

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Hybrid Organic/Inorganic Single Nanorod Solar cell

유상훈, 김태헌, *조성환, 박성호

*성균관대 화학과 *성균관대 에너지과학학과*

This presentation describes the electrical properties of template-synthesized core-shell nanorods consisting of organic (polypyrrole) -inorganic (CdSe) domain. The organic domain works as a p-type semiconductor and the inorganic CdSe domain acts as a n-type semiconductor. The resulting heterojunction could separate exictons into electrons and holes when the white light was introduced. The efficiency was affected by polymer domain thickness, which is related to the effectiveness of exciton separation. We will show how the photovoltaic effect of single nanorod depends on the morphology of nanorod structures.

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Surface Plasmon Coupling for the Bimetallic Gold-Platinum Nanorods

정수진, 김현정, 홍순창, 박성호

성균관대 화학과

We report the surface plasmon coupling for the bimetallic gold and platinum nanorods. The platinum nanorod has rather weaker and broader LSP bands than gold nanorod. Surface plasmon of platinum nanorod can be coupled with gold blocks, when there are two distinct domains consisting of gold and platinum. The degree of coupling depends on the relative length of two metal domains. For instance, when the platinum portion is longer than gold, they do not show the surface plasmon coupling phenomenon. In this case, they just show the optical properties of each Gold and Platinum blocks. However, when the dominant block is gold, the free electrons on platinum coupled with the surface plasmon band of gold and exhibited optical behavior like a single gold nanorod.

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Synthesis of Gold Nanoparticles and Association of DNA-Gold Nanoparticles

고원배, 홍성규, 이정호

삼육대 화학과

This study examined the synthesis of gold nanoparticles using a non-ionic surfactant, polysorbate 80, and $KAuCl_4$in water. The gold nanoparticles, which were well dispersed in water, were analyzed by UV-vis spectroscopy and transmission electron microscopy (TEM). In addition, the SRY(sex-determining region Y) gene of the *Bos taurus* specific primer was designed, and this primer solution was mixed with the aqueous gold nanoparticle solution. The binding ability of DNA and gold nanoparticles was identified by polyacrylamide gel electrophoresis. The products of DNA linked with gold nanoparticles were also characterized by UV-vis spectroscopy and TEM

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Optical Property of Au Nanorods as a Refractive Index Sensor

정이든, 오민경, 백효진, 박성호

성균관대 화학과

Surface plasmon resonance (SPR) condition of metal nanoparticles depends on the size, shape, composition, and dielectric constants of the metal and the surrounding media. Herein, we electrochemically synthesized Au nanorods (NRs) with a diameter of 65nm and investigated their optical properties as a function of lengths and refractive indexes of dispersion medium. As the refractive index of solvent increases, all SPR bands associated with NRs red-shifted. The magnitude of band shift was different for transverse, longitudinal dipole, and quadrupole modes. The longitudinal dipole mode showed the largest sensitivity towards the change of refractive index of medium.

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Size-control of silica nanoparticles using mixed alcoholic solvents

임주현, 하신우, 이진규

서울대 화학부

Even though silica nanoparticles have been synthesized and used in various fields such as bioimaging, drug- and gene-delivery, and composite polymers, a solvent effect during the well-known Stöber method of hydrolysis-and-condensation of tetraethyl orthosilicate (TEOS) is not completely understood yet. We could control the size of silica nanoparticles in the range from 20 nm to few hundred nm by simple changes of solvent ratio and all the resulted silica nanoparticles were characterized by TEM, and FE-SEM. An alkoxy exchange reaction of TEOS in alcoholic solution seemed to play the major role of size control, and the several intermediates were characterized by GC-MS. We will discuss the mechanistic understandings of the relationship between solvent ratio and size of silica nanoparticles.

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Synthesis of dispersible Fe_3O_4 magnetic nanoclusters

문두식, 차진명, 이진규

서울대 화학부

We synthesized the Fe_3O_4 magnetic nanoclusters with a high magnetic response by the method of reducing $FeCl_3$ with $Na(O_2CCH_3)$ in ethylene glycol. By refluxing at atmospheric pressure, unlike the conventional autoclave method, we could enhance the dispersibility of nanoclusters by controlling the size smaller than 100 nm in a large-scale synthesis of few grams. For various applications, we overcoated the surface of the nanocluster with silica shell by inducing ligands on the surface and growing an amorphous or mesophorous silica by the modified Stöber method. The synthetic process of these magnetic nanocomposite particles and various applications will be discussed, where wettability, biocompatibility and easiness of surface modification are very critical.

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Electrochemical and In Situ Mn K-edge X-ray Absorption Spectroscopy Studies of TiO_2-pillared MnO_2 Nanohybrid

강주희, *백승민, 최진호

*이화여대 화학.나노과학과 *포항가속기연구소*

Porous structure of layered manganate pillared with titania nanoparticles has been realized by exfoliation and reassembling route. X-ray diffraction (XRD), cross-sectional transmission electron microscopy (TEM), and N_2 adsorption-desorption isotherms clearly show that the titania nanoparticles are successfully intercalated into the two dimensional manganate lattice with a high specific surface area (106 m^2 g^{-1}). The application potential of the present nanohybrid as a cathode material in a rechargeable lithium battery is also demonstrated by electrochemical experiments, where the enhanced discharge capacity (288 mA h g^{-1}) is observed compared to the theoretical value (210 mA h g^{-1}) of the physical mixture between MnO_2 and TiO_2. Finally, in-situ X-ray absorption spectroscopy (XAS) at Mn K-edge has been systematically examined to elucidate the changes in local symmetry and electronic structure for the TiO_2-pillared layered MnO_2 electrode during the first charge/discharge process. This study clearly demonstrates that the average oxidation state and local coordination environment around manganese ions in the electrode change reversibly during the redox reaction.

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Preparation and characterization of phosphorescent silica nanoparticles incorperated with cyclometalated iridium(III) complexes

김옥희, 하신우, 이진규

서울대 화학부

Phosphorescent Ir(III) complexes were modified by allylation and consecutive hydrosilylation of ligands, and covalently incorporated into the silica nanoparticles by a hydrolysis-and-condensation reaction with TEOS. These nanoparticles showed an excellent photochemical and thermal stability, and a very high luminescent efficiency probably due to the blocking of O_2 quenching and self quenching through the amorphous silica solid solution. Modified Ir(III) complexes were characterized by 1H-NMR, FAB-MS, and MALDI-TOF. Size and shape of silica nanoparticles containing Ir(III) complexes were confirmed by TEM and FE-SEM. Their luminescent properties were characterized by UV-Visible spectrometer and spectrofluorometer. Lifetime was measured by TCSPC (Time Correlated Single Photon Counting Spectrometer), and porosity and surface area were also measured. These luminescent nanoparticles could be used to many interesting application fields such as bioimaging, photonics, and optoelectronics where the long-term stability and the high luminescent efficiency are necessary.

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Exploring Cellular Uptake Mechanism and Intracellular Fate of Lipid-Gold Nanoparticle Hybrids in Gene Delivery

임원규, 남좌민

서울대 화학부

We devised lipid-DNA-AuNP (L-DNA-AuNP) hybrid-based gene delivery system for better transfection efficiency and reduced cytotoxicity by taking advantages of both AuNPs and liposomes as gene delivery vehicles. However, the mechanism of gene delivery using these hybrids has not been explored. Here, we studied their cellular uptake mechanism and intracellular fate using various techniques including endocytosis inhibitors, fluorescently labeled lipid molecules and TEM imaging of AuNPs

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Synthesis and Characterization of Novel Mesoporous Manganese Oxide by Hybridization of Colloidal Mn_3O_4 Nanoparticles and Exfoliated MnO_2 layers

이나라, 권법진, 정현

동국대 화학과

To fabricate a novel mesoporous manganese oxide structures, the exfoliated MnO_2 layers in aqueous solution was reassembled in the presence of surface modified Mn_3O_4 nanoparticles to produce a great number of mesopores and eventually a large surface area of manganese oxide. The exfoliated manganese oxide nanosheets were obtained by tetrabutylammonium cation into the layered protonic manganese oxide, $H_{0.13}MnO_2$•$0.7H_2O$. The colloidal monodispersed Mn_3O_4 nanoparticles were prepared by thermal decomposition reaction of $Mn(acac)_2$ in the presence of oleylamine. In order to obtain hybrid mesoporous structure, the surface of Mn_3O_4 nanoparticles was functionalized by cationic surfactant molecules. Finally, the mesoporous manganese oxide materials were obtained by electrostatic reassembling route between negatively charged manganese oxide nanosheets and positively charged Mn_3O_4 nanoparticles. X-ray diffraction (XRD), N_2-adsoption-desoption isotherms, Fourier transform infrared (FT-IR) spectroscopy and thermal analysis were carried out to study the hybridizing process and the porous structure of hybrid mesoporous manganese oxide.

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Synthesis and photophysical studies of Carbazole derivatives

유득남, 한만소, 채원석

대진대 화학과

We were synthesized multi-phenylated carbazole derivatives known as emitting and hole-transporting materials of OLED, such as (E)-9-(4-(2-(naphthalene-1-yl)vinyl)phenyl)-9H-carbazole(CZN), (E)-9-(4-(2-(naphthalene-1-yl)vinyl)phenyl)-9H-carbazole-3,6-dicarbonitrile(CZN$(CN)_2$), (E)-3,6-dibromo-9-(4-(2-(naphthalene-1-yl)vinyl)phenyl)-9H-carbazole(CZN$(Br)_2$). To obtain the electronic properties of products, the level of HOMO and LUMO was determined by a cyclic voltammetry. The band-gap energies and quantum yields were measured by using an UV/Vis and fluorescence spectrophotometer. The maximum PL peak of CZN, CZN$(CN)_2$, and CZN$(Br)_2$ appeared in blue region, each PL-λ_{max} was 422 nm, 417 nm, and 421 nm, respectively. Especially, The CZN$(CN)_2$ compound was shown high quantum yield.

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Synthetic melanin nanoparticles and their application of removing metal ions

김다정, 주국연, 이진규

서울대 화학부

Melanin is dark brown or black natural pigment with high molecular weight, which protects cells from high energy ultraviolet lays and scavenges radicals and heavy metal ions. By absorbing some of harmful heavy metal ions, it controls the toxicity of heavy metal ions in living systems. We have synthesized several artificial melanin nanoparticles having excellent stability in water, and investigated the ability to absorb the metal ions. Various melanin nanoparticles could be prepared from 2-(3,4-dihydroxyphenyl)ethylamine (dopamine) and 3,4-dihydoxyphenylalanine (DOPA) in the presence of oxidants. The shape, size, size distribution of melanin nanoparticles were characterized by SEM and TEM, depending on a concentration of precursor compounds, an amount of base, and a type of oxidants. The absorption ability of prepared melanin nanoparticles towards various heavy metal ions will be discussed.

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Scattering layer of nanoporous TiO_2 spheres for high efficiency dye-sensitized solar cell (DSSC).

유인경, 김경하, 장세희, 김학진, 이완인

인하대 화학과

We synthesized nanoporous TiO_2 spheres of various sizes and applied them as the scattering layer (SL) in dye-sensitized solar cell. For the synthesis of nanoporous TiO_2 spheres, the acetonitrile in ethanol, the mixture of H_2O and methylamine and the $Ti(O\text{-}iPr)_4$ in ethanol were mixed and stirred for 1 hr. Highly crystallized nanoporous TiO_2 spheres were formed by hydrothermal reaction at 230℃ for 5 hr and the size of TiO_2 spheres was controlled by adjusting the ratio of H_2O and Ti precursor. For the formation of main TiO_2 layer, the TiO_2 paste purchased from Dyesol Co. was employed while the nanoporous TiO_2 spheres with a size of 200 ~ 800 nm were used as SL. The increase in photovoltaic-conversion efficiency (η) is due to the efficient scattering effect of nanoporous TiO_2 spheres. Particularly, 450 nm-sized spheres induced the most efficient scattering efficiency.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 14:00~16:00

Synthesis and characterization of highly soluble perylene dyes for LCD color filter.

최준, 사공천, 김재필

서울대 재료공학부

There are growing requirements of development of dye - based LCD color filter because of its superior color purity and contrast ratio compared to pigment - based one. In order to enhance thermal and light stability of dyes, we have modified red pigment, perylene, into dyes by introducing steric hindrance with various bulky substituents at bay and terminal positions. The sterically hindered non planar perylene dyes were highly soluble in most organic solvents. The optical properties and thermal stabilities of the synthesized dyes were estimated with UV-visible spectrometer, TGA and DSC. It is notable that synthesized dyes were prevented aggregation with appropriate absorption spectra for red colorants of color filters.

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Direct Synthesis of Polymer Nanocapsules Containing Disulfide Linkages and Their Redox-Triggered Release of Encapsulated Substances

김은주, *정현태, 이지영, N. Selvapalam, **김기문

*포항공과대 지능초분자연구단, 화학과 *포항공과대 시스템생명공학부 **포항공과대 지능초분자 연구단, WCU 첨단재료과학부, 화학과*

Here we present a novel and straightforward synthetic approach to redox-labile polymer nanocapsules with disulfide bridges. The recently developed, direct synthetic approach was extended to another polymerization method based on the formation of multiple amide linkages using a cucurbit[6]uril derivative containing twelve amine groups. Polymer nanocapsules containing disulfide bridges, which are chemically labile and can be cleaved under reducing condition, were also directly synthesized by a reaction of cucurbit[6]uril derivative containing twelve amine groups and disuccinimidyl linkers having a disulfide bridge. The redox-labile polymer nanocapsules can also encapsulate dye molecules in their interior, and the shell of polymer nanocapsules consisting of host molecules were easily tailored using host-guest chemistry between the accessible CB[6] units on the surface and polyamine derivatives. Furthermore, the destruction of polymer nanocapsules triggered by a reducing agent such as dithiothreitol (DTT), which leads to release of encapsulated contents from the polymer nanocapsules was demonstrated. Finally, the redox-triggered release of a dye from polymer nanocapsules inside the cytoplasm of a target cell was also investigated.

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Synthesis of Very Stable Artificial Melanin Nanoparticles[발표취소 9-30]

주국연, 이유원, 이진규

서울대 화학부

Melanins are one of the well-known bio-polymers widely distributed in many part of the living organisms. They have attracted much attention as bio-materials because of their interesting properties with various biological functions and coloration. Partial understandings of the primary role of melanins in the bio-system have been reported as very diverse including photo-protection to absorb a broad range of the electromagnetic radiation, photosensitization, metal ion chelation, antibiotic, thermoregulation, free radical quenching and some involv[illegible]ll the reported synthetic melanins could not provide the particlar sh[illegible]e in water, which was a serious problem to control them in ana[illegible]We have synthesized eumelanin nanoparticles with controllable sizes ranged from 80 to few hundred nm by the neutralization of dopamine hydrochloride with NaOH and spontaneous oxidation of dopamine in the air. The shape, size, size distribution of melanin nanoparticles were characterized by SEM and TEM, depending on a concentration of dopamine hydrochloride, an amount of base, and a type of oxidants. All the characterization results and possible applications of artificial melanin nanoparticles will be discussed.

발 표 취 소

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Wet-chemical deposition of $CuInGaSe_2$ thin films for thin film photovoltaic device

차지현, 장주연, 이종현, 손현영, 정덕영

성균관대 화학과

Non-vacuum technique is described for the fabrication of a $CuInGaSe_2$(CIGS) absorber layer using solution precursor. The process was organized incorporation of metal and selenium, deposition of precursor and annealing as-deposited film, to form thin and dense CIGS films. The precursors containing Cu-, In-, Ga- and Se- related chemical were coated onto glass substrate by using the spin-casting method and then dried in air. The as-deposited layer showed amorphous Cu-In-Ga-Se phase, which were converted to chalcopyrite CIGS phase by heat treatment. Morphological, crystallographic and compositional analyses were performed at each step of the fabrication process by SEM, XRD and EDS. Hall measurement and electrical properties of CIGS thin film were investigated. Our facile method is expected to cost and fabrication time of CIGS thin film solar cells.

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Simple hydrothermal synthesis of Ru-CNT, Pd-CNT and Ag-CNT nanocomposites

송재희, 김승우

순천대 화학과

We describe a synthetic route for the high yield production of Ru-CNT, Pd-CNT, and Ag-CNT nanocomposite materials at low temperature. Pristine-MWCNT(MWCNT), thiol modified MWCNT(MWCNT-SH) were dispersed in an aq. SDS(Sodium dodecyl sulfate) solution. MWCNT, MWCNT-SH were mixed with metal ion precursors and refluxed at 100°C for 14 hrs. Only MWCNT-SH was densely decorated with corresponding metal naoparticles. Metal-CNT nanocomposites were characterized by UV-Vis, TEM, EDS, and XRD.

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Facile one step synthesis of Au, Ag, and Ru nanoparticles

송재희, 신철우

순천대 화학과

We describe a synthetic route for the high yield production of nanomaterials via a simple one step reduction process. Uniform Au and Ag, Ru nanoparticles were synthesized by simply mixing metal ion precursors and N,N-dimethylacetoacetamide, thenoyltrifluoroacetone, and 4,4,4-trifluoro-1-phenyl-1,3-butanedione.By simply varying the reaction temperature and the concentration of reducing agent, the shape and size of the resulting nanoparticles were easily controlled.

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Measurement of Heat-Dissipating Temperature of the Organic-Inorganic Composite Coated Electrogalvanized Steel Sheets

조두환

(주)포스코 기술연구소 표면처리연구그룹

The electrogalvanized steel sheets have been produced via organic-inorganic coating process on the zinc surface to enhance corrosion resistance and afford additional functional properties. Recently, LCD and PDP TV industry are inclined to adopt cost-saving materials such as steel panels instead of expensive materials to reduce production cost. Aluminum panels have widely used as an inner panels of TV because of high heat-dissipating property by thermal conductance. To replace this expensive aluminum, we measured heat-dissipating temperature of a varity of electrogalvanized steels sheets that coated organic-inorganic composite and discussed in detail.

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다공성 금나노입자의 표면증강라만 신호분석

이남훈, *박민규, 이치우, **유현웅

*고려대 신소재화학과 *충북대 공업화학 **한국표준과학연구원 미래융합기술부*

금속 나노입자의 표면 플라즈몬 공명 (surface plasmon resonance, SPR)의 독특한 광학적 성질은 전자탐지 시스템, 표면증강라만분광학(SERS)광소자의 개발 등 다양한 곳에 응용가능하다. 특히 귀금속나노입자 중 금나노입자는 가시광선영역에서 뚜렷한 표면 플라즈몬 공명대역(SPR band)을 가지며 우수한 표면 안정성을 가지므로 나노센서, 광전자 탐지 시스템, 약물전달 시스템 등에 다양하게 응용할 수 있다. 우리는 다양한 크기의 구(sphere)형태와 다공성입자(Porous gold structures)를 제조하여 FESEM 을 통해 제조된 나노입자의 크기와 표면 관찰을 확인하였고 마이크로 Raman 분광기를 사용해 SERS (surface-enhanced Raman scattering) 신호의 증강효과를 비교분석하였다. 이들 금나노입자는 고효율의 안정한 분자센서 플랫폼으로 이용가능하다.

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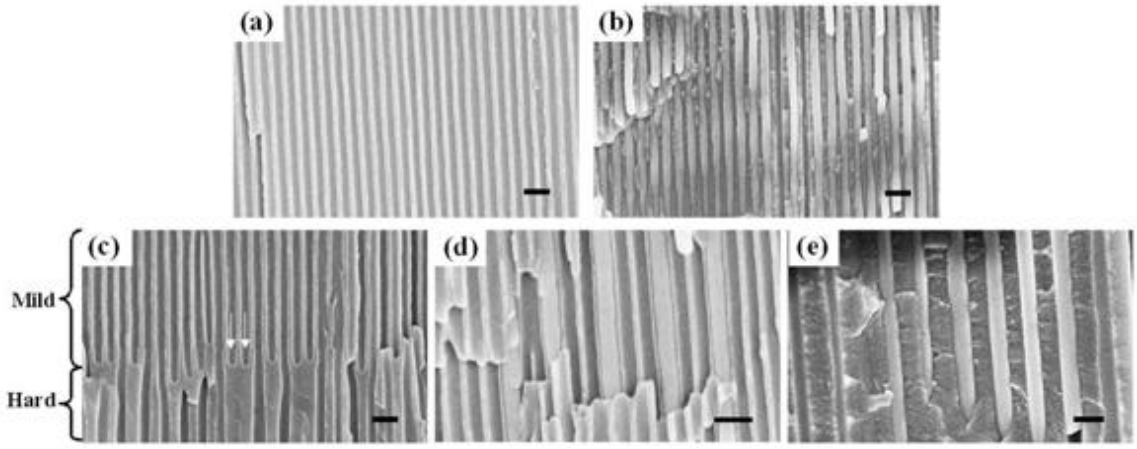
Synthesis and Characterization of Fe Nanostructures in AAM

정진승, 함성경, *이희옥

*강릉대 화학과 *한국기초과학지원연구원 강릉센터*

One dimensional ferromagnetic nanostructures, such as Fe, Co, and Ni has been attracted much attention because of their unique physical properties and potential applications in high density recording media and spin electronics. These materials have been synthesized by electron-beam lithography, self-organization-based mehod, or template-assisted electrodeposition. The template-assisted electrodeposition is simple technique to achieve highly ordered nanostructure arrays rather than other methods. We synthesized and characterized Fe nanostructures in two different AAMs; normal AAM anodized at 40V in 0.3M oxalic acid and mild-hard AAM anodized at 40-100V in 0.3 M oxalic acid.



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Hydroxylated CdSe/ZnS Nanocrystals for Biological Application

김용욱, 김원정, 윤혜주, 신승구

포항공과대 화학과

Zinc-blende CdSe/ZnS nanocrystals are hydroxylated with bifunctional thiol and then conjugated with biomolecules, such as biotin, DNA and hemagglutinin tag (HA-tag). Optical properties (absorption, emission and fluorescent lifetime) are characterized to examine the effect of bioconjugation on photoluminescence. For comparison, carboxylated CdSe/ZnS nanocrystals are prepared and conjugated with biomolecules. Both hydroxylated and carboxylated CdSe/ZnS nanocrystals are used in DNA chip detection as fluorescent probes.

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Synthesis of Tetrahexahedral Gold Nanocrystals with High-Index Facets

김도엽, *박오옥

*KAIST 생명화학공학과 *KAIST 생명화학공학과*

Metal nanocrystals with high-index facets are of great interest owing to their higher catalytic activity than those with low-index facets. The high-index facets, compared with low-index facets such as {111}, {100} and even {110}, have much higher density of low coordination number step atoms, ledges, and kinks, and therefore exhibit high activity for breaking chemical bonds. However, those facets will disappear during growth due to their relatively high surface energies since facets with high surface energies usually grow much faster than others. It is, thus, a challenging work to synthesize metal nanocrystals with high-index facets. In this poster, we report on the synthesis of tetrahexahedral gold nanocrystalas with high-index facets by a simple colloidal method which using *N,N*-dimethylforamide (DMF) both as solvent and reducing agent in the presence of poly(vinylpyrrolidone) (PVP) as a surfactant. The as-prepared THH gold NCs were single-crystalline and bounded 24 high-index {210} facets. They are expected to exhibit high catalytic activity since they are bound by high-index facets.

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Fabrication of Photo-induced Patterned Conducting Polymer Films Containing Gold Nanoparticles

허성, 김승빈

포항공과대 화학과

Novel multifunctional nanocomposite, conducting polymer poly(thiophene) coated gold nanoparticles including photoreactive moiety (P3OT-AuNPs-CI), is newly developed. We can obtain patterned P3OT-AuNPs-CI thin film using this fast and easy UV irradiation system. This new nanocomposite provides a convenient patterning technique, which can alternate the conventional lithography on the patterning process of conducting polymer, as well as sufficient conductivity for sub-micro and microscale electronic devices. We suggest that this new multifunctional nanomaterial can be applied to manufacture microelectronic devices and circuits, solar cells, diode, and chemical sensor.

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Determination of solubility parameter of multi-walled carbon nanotubes by inverse gas chromatography technique

임형준

서울대 재료공학부

Carbon Nanotubes(CNTs) have good electrical, mechanical and optical properties. They usually aggregate and take bundle shape, because of strong interaction and high aspect ratio of CNTs, which are obstacles to process. To adapt the CNTs for many potential practical applications, dispersion of CNTs in various solution or polymer composites is required. For predicting of the solubility and/or miscibility of many different chemical species, the solubility parameter is widely used. However, in the case of CNTs, there has been little information on such solubility parameters. This study thus tried to determine the solubility parameter, including the Hildebrand solubitily parameter and the Hansen solubility parameter, of as-produced multi-walled carbon nanotubes(MWNT) which produced by CVD and surface functionalized MWNT, using an inverse gas chromatography(IGC) technique.

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1,6-Bis(N-phenyl-p-R-phenylamino)pyrene화합물의 색 변화와 청색 도판트 물질의 적용

김주은, 위경량, 강상욱

고려대 소재화학과

소자 구조의 최적화와 고효율 청색 형광 재료의 개발은 현재 많은 연구자들에게 관심의 대상이 되고 있다. 이번 연구에서는, 효율적이고 진한 청색 pyrene 유도체를 얻기 위해서 electron-withdrawing (EW) 과 -donating (ED) 그룹을 이용해서 pyrene 에 체계적인 전자밀도 변화를 주었다. 최종 화합물인 1,6-bis(N-phenyl-p-R-phenylamino)pyrenes, 2R, 은 N-phenyl-p-R-phenylamines 유도체 와 1,6-dibromopyrene 을 Buchwald-Hartwig coupling 반응을 이용해서 합성하였다. 전 색체를(454 nm ~ 620 nm) 보이고 있는 2R 의 광 물리적 특성은 diarylamine 에 치환된 EW 과 ED 정도에 따라서 잘 일치 하고 있다. 특히, 가장 진한 청색을 나타내고 있는 2CN 화합물의 경우 2.85 × 108 s-1 의 높은 radiative rate 상수를 보여 주고 있을 뿐 만 아니라 높은 형광 양자 수율을 (79%) 보여주었다. 최종적으로 고효율 진한 청색 소자를 만들기 위해 2CN 을 도판트로 사용한 다층 소자를 제작 하였고, 최대 전류 효율이 3.98 cd/A 이고 색 좌표가 x = 0.14, y = 0.10 인 소자 결과를 얻을 수 있었다.

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Polymer-Protected DNA-Au Nanoparticle Conjugates with High Solubility and Stability

임동권, 남좌민

서울대 화학부

Here, we developed a polymer-based method to prepare DNA-modified AuNP conjugates with a high solubility and stability in various environments. We found out that PVP polymers form layers around DNA-AuNPs to greatly enhance particle stability at very low pH, high temperature and high salt concentration. Moreover, these PVP-DNA-AuNPs exhibited a long-term stability even under 60 ˚C and pH 2.5. In addition, the PVP layer on DNA-AuNP enabled the DNA-AuNP conjugates to be soluble in hydrophobic organic solvent. Finally, the PVP protection layer could be readily removed with a simple chloroform washing procedure for the effective use of AuNP surface-modified DNA as biosensing applications. We believed that the PVP-coated DNA-AuNP conjugates could expand the applications of DNA-AuNPs, including artifical coding applications in various conditions and environments, and our strategy opens revenues of improving probe stability using a polyrmer-based probe protection strategy.

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Photoinduced Energy Transfer Efficiency of Tunable Phosphorescence Iridium Dendrimers Bearing Carbazole Groups

황아름, *손호진, **조대원, *고재중, *강상욱

*고려대 신소재화학과 *고려대 소재화학과 **고려대 광전자신소재연구소*

We have investigated the phosphorescence properties of dendrimers (Gn is the dendrimer generation number) containing four different luminophores, namely nonconjugated dendritic iridium(III) based on tunable pyridine based ligands. These dendritic iridium(III) complexes exhibiting tunable photoluminescence from blue to red were obtained. In this system, host/dopant ratio can be systematically adjusted by varying dendritic generations. The light-harvesting ability of Ir(III)(C^N)2-(Gx, x = 1-3)-CBP increases with the number of energy donor phenyl carbazole units. Photoluminescence excitation measurements showed that energy could be transferred efficiently from the dendrons to the core in blue series. The energy transfer efficiency is higher in blue series than green and red series. The detail optical study, such as excited-state life time, low temperature PL, transient UV/PL, and quantum efficiency, showed the efficient S-S and T-T energy transfer from the dendritic carbazole unit to the core acceptor.

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Ligand-Dependent Photoluminescence Properties of Zinc-Blende CdTe-based Core/Shell Nanocrystals

정화준, 김원정, 임성준, 신승구

포항공과대 화학과

Zinc-blende CdTe-based core/shell nanocrystals such as CdTe/CdS and CdTe/CdS/ZnS are synthesized from non-coordinating solvent systems using a layer-by-layer shell growth technique. Structures of core/shell nanocrystals are analyzed by both high resolution transmission electron microscopy and powder X-ray diffraction measurements. Effects of the nanocrystal band structure and the surface states on the photoluminescence properties of nanocrystals are studied by observing the absorption and emission spectra and the fluorescence lifetimes of core/shell nanocrystals in solution depending on the shell type and the surface ligand composition.

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Dye-Sensitized Solar Cell with Multi-layered TiO_2 Structures

황윤화, 김소영, 표명호

순천대 화학과

Since gratzel et al. discovered efficient solar energy conversion based on TiO_2/Ru complexes/redox couple, Dye-Sensitized Solar Cell (DSSC) has been extensively studied due to its easy-to-fabricate, colorful appearance, and transparency with reasonable power conversion efficiency. Many factors can determine the cell's performance, but one of the important determinants is the nanoprous structure of TiO_2. In this work, we prepared multi-layered TiO_2 films, each layer of which consists of different size of TiO_2 particles. The improvement of cell performance was observed by optimizing the composition of TiO_2. In addition, SiO_2 insulating layers were introduced as a bolcking layer on FTO by the control of thermal decomposition of PDMS. It was found that SiO_2 can effectively reduce the electron recombination by blocking the diret contact between the redox electrolyte and the conductive FTO surface.

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Polymer photovoltaic cells based on low band gap polymer-wrapped single-wall carbon nanotubes

표명호, *정규관, 배은경

*순천대 화학과 *전북대 과학교육학부*

Single-wall carbon nanotubes (SWNT) have been utilized with light harvesting polymers in photovoltaic cells since favorable energy levels and high electron affinity of SWNT can lead to efficient charge separation at the polymer/SWNT imterface. In addition, incorporation of SWNT to polymer can facilitate SWNT's unique morphological properties such as high surface area and extremely low percolation threshold (0.1 ~ 0.2%), which are also prerequisites for efficient exciton dissociation and fast charge carrier transport. In this work, we present that SWNT wrapped with a low band gap polymer can function as an efficient charge separation layer. The band gap and levels were confirmed by cyclic voltammetry and UV-Vis-NIR. The existence of polymer on the surface of SWNT was -wrapping was also confirmed by UV-Vis-NIR, FT-IR, and FESEM. After blending low band gap polymer-wrapped SWNT with regioregular poly(3-hexylthiophene), the performance of the whole cells was compared with that of SWNT/poly(3-hexylthiophene) to elucidate the role of low band gap polymer in between electron donors and acceptors.

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Dendritic Modification of Organic Dyes for the Production of Hydrogen under Visible Light

이수현, *박이슬, **손호진, ***조대원, **고재중, *최원용, **강상욱

*고려대 신소재화학과 *포항공과대 환경공학부 **고려대 소재화학과*
****고려대 광전자신소재연구소*

A hydrophilic group substituted organic dye, (E)-3-(5'-(4-(bis(4-(2,5,8-trioxanonyl)phenyl)amino)-phenyl)-2,2'-bithiophen-5-yl)-2-cyanoacrylic acid (HOD-3), has been synthesized, and the effect of hydrophilic group on its performance in hydrogen production on platinized TiO2 particles (Pt/TiO2) and Dye Sensitized Solar Cells (DSSCs) has been investigated. With the adsorption of HOD-3 to Pt/TiO2, we observed increased miscibility between photocatalyst and aqueous solvent, contrary to a non hydrophilic group substituted dye (ref) which displays a large aggregate themselves. As a result of good miscibility with water, in a standard photo-induced hydrogen production system HOD-3 exhibited an enhanced photocatalytic activity when compared to ref, indicating facile proximity of proton source to the reduction center (Pt). In addition, we studied the effect of hydrophilic substitution in DSSCs.

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Polypyridyl Bridging Ligand를 포함하는 Dendritic 이핵체 (Ir-Pt) 화합물 시리즈의 빛에 의한 효율적인 에너지 전달: 합성, 분석, 광물성 연구

민경태, *조대원, 고재중, 강상욱

*고려대 소재화학과 *고려대 광전자신소재연구소*

Ir(III)을 기본으로 하는 광촉매 시스템은 리간드와 치환체효과에 의해 조절이 가능한 전자적 특성의 큰 다양성으로 많은 관심을 받고 있다. 덴드리머를 이용한 효율적인 광흡수 시스템(Ir-PtGx, x = 0-2)을 개발하기 위한 노력으로서 새로운 platinum 이핵체 시리즈 화합물[(dfppy)2Ir(BL)PtCl2](PF6)2 을 합성하고 확인하였다. 새로운 화합물들의 흡수스펙트럼은 이핵체 시스템 고유의 특수한 성질을 나타내었으며 이러한 시스템의 여기된 상태에서의 MLCT (metal-to-ligand charge transfer)특성은 전자 이동에서의 빛의 흡수와 광화학적 반응의 성질의 연구를 가능케하였다. 흡수 스펙트럼은 It-Pt 화합물내에서의 효과적인 광흡수를 위한 덴드리머 작용기로부터 빛을 감지하는 core sensitizer 에서 일어나는 빛에 의한 효율적인 S–S 와 T–T 의 에너지 이동을 보여주며, 이는 carbazole unit 이 효과적인 광흡수체이며, core Ir sensitizer 는 에너지 집합체로서의 기능을 하고 있음을 보여준다. 이러한 결과는 Ir sensitizer 와 reactive center 인 Pt 사이의 보다 효과적인 광유발 전자의 이동을 위한 이핵체 전자전달시스템으로서의 한 모델을 제시한다.

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Antibody Structure and Activity Test Assay Using Gold Nanoparticle Probes

우정림, 임동권, 남좌민

서울대 화학부

Evaluating structure and activity of antibodies of interest in a simple and rapid manner would be quite useful. Herein, we introduce a gold nanoparticle probe-based antibody structure and activity test method without using complicated and expensive instruments. In this assay, the conformational change of surface-modified antibodies affects the stability of gold-nanoparticles and results in salt-induced aggregation. The degree of nanoparticle aggregation was measured and quantified via color change of the gold nanoparticle probe solution. This strategy should be applicable to all kind of antibodies and an easy, rapid and cheap method for detecting the conformational change of proteins.

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Electrofluidic Biosensor Based on Patterned Lipid Bilayer

이영광, *남좌민

*서울대 화학과 *서울대 화학부*

Here, we fabricated patterned supported lipid bilayer (SLB) substrate and electrofluidically controlled the flow of charged, fluorescent lipids for the development of electrofluidic lipid membrane biosensor. Electrophoretic accumulation of the charged lipid components allows one to obtain significant signal amplification in a controlled manner. The resulting fluorescence distribution of TR-DHPE was quantitatively evaluated by epifluorescence microscopy in a straightforward fashion. Current detection limit of our electrofluidic sensing platform is 10 fM (>10,000 improvement over conventional optical detection methods) and it works in a range from 10 fM to 10 nM.

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Melamine mediated synthesis of silver/organic nano-needle and its application

박금환

KAIST 생명화학공학과

We have investigated the generation of silver nanoparticles embedded organic nano-needle particles firstly by introducing melamine. Melamine and silver nitrate can be made linear chain with forming 1:1 complex, and this phenomenon might be the reason for being generated linear particles. This study shows that the shape of synthesized particles can be affected by the structure of organo-metal complex. Surprisingly, the melamine plays curial role to form nano-needle in early reaction stage but the organic frame disappeared in final reaction stage leaving only silver nanoparticles. This disappearing organic part seems to be imine and amide mixture and we confirmed that by IR spectrum. This simple synthetic route will be one protocol to make one dimensional metal-organic nanocomposite. In addition we found that these particles could be use for Nonvolatile memory. Reported studies about polymer/metal nonvolatile memory have been using conductive polymer such as polyaniline decorated with metal nanoparticles. While these methods need two steps for fabrication of materials, our process needs only one step because the synthesized particles have the character for nonvolatile memory. Not only far easier process, but smaller size is another merit for fabrication of device. Without any process, we could fabricate nano-scaled nonvolatile memory device and confirmed write-read-erase-rewrite cycle.

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Characterization of chemical sensor arrays using functional dyes for the detection of unknown VOCs

성은숙

한국화학연구원 산업바이오화학연구센터

공기중의 VOCs(휘발성 유기물)는 인체에 유해하기 때문에 그것을 검출하고 농도를 알아낼 수 있는 센서의 연구는 중요하다. 공기 중에 포함된 저농도의 VOCs 를 검출하고 육안으로 쉽게 확인할 수 있는 Colorimetric sensor array(CSA)를 제조하기 위하여, VOCs 와 반응하여 강한 색변화를 일으키며 공기 중 습도에도 안정한 화학감응성염료인 Metalloporpyrins, pH indicator 를 sensor 물질로 사용하고 이런 화학감응성염료를 용매에 용해하여 revere-phase silica gel plate 에 패터닝하였다. VOCs 에 의한 CSA 의 색변화 패턴을 연구하기 위하여, Aldehyde, carboxylic acid, amine, phosphine, thiol 등과 같은 다양한 VOCs 를 농도범위 500ppb 에서 200ppm 까지 실험하였다. VOCs 노출 전과 후의 CSA 의 색변화 차이는 색변화 정량화 장치를 이용하여 조사하였으며, 이러한 과정을 통하여 미지의 VOC 검출과 이들의 농도 결정에 필요한 데이터베이스를 얻을 수 있었다. CSA 는 여러 분야에서 발생하는 VOCs 을 잘 검출할 수 있고 사용이 간편하여 경제적으로 경쟁력이 있을 것으로 기대된다.

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Synthesis and Bio-application of Novel Semiconductor Nanocrystals

유화성, *김창해

*고려대 화학과 *한국화학연구원 화학소재연구단*

Fluorescent semiconductor quantum dots (QDs) are a novel class of fluorescent probe whose unique optical properties suggest that they are superior to conventional organic dyes for many biological applications. QD properties include high quantum yields, broad absorption spectra, narrow symmetric, materials- and size-dependent emission spectra, and excellent resistance to photobleaching.1 Because of these characteristics, QDs are an interesting alternative to organic fluorophores in some biotechnological and biomedical applications.2 These attractive fluorescence properties are particularly appealing for the visualization of cellular processes, as they can potentially facilitate long-term and multicolour labeling of both fixed and living cells.

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3, 3'- Dithiodipropionic acid as co-adsorbent along with poly(ethyl thieno[3,4-b]thiophene-2-carboxylate) for efficient NIR sensitization of TiO_2 photoelectrode

Viswanathan S. Saji, 표명호

순천대 화학과

Recently, organic dyes have attracted considerable research interest as potential substitutes for the Ru-based metal-ligand counterparts for sensitization of nanocrystalline photoelectrode in dye sensitized solar cells; as they are attractive in terms of easy availability, cost and environmentally friendly nature. When considering the quantum of research done in organic dyes, reported information available on conjugated polymer based dyes is limited. It has been proved that the possible polymer aggregation onto the photoelectrode can be minimized by effective use of small molecular weight co-adsorbents. In the present investigation, we have employed a newly synthesized thieno[3,4-b]thiophene based polymer, having near infra red region (NIR) absorption as the sensitizer. NIR sensitization of the nanocrystalline TiO_2 electrode can significantly improve the cell efficiency. 3,3'-dithiodipropionic acid was investigated as a novel co-adsorbent. Photoelectrodes sensitized with the NIR dye, with and without co-adsorbent, were characterized using UV-Visible spectroscopy, SEM, TEM and XRD. The photocurrent and photovoltage were measured using a Potentiostant/Galvanostat under AM 1.5 simulated sunlight at 100 mW cm^{-2}. The results of the study revealed that the co-adsorbent in optimum composition significantly enhanced the polymer adsorption onto the nanocrystalline electrode which further enhanced the current conversion efficiency. The study proved that 3,3'-dithiodipropionic acid is a promising co-additive that enhanced the conjugation length of the adsorbed polymer. The newly synthesized polymer dye possesses significant promise as an efficient NIR sensitizer in DSSC applications.

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Low-Band-Gap Conjugated Polymers Based on Thiophene for Organic Photovoltaic Cell

정연수, 조연경, 표명호

순천대 화학과

Over the past decades, solar cells based on organic semiconductors or hybrid organic/inorganic composites have been very attractive topic because of the advantages which include low fabrication cost, simple fabrication process and flexibility. Although their photovoltaic (PV) performance were very poor than other inorganic based solar cell, recent studies have reported improved PV performance with low-band-gap conjugated polymer. In thisk work, composites of poly(3-heylthiophene) (P3HT) with poly(thieno[3,4-b]thiophene-2-carboxylic acid) (PTTA) or poly(3-thiophenecarboxylic acid) (PTCA) on TiO_2 nanoparticles were investigated by UV-visible spectroscopy (UV-Vis), photoluminescence (PL), fourier transform infrared absorption (FT-IR), thermo gravimetric analysis (TGA) and field emissionscanning electron microscope (FE-SEM). Chemically prepared PTTA and PTCA were absorbed on TiO_2 nanoparticles for the improvement of the electron transfer process from thiophene polymers to TiO_2. PTTA and PTCA were expected to mediate electron transfer, resulting in efficient charge separation between P3HT and TiO_2. We also examined how these polymers affect the performance of organic photovoltaic (OPV) cells.

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Synthesis and Characterization of New Thin Film Materials Based on Epitaxial Growth of Metal-Organic Porous Materials

윤민영, *이다미, 윤경원, 정민선, **김기문

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Recently an application area of thin film has expanded drastically because of a various interesting properties of the thin films according to consisting materials. There are many reported thin film materials, such as metal oxides, polymers, organic materials according to their functions. However, even though metal-organic polymeric materials are one of the hot topic materials due to their wide range of application area, such as catalyst, separation, and storage, there has not been hardly reported metal-organic hybrid crystalline thin film. Here we present new route to synthesize new family of thin film materials through epitaxial growth of metal-organic porous materials (MOPMs). New 2-D porous MOPM crystals have grown on gold surface. To prevent random orientation of crystalline materials, we have designed and prepared amine terminated gold SAM and grown crystalline MOPMs epitaxially on gold SAM. The epitaxial growth and thickness of the crystalline thin films have been characterized by XRS of Pohang Accelerator Laboratory. Details of the thin films syntheses and their characterization will be presented.

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Syntheses Characterizations and Applications of Metal Oxide Nanoparticles

한종석, 황풍곡, 정동운

원광대 화학과

A flood of research has been made to develop and characterige Titanium Oxide(TiO2) for Photocatalyst since it absorbs Ultra-violet light under 400nm. N, S substituted TiO2's were synthesised and substituted and characteriged in this work.

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Preparation of Bimodal Mesoporous Silica with High Pore Volume by Using Inorganic-Organic Templates

문기홍, *김호건

*한양대 응용화학과 *한양대 화학과*

Mesoporous silica with bimodal pore size distribution was prepared using Fe_3O_4 particles as inorganic sacrificial template. Sodium oleate and cetyltrimethylammoniumbromide (CTAB) were used as a dispersant and a structure-direct agent respectively in the first step of reaction. In the second step tetraethylorthosilicate (TEOS), was used as an silica source under acidic condition. Organic residue and Fe_3O_4 were removed through heat treatment and acid leaching process. Silica with relatively high pore volume of 3.3 cm^3/g was obtained and the pore size of silica showed bimodal distribution at about 7nm and 30nm.

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탈염소화 촉매반응을 통한 사슬형, 고리형 유기규소화합물의 합성 및 액상 수소저장물질로서의 응용

한원식, *김민혜, **정일남, 고재중, 강상욱

*고려대 소재화학과 *고려대 신소재화학과 **제이에스아이실리콘(주) 사장실*

최근 인 촉매를 이용한 새로운 유기규소화합물의 합성방법을 발견하였으며 이 연구결과를 토대로 간단한 방법을 통해 사슬형, 고리형 유기규소화합물의 합성에 성공하였다. $HCl_2SiCH_2SiCl_3$ 와 인 촉매를 함께 반응하여 사슬형 화합물인 $SiH_2(CH_2SiH_3)_2$ 와 고리형 화합물인 $(CH_2SiH_2)_3$ 를 합성하였다. 합성된 두 가지 화합물은 $LiAlH_4$ 를 통해 높은 수율로 환원할 수 있으며 환원된 두 가지 화합물 $SiH_2(CH_2SiH_3)_2$ 와 $(CH_2SiH_2)_3$ 의 액상수소저장물질로서의 응용에 관한 실험을 진행하였다. 메탄올과의 반응을 통하여 각각의 화합물은 6 당량, 8 당량의 수소를 정량적으로 방출함을 확인하였다. 각각의 화합물은 전제 반응에서 3.76 wt%, 4.30 wt%의 수소저장용량을 가졌으며 수소 방출 시 14.23, 8.23 kcal/mol 의 활성화에너지를 가졌다. 또한 수소 방출 후 생성된 실라놀화합물은 $LiAlH_4$ 를 통하여 정량적인 재생이 가능하였다.

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발표종류: 포스터, 발표일시: 금 14:00~16:00

청색 인광 OLED를 위한 고효율 전자 수송 재료의 개발: Bis(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)dimethylsilane의 합성, 광물리적 특성 연구, 그리고 소자제작

위경량, 김애리, 강상욱

고려대 소재화학과

최근 들어, Fir6 (ET =2.82 eV)와 같은 진한 청색 도판트에 맞는 호스트 물질은 여러 개 보고가 되었지만, 여전히 넓은 밴드 갭을 가지는 HTL 물질과 ETL 물질은 많이 보고 되고 있지 않다. 이 연구에서는, 넓은 에너지 갭을 가지면서 뛰어난 열적 안정도와 높은 전자수송 물질을 가지는 청색 인광 OLED 용 ETL 물질을 개발하기 위해 실리콘 원자를 3,4,5-triphenyl-1,2,4-triazole 분자 사이에 넣었다. 최종화합물인 bis(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)dimethylsilane (SiTAZ)은 2 당량의 3-(4-lithiumphenyl)-4,5-diphenyl-1,2,4-triazole (LiTAZ)과 dichlorodimethylsilane 을 이용해서 치환반응으로 합성 하였고, 합성된 SiTAZ 는 2.84eV 의 높은 triplet energy, 115°C 의 높은 열적 안정도, 그리고 1 x 10-4cm2 V-1 s-1 의 높은 전자 이동도를 보여 주었다. 최종적으로 고효율의 진한 청색 소자를 만들기 위해 SiTAZ 을 ETL 물질로 사용한 다층 소자를 제작 하였고, 최대 외부 양자 효율이 16.2 % 이고 색좌표가 x = 0.16, y = 0.23 인 소자 결과를 얻을 수 있었다.

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Localized surface plasmon resonances of colloidal Cu nanorprisms

박영석, 권태정, 채희권

서울대 화학교육과

Localized surface plasmon resonances (LSPRs) have been observed from nanostructured particles and cavities composed of noble metals such as Au, Ag, Cu, and Pd. Cu nanostructures have been studied due to their characteristic LSPRs, and especially, anisotropic Cu nanoparticles have shown intense dipolar plasmon resonances. Herein, we describe a microemulsion strategy for preparation of colloidal Cu nanoprisms. As a result, intense dipolar resonances were observed by monitoring the optical response of resulting Cu nanoprisms. To explain the relation between resulting morpologies and corresponding optical response, the simulated optical spectra were calculated for the comparison between measured and simulated optical spectra. Spectral enhancement and red-shift of LSPRs were confirmed from measured and simulated spectra with anisotropic control of resulting mophologies.

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A miniaturized reference electrode based on a biocompatible epoxy membrane: Voltammetric determination of dopamine in biological samples

조백현, 권기학, 김승기, *Robert K. Franklin, **Richard B. Brown, 차근식, 남학현, 신재호

*광운대 화학과 *Departmen of Electrical Engineering and Computer Science, University of Michigan, U.S.A. **College of Engineering, University of Utah, U.S.A.*

The potential of Ag/AgCl electrodes caused commonly used in electrochemical measurements as a reference electrode. However, Ag/AgCl reference electrodes have a low biocompatibility in the whole blood because the electrode can cause adverse response from blood such as clot formation. So, an epoxy membrane is introduced to improve biocompatibility. The immobilized quaternary ammonium moiety are known to behave as an anion-exchanger and to induce anionic potential response across the membrane. Therefore, the epoxy-based Ag/AgCl electrode can be used chloride sensors. The novel epoxy-based Ag/AgCl electrode exhibits a Nernstian potentiometric slope of -51.89 mV/dec. in the whole blood. Cyclic voltammograms does not change over time when the electrode is immersed in the whole blood sample for 24 hours. In conclusion, we developed a novel epoxy-based chloride sensor with an improved biocompatibility. This sensor will take a role of a reference electrode for determination of sensing analytes in blood.

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Potentiometric nanopore oxygen sensors using an electrochemically etched cobalt wire

조백현, 김승기, 강영재, *강태영, 신재호, 차근식, 남학현

*광운대 화학과 *(주)아이센스 부설연구소*

Determination of oxygen levels (PO_2) in blood is critically important in the clinical and physiological fields. For several years, many electrochemical oxygen sensors have been reported, which mostly employed amperometric detection techniques. Recently, a potentiometric oxygen sensor was proposed by Meyerhoff group based on a cobalt electrode. The potentiometric technique does not change the local concentration of oxygen during measurements, making this type of sensors more advantageous than the conventional amperometric sensors. In addition, since potentiometric signals are dependent on the electrode size, the miniaturization of oxygen sensors may be feasible. The potentiometric oxygen sensor is based on measuring a mixed potential at the surface of the cobalt metal. The mixed potential comes from the slow oxidation of cobalt and simultaneous reduction of oxygen at the cobalt surface. In this work, the cone-shape cobalt wire is prepared and studied for the detection of oxygen level in the microscopic region. This miniaturized oxygen sensor has a great potential in the biological application including monitoring of cellular respiratory activity. But, this oxygen sensor has a problem as a heat treatment in the fabricating of electrode. So, the epoxy membrane is applied to solve the problem. In this presentation, we report on an improved potentiometric oxygen microsensor fabricated on a novel nanopore electrode with electrochemically etched cobalt wire.

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Influence of Crystallinity on Ion Conductivity of PEO-based Solid Electrolytes

한아름, 신재섭, *김석, **박수진

*충북대 화학과 *부산대 화학공학과 **인하대 화학과*

Polymer blends of poly(vinyl chloride)(PVC)/poly(ethylene oxide)(PEO), were prepared by a solution casting technique for solid electrolytes. A binary mixture of carbonate solvent was used as a plasticizer, and lithium perchlorate ($LiClO_4$) as a salt. The morphology, ionic conduction and mechanical properties of the polymer electrolytes were characterized by SEM, FRA, DSC, and UTM experiments. As a result, the mechanical properties of polymer electrolytes didn't show significant change up to 5 wt.% even though the phase separation of the composites. The ionic conductivity of the polymer electrolytes containing 2 wt.% PVC showed the highest ionic conductivity, 2.35 x 10^{-3} (S/cm) at 25℃. This ion conductivity was dependent on the reduced crystallinity by adding PVC moieties.

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Enhancement of Ionic Conductivity of Solid Electrolytes PMMA/PEO Membranes for Lithium Batteries

한아름, 신재섭, *김석, **박수진

*충북대 화학과 *부산대 화학공학과 **인하대 화학과*

To investigate the effects of blending concentration, PMMA was incorporated into a PEO-based polymer blend and thin electrolytes were prepared by solution casting technique. A polymer electrolyte of a blend of poly(methyl methacrylate) and poly(ethylene oxide) as a host polymer, the mixture of carbonate as a solvent, and $LiClO_4$ as a salt was studied. DSC data indicate that the amorphous nature of solid polymer electrolyte (SPE) increased with PMMA concentration. Impedance spectra of SPEs have also been made to provide an idea about the phase boundary resistance of the polymer electrolytes. As a result, the ionic conductivity of the polymer electrolytes containing 20 wt.% PMMA showed the highest ionic conductivity, 5.80 x 10^{-5} (S/cm) at 25℃. However, when PMMA content exceeds 20 wt.%, the ionic conductivity was decreased due to the slow ionic transport through the phase separation.

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Determination of Humic Acid in Soil by Employing a Potentiometric Polyanion Sensor

정연호, 강영재, *임우진, *이상은, 신재호, 차근식, 남학현

*광운대 화학과 *한경대 식물자원과학과*

Humic acid is one of major organic components in soil, and is formed by microbial degradation of plants and animal bodies. Humic substances consist of phenolic and carboxylic groups around the aromatic and aliphatic backbone. The presence of humic acid in soil significantly improves the bioavailability of physiologically important inorganic cations (e.g., Ca2+, Mg2+, and Fe2+) required for growth of plants. Indeed, the chelating effect of humic acid is able to prevent those cations from being washed away from the soil. Therefore, the determination of humic acid concentration in the soil samples is an important process to assess the quality of soil in the agricultural aspect. The standard method for the humic acid analysis is based on the measurement of total organic carbon (TOC) in the soil samples, which is not suitable for the on-site analysis. Herein, we present a simple and fast approach to determine humic acid in soil by employing a potentiometric polyanion sensor. Humic acid is deprotonated under the basic conditions (typically pH > 12), forming polyanionic species with high charge density. The anion-selective electrode based on the plasticized polymeric membrane containing lipophillic anion exchanger (i.e., tridodecylmethylammonium chloride) yields a significant potential response as the anionic humic acid is extracted into the mamebrane from the aqueous sample phase by the ion-exchange process with chloride. By monitoring this EMF change, the concentration of humic acid in the soil extracts can be determined. The result from the potentiometric measurement will be correlated to that of the conventional TOC method in order to discuss the validity of this new method.

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Electrochemical enzyme immunoassay of a cardiac biomarker, B-type natriuretic peptide (BNP) at picomolar levels

정연호, 권기학, 임은혜, 구현우, *최문희, *송규정, 차근식, 남학현, 신재호

*광운대 화학과 *(주)아이센스 부설연구소 바이오센서 2팅*

There are approximately 500,000 new cases of heart failure in the United States each year. B-type natriuretic peptide (BNP) consists of 32 amino acid secreted by the ventricles of the heart in response to excessive stretching of heart muscle cells (cardiomyocytes). BNP levels are correlated with both the severity of symptoms and the prognosis in congestive heart failure. Therefore, BNP is as a biomarker of heart faliure. We have developed an electrochemical immunosensor for based on the well-known correlation between BNP and heart failure. We have introduced streptavidin-biotin chemistry to increase low electrochemical signal and as a result, we can measure very low concentration of BNP (1pg/ mL). We think that thus BNP immunosensor developed is a fast and simple instrument and it helps to monitor BNP concentration of a cardiac disorder patients.

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Enhancement of Electrocatalytic Activity of DNA-Conjugated Gold Nanoparticles and Its Application to DNA

Das Jagotamoy, Aziz Abdul, 이정아, 양해식

부산대 화학과

Hydrazine electrooxidation readily occurs on bare Au nanoparticle (AuNP), whereas it does not on DNA-conjugated AuNP. Thus, when DNA-conjugated AuNPs are used as electrocatalytic labels in electrochemical DNA detection, anodic current of hydrazine is not easily observed within potential window because of the high overpotential caused by the slow electron-transfer kinetics on DNA-conjugated AuNP as well as the slow electron tunneling between AuNP and indium-tin oxide (ITO) electrode. NaBH4 treatment significantly enhances the electrocatalytic activity of DNA-conjugated AuNPs. This enhancement substantially decreases the overpotential caused by the slow electron-transfer kinetics, and anodic current of hydrazine can be measured within potential window if the distance between AuNP and ITO electrode is not too large. The enhancement with NaBH4 treatment allows high signal current, and the low intrinsic electrocatalytic activity of ITO electrodes allows low background current. The high signal-to-background ratio enables us to detect 1 fM target DNA without target amplification or enzymatic signal amplification. The ultrasensitive detection using versatile AuNP and simple chemical treatment is practically appealing.

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Selective deposition of Pt on Au nanoparticles using hydrogen presorbed into Au nanoparticles during NaBH4 treatment

Patra Srikanta, *강현주, *이정아, *양해식

*IIT, Bhubaneswar *부산대 화학과*

We have developed a facile chemical method to prepare a Pt layer selectively on the AuNPs of AuNP/APTES/ITO electrodes. Hydrogen presorbed into AuNPs during NaBH4 treatment led to the formation of a thin Pt layer on the AuNPs. NH3 treatment facilitated the removal of Pt ions unreduced but absorbed on the AuNPs and the APTES layer. The Pt-coated AuNPs exhibited significantly improved electrocatalytic activity for the electrooxidation of formic acid. The formation of other metal-coated AuNPs via NaBH4 treatment could be possible, and the formation of other metal layers on Pt or Pd nanoparticles might be possible without using explosive hydrogen gas.

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Preparation and Characterization of PtRu Catalysts Supported on Graphene Nanosheets for Direct Methanol Fuel Cells

박정민, 박수진

인하대 화학과

In this work, graphene nanosheets (GNSs) were introduced as PtRu catalyst supports because of their unique physical properties and electronic structure. The GNSs were synthesized using a chemical reduction approach of graphite materials. And, the PtRu particles deposited on GNSs were prepared via chemical reduction method. The surface and structural properties of the GNSs were characterized by Raman spectroscopy and X-ray diffraction (XRD), respectively. The morphological structures of the PtRu/GNSs catalysts were analyzed by transmission electron microscopy (TEM) and scanning electron microsopy (SEM). The electrocatalytic activity of the catalysts was investigated by cyclic voltammetry measurement. As a result, catalytic performance of the PtRu/GNSs was exhibited better electrocatalytic activity than derivative of carbon blacks (CBs) for methanol oxidation. Consequently, it was found that GNSs could largely influence on the characterization of the catalysts, indicating GNSs might have potential application as catalyst supports for fuel cells.

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Electro-catalytic Performance of Pt-Ru Nanoparticles Deposited on Modified Carbon Substrates for Direct Methanol Fuel Cells

박정민, 박수진

인하대 화학과

In this work, carbon supported metal nanoclusters as fuel-cell catalyst electrodes were prepared by a chemical method of H2PtCl6 and RuCl3 reduction on base treated multi-walled nanotubes (MWNTs). The size and loading efficiency of the metal clusters were dependent on the preparation method and the surface characteristics of the MWNTs. In the process of catalyst preparation, the urea concentration was a critical factor in obtaining PtRu nanoclusters of small size and high loading efficiency. The catalysts were characterized by means of elemental analysis, nitrogen adsorption, and X-ray photoelectron spetroscopy (XPS). And the structure and morphological characteristics of the catalysts were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). As a result, the PtRu nanoparticles were impregnated on the MWNTs with good formation in 3-5 nm. And, the cyclic voltammograms for methanol oxidation revealed that the methanol oxidation peak varied depending on changes of surface functional groups of the MWNTs. It was thus concluded that the changes of surface functional groups of the MWNTs were related to reduction of PtRu, significantly affected the methanol oxidation activity of anodic electrocatalysts in DMFCs.

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Synthesis and Electrochemical Characterization of 2,2´:5´,2´´-terthiophene-3´-propiolic acid

황재영, 손정익, 윤상수, *윤장희, *원미숙, 심윤보

*부산대 화학과 *한국기초과학지원연구원 부산센터*

Synthesis of a terthiophene functionalized monomer, 2,2´:5´,2´´-terthiophene-3´-propiolic acid (TTPA), was successfully achieved. A new polythiophene derivative was synthesized by electrochemical polymerization. The study for the properties of the polyTTPA film were performed with cyclic voltammetry (CV), in-situ UV-vis spectroscopy, atomic force microscope (AFM), in-situ conductivity and X-ray Photoelectron Spectroscopy (XPS) measurement. Spectroelectrochemical study indicated that the polymer switch from a highly opaque dark-blue reduced state to highly transmissive oxidized state with a contrast of 89% in polyTTPA. Spectroelectrochemistry, switching ability and the electrochromic behavior of the devices were investigated.

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Towards Donor -Acceptor Double Cable Polymeric Material: Synthesis and electrochemical properties of vinylcyanoacetic acid-substituted terthiophene derivative and its polymer

황재영, 윤상수, 손정익, *원미숙, 심윤보

*부산대 화학과 *한국기초과학지원연구원 부산센터*

3´-benzaldehyde-2,2´:5´,2´´-terthiophene with vinylcyanoacetic acid substituent at benzyl para-position were synthesized. The monomers were characterized by NMR, FT-IR and mass spectroscopy. Density functional theory has employed to study the electron distribution and the interamolecular charge transfer (HOMO→LUMO) of the monomer. The monomer was polymerized on a glassy carbon electrode in 0.1M TBAP/dichloromethane solution. The polymer consists of covalently linked electron acceptor moieties to an electron donor polymeric backbone. The polymer films were characterized with cyclic voltammetry (CV), in situ UV-vis spectroscopy, and atomic force microscope (AFM), X-ray photoelectron spectroscopy (XPS) and in-situ conductivity measurement. Spectroelectrochemistry, electrochromic switching, and open circuit stability of the device was studied. They were found to have good switching times, reasonable contrasts and optical memories.

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Electrochemical behavior of water-splitting cobalt(II) in potassium dihydrogen phosphate buffer

K.N. Shashikumar, *석진호, **이치우

*고려대 소재화학과 *고려대 **고려대 신소재화학과*

The utilization of solar energy under dark requires its storage. In natural system, light energy is used to rearrange the chemical bonds of water to oxygen and hydrogen equivalents. The realization of artificial systems that perform “water splitting” requires catalyst that produces oxygen from water, which normally requires high over-potential, without the need for excessive driving potentials. Here electrochemical behavior of cobalt(II)ion in potassium dihydrogen phosphate buffer were studied by various electrochemical techniques at glassy carbon working electrode at different scan rates and ITO electrode at the time dependence. Cyclic voltammogram shows that a single electron- transfer reaction taking place at 0.89V is due to the oxidation of Co(II). The heterogeneous rate constant value k=0.2743 was obtained by the slop of charge vs time. Increase of scan rate and time increases the peak current and shifts the anodic peak potential toward positive direction. This indicates a irreversibility of electrooxidation of cobalt(II).

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Carbon-supported Metal/Conducting Polymer Composites for Oxygen Reduction Reaction

한수정, *정현정, **이영미, 이종목

*이화여대 화학과 *이화여대 화학나노과학과 **이화여대 자연과학대학/화학전공*

Recently several carbon-supported non-Pt-based materials have been reported as alternatives of Pt-based catalyst materials for fuel cell. In this study we have synthesized several carbon-supported metal-conductive polymer (M-CP) composites by chemical method. The composites were prepared with various metals (M = Pd, Fe, Co, Ni, Ru, Sn, Ir) and either polypyrrole (M-PPy) or polythiophene (M-PTh) as conducting polymers. The catalytic activities of these materials for oxygen reduction reaction were examined by cyclic voltammetry and rotating disk electrode experiments using M-CP modified glassy carbon electrodes.ORR activities of various M-CP composites in 0.5 M H_2SO_4 depending on the types of CP as well as M will be demonstrated. Some M-PTh with substituents on 3-position of Th are also under investigation in this group.

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Preparation of Prussian blue analogues film on flexible ITO substrate

정영희, 안준영, *곽준영, 김영일

*부경대 화학과 *(주) 마프로 연구개발*

Electrochromic device technology can be used for modulating the transmittance of visible light and solar radiation in windows in buildings by external voltage.Among the various electrochromic materials, Prussian blue(PB), FeⅢ4[FeⅡ(CN)6]3 has been known that the chemical reduction and oxidation of PB can lead to Prussian white and Prussian green(Berlin green). Thus PB exhibits an attractive electrochromic behaviour. Size controlled PB analogues were synthesized at 0℃, 25℃, 50℃, 80℃ and characterized using TGA, XRD, SEM, TEM, Cyclic voltammetry and UV-vis spectrometer.For commercial Applications, PB analogues films were prepared by sol-gel coating on flexible ITO substrate. For Optimization of PB analogue film, various binders, organic solvents and inorganic solvents were investigated. Optimized conditions and durability of PB analogues films were estimated by cyclic voltammograms and transmittance spectrum.

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Modified GCE with 3,4-Ethylenedioxy pyrrole(EDOP) and single-walled carbon nanotubes and its application to the selective determination of serotonin

김슬기, 유정민, 전승원

전남대 화학과

GCE modified by 3,4-Ethylenedioxy pyrrole(EDOP) and single-walled carbon nanotubes(SWNTs) was investigated by voltammetric methods in phosphate buffer saline (PBS) solution at pH 7.4. The electropolymerization of 3,4-Ethylenedioxy pyrrole and single-walled carbon nanotubes exhibited strongly enhanced voltammetric sensitivity and selectivity towards serotonin detection in the presence of ascorbic and uric acid. Voltammetric techniques separated the anodic peaks of 5-HT and interferences, and the interferences were effectively excluded from 5-HT determination. Linear calibration plot was obtained in the 5-HT concentration range of 0.1 μM 10 μM.

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A copper(Ⅱ)-selective PVC membrane based on a Schiff base complex of 1,2-bis((E)-2-hydroxybenzylideneamino)anthracene-9,10-dione

정은선, 서형란, 전승원

전남대 화학과

In this study, 1,2-bis((E)-2-hydroxybenzylideneamino)anthracene-9,10-dione was used as an ionophore for preparing PVC membrane ion-selective electrodes for copper ion.Among their membranes, a membrane electrode containing DOP as a plasticizer and 50 mol% KTpClPB as an additive shows good Nernstian response and the limit of detection of –log a(M)=6.60 to Pb2+ in Cu(NO3)2 solutions at room temperature. It has a rapid response time within 15 s over the entire concentration range. The proposed sensor revealed good selectivity andresponse for Cu2+ over a wide variety of other metal ions in a pH 5 buffer solutions.

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Silver(I) ion selective electrode based onN1,N2-bis(pyridin-2-ylmethylene)benzene-1,2-diamine

서형란, 정은선, 전승원

전남대 화학과

PVC-membrane electrodes based on (N2E)-N1,N2-bis(pyridin-2-ylmethylene)benzene-1,2-diamine ionophore were prepared. The effects of polymeric-membrane composition and buffer solution pHs were tested. Among their membranes, membrane electrode containing o-NPOE as a plasticizer and 50 mol% additive displays an good selectivity and response in Ag ion over a wide variety of other metal ions in a pH 5 buffer solutions at room temperature

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Formation of 1D nanostructured $Cu(OH)_2$ by Electrochemical Anodization of Cu Foil

라덕동, 김용신

한양대 바이오나노대학원

Copper hydroxide films with 1D nanostructures were prepared by anodizing copper foil in an aqueous NaOH solution. The optimized conditions for nanowire and nanotube formation were found to be 0.5M and 1M NaOH, respectively, at a reaction temperature of 20°C and current density of 2 mA cm^{-2}. The growth mechanism was interpreted by the formation of anisotropic $Cu(OH)_2$ lamellate followed by scrolling the sheet. In addition, copper compound films comprised of Cu_2O agglomerates or CuO nano-leaves were formed under non-optimized conditions, suggesting that there are side reactions that hamper the formation of nanotubes or nanowires. Consequently, single crystalline quasi-aligned $Cu(OH)_2$ nanotubes or nanowires can be prepared on a large scale by using this simple electrochemical anodization process. This protocol for the production of 1D nanostructured $Cu(OH)_2$ films can be widely utilized to prepare promising CuO nanomaterials and superhydrophobic surfaces.

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Growth kinetics and electronic properties of passive film of Zinc in borate buffer solution

유지선, *천정균, *김연규

*한국외국어대 생명화학과 *한국외국어대 화학과*

We have investigated the reaction mechanism of passivation and corrosion of Zinc in borate buffer. The oxide film formed from this process is composed of ZnO and $Zn(OH)_2$ and showed the property of n-type semiconductor based on Mott-Schottky equation. We found out that the n-type semiconductor in oxide film has deep donor and shallow donor.

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Mesoporous Pd-Co Bimetallic Films for Oxygen Reduction Reaction

김연수, *이영미, **이종목

*이화여대 화학나노과학과 *이화여대 자연과학대학/화학전공 **이화여대 화학과*

Efficient and economic electrocatalytic materials as substitutes of Pt-based oxygen cathodes in polymer electrolyte membrane fuel cells (PEMFCs) have been investigated extensively. It is reported that the catalytic efficiency of Pt can be enhanced when it has finely regulated microstructure called mesoporous.In this research we prepared the mesoporous bimetallic films (Pd-Co) with various compositions via the electrochemical deposition on Au surface in the reverse micelle solution of nonionic surfactant. The catalytic activities of the prepared films were evaluated for oxygen reduction reaction (ORR) using cyclic voltammetry and rotating disk electrode experiments. The activities for ORR were tested in both acidic (0.5 M H_2SO_4) and alkaline (0.1 M NaOH) conditions. Mesoporous Pd showed more positive peak potential for ORR than bare (non-mesoporous) Pd did. The compositions of the electroplating solution were also optimized. For Pd-Co bimetallic system, the molar composition of solution with [Pd]/[Co] = 8/2 or 9/1 showed the better results than the others.

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Electrochemical Impedance Measurement for the Anodic Deposition of V_2O_5 on the Polyaniline film from a $VOSO_4$ Solution

박경일, 송한목, *조원일, 모선일

*아주대 에너지시스템학부 *KIST 에너지환경연구부*

It is known that the intercalation capacity and charge/discharge rate of vanadium oxides as electrode materials for lithium batteries are limited by the moderate electrical conductivity and the low diffusion coefficient of lithium ions in the vanadium oxide matrix. Conducting polymer and vanadium oxide composite materials are of great interest to improve the mechanical property, and the conductivity of the electrodes for rechargeable lithium batteries. The V_2O_5 and PANi composite films on a stainless steel substrate were prepared by two-step electrochemical process in a conventional three-electrode cell system. Firstly, the PANi film was grown by a potentiodynamic polymerization method scanning the potential between -0.5 V and +1.0 V in a solution containing aniline monomer. Vanadium oxide was then deposited on this polymer film as a second step by a potentiostatic anodization method from a $VOSO_4$ solution. Temperature of the $VOSO_4$ solution and the anodization charge (Q) were modulatd to control the composition of the V_2O_5/PANi composite films. Oxidation deposition process of V_2O_5 from the $VOSO_4$ solution was monitored by measuring the electrochemical impedance in the frequency range of 100 mHz ~ 100 kHz and analyzed by a simple equivalent circuit to explain the interfacial phenomenon.

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Improved electrochemical performance of nano-V_2O_5/polypyrrole composite film cathodes in lithium batteries

김유나, *김주성, **조원일, 모선일

*아주대 에너지시스템학부 *아주대 화학과 **KIST 에너지환경연구부*

The vanadium oxide and polypyrrole composite(V_2O_5/PPy) materials are of great interest as cathodes for the rechargeable Li batteries. Nano structured V_2O_5 is one of the most beneficial and novel cathode materials with high capacity and with structural flexibility for the reversible insertion/release of guest Li^+. Kinetic barriers due to Li access and transport within the crystalline lattice can pose limits to attaining theoretical capacities. Neither of these material fully capitalize on the high surface area available. Their low electrical conductivity can be partially overcome by the incorporation of conductive polymer. PPy is an electronically conductive polymer which has received considerable attention due to its high electrical conductivity and stability in electrochemical environments. In this work, V_2O_5 and polypyrrole composite films was prepared by a one-step anodic(+1.75V vs. Li) polymerization method, on a stainless steel gauze electrode in an aqueous solution containing pyrrole monomer and well dispersed V_2O_5 particles. Electrochemical performance of the nano-V_2O_5/PPy composite electrodes was tested by assembling coin-type (CR2032) cells with a battery test system (Maccor series 4000). The cell was assembled in a dry room and cycled galvanostatically on a multichannel battery test mode. The initial discharge capacity above 250 $mAhg^{-1}$ in the voltage range of 1.5-4.0 V. The intercalation capacity and discharge/charge rate of the nano-V_2O_5/PPy composite film cathode has been shown to be enhanced V_2O_5-only electrodes.

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Selective Surface-Modifications by Electrochemical Reactions for Cell Chip Development

최인성, *김소현, *서현정, *김재일, *여운석

*건국대 생명과학과 *건국대 생명공학과*

The ability to control the placement of cells on surface is important for many research applications such as diagnostics, cell based drug screenings, and basic researches. One of the important challenges in those studies is to induce the cell placement on-demand. In this work, we report new methods to control the placement of cells at the molecular level by electrochemically induced reaction. The strategy relies on the electroactive moieties on the substrate which reveal the organic functional groups. The subsequent chemical reactions with these groups afford 'RGD' surfaces which mediate cell adhesions. Our approach is based on self-assembled monolayers (SAMs) on gold fabricated on the glasses with spatially addressable manner. The application of an electrical potential induces the specific chemical reactions to give organic functional groups which play a role of molecular handles for the immobilization of cell adhesion peptides. As expected, NIH 3T3 fibroblast selectively adhered to electrochemically induced regions. We believe this method can be used for selective cell patterning and cell chip development.

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Preparation and Characterization of V_2O_5/copolymer(Polyaniline-co-Polypyrrole (PANi-co-PPy)) Composites prepared by Chemical Method

THIEU MINH TRIET, 모선일, *여인형

*아주대 에너지시스템학부 *동국대 화학과*

Conducting polymers such as Polyaniline (PANi) and polypyrrole (PPy) are promising components to construct a cathode material in lithium batteries for their relative high conductivity, easy preparation and environment stability. It has shown from our previous works that composites of V_2O_5/PANi or V_2O_5/PPy can be chemically synthesized. The battery performance indicates that the specific capacity with the V_2O_5/PANi cathode is in the range of 320 mAh/g to 145 mAh/g and that of the V_2O_5/PPy covers from about 420 mAh/g to 160 mAh/g with repeated cycling of 50 times.In this work, we have prepared new composites of V_2O_5/(PANi-co-PPy), expecting any synergistic effect by making conducting copolymers. The composites of V_2O_5/(PANi-co-PPy) were prepared by a chemical method under different acidic solutions such as HCl (1M), H_2SO_4 (0.5 M) and $HClO_4$ (1M). The resulting composites were analyzed by XRD, FT-IR, TGA, and SEM. Also, electrochemical features of the V_2O_5/copolymer composite were compared with those of the V_2O_5/PANi and V_2O_5/PPy composites. It will be discussed on the structure, morphology, and amount of active material, V_2O_5 in the various composites with battery performances in detail.

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Preparation of nanostructured LiV_3O_8 cathode material

Quang-thao Ta, 모선일, *여인형

*아주대 에너지시스템학부 *동국대 화학과*

Lithium ion/lithium batteries are of great interest as energy storage and conversion devices and have become commercial reality during the past several decades. With the successful introduction, intensive efforts are still underway to explore new and advanced materials and to improve this technology. Lithium trivanadate (LiV_3O_8) is an attractive electrode material for lithium ion batteries due to its very attractive characteristics, such as structural flexibility with Li^+ insertion, high specific capacity and long cycle life. Nanostructured LiV_3O_8 will give large surface area and high specific capacities because the electrochemical properties of electrode materials depend strongly on the particles size: the bigger particles size, the higher the cell polarization and the lower the cell capacity and vice versa. In order to prepare LiV_3O_8 nanostructure, the nucleation rate and particle growth rate were modulated by controlling the solution pH, temperature, and concentration in the reaction from LiOH and V_2O_5 or NH_4VO_3. The crystal structure and surface morphology of the samples were characterized by X-ray diffraction (XRD) and scanning electron spectroscopy (SEM) or transmission electron spectroscopy.

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Electrochemical preparation and characterization of poly(3,4-ethylenedioxythiophene) films

송한목, *김주성, **여인형, 모선일

*아주대 에너지시스템학부 *아주대 화학과 **동국대 화학과*

Rechargeable lithium/ lithium-ion batteries and electrochemical capacitors are of great interest as electrochemical power sources for diverse applications. Composites of metal oxide and conductive polymer are expected to show mechanical flexibility with enhanced conductivity as electrode materials for the electrochemical power sources. Poly3,4-ethylenedioxythiophene (PEDOT) is one of the most successfully conjugated conducting polymers because of its remarkably high conductivity ($600\Omega^{-1}cm^{-1}$) and excellent environmental stability. It combines a low oxidation potential and moderate bandgap with good stability in the oxidized state. Conductive PEDOT is the candidate orgamic material for this work to make a composite electrode with inorganic oxide lattices. PEDOT film was prepared on a stainless steel electrode and ITO (Indium Tin Oxide) glass electrode by electrochemical polymerization from a 0.01M EDOT solution in acetonitrile with 0.1M $LiClO_4$ using a three electrode cell system. Polymerization of EDOT was processed by a potentiodynamic method, potentiostatic method and galvanostatic method. The electrochemical and spectroscopic properties of PEDOT electrode material was characterized by cyclic voltammetry(CV) and Infrared Spectroscopy (FT-IR). The morphology of the PEDOT film was observed using a scaning electron spectroscope.

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Comparison of polypyrrole coating and carbon coating on nanostructure $LiFePO_4$ cathode material

Hung-Cuong Dinh, *여인형, **조원일, 모선일

*아주대 에너지시스템학부 *동국대 화학과 **KIST 에너지환경연구부*

$LiFePO_4$ becomes one of the most promising candidates for rechargeable lithium ion batteries in terms of its structural stability and flexibility with lithium ion insertion, attractive voltage of 3.5 V, high theoretical capacity of 170 mAh/g, low cost, and ease of synthesis. However, the relatively poor electronic conductivity limits its application for cathode of lithium ion battery. Considerable efforts have been made to improve the conductivity, the charge/discharge rate performance of $LiFePO_4$, such as particle size minimization, carbon coating, cation doping or polymer coating. In my work, $LiFePO_4$ nano-sized crystals were prepared by a hydrothermal process from the solution of LiOH, $FeSO_4$, and H_3PO_4, adding glucose as a reductant of Fe^{3+} to Fe^{2+} and a surfactant in order to increase the specific surface areas. Carbon-coated $LiFePO_4$ ($LiFePO_4$-C) was prepared using the acetylene black during the heat treatments that occurred between 400 and 870° C. The polypyrrole coated $LiFePO_4$ ($LiFePO_4$-PPy) was synthesized by polymerising pyrrole monomers on the surface of lithium iron phosphate nanoparticles. The morphology, the spectroscopic and the electrochemical properties of the as-prepared $LiFePO_4$-C and $LiFePO_4$-PPy composite cathode materials were systematically characterized by X-ray powder diffraction, scanning electron microscopy, transmission electron microscopy, thermal gravimetry analysis, cyclic voltammetry, and battery test with constant current charge-discharge cycling.

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A Neomycin Immunosensor Based on Gold nanoparticles Decorated Carbon Nanotube Amplification Strategy

Ye Zhu, 황재영, 김동민, 심윤보

부산대 화학과

In the present work, the monoclonal neomycin antibody was covalently immobilized onto the gold nanoparticles deposited conducting polymer poly-[2, 5-di-(2-thienyl)-1*H*-pyrrole-1-(*p*-benzoic acid)] (pDTPyBA) to fabricate an amperometric immunosensor for the detection of neomycin. The immunosensor was designed based on a sandwich type immunosensing approach, where gold nanoparticles decorated multiwall carbon nanotubes were used as the linker for the secondary antibody and hydrazine label to achieve a multi-label strategy. The hydrazine labeled unit was used as a catalyst for the reduction of hydrogen peroxide, and the catalytic signal was monitored at −0.4 V vs. Ag/AgCl. The use of gold nanoparticles/carbon nanotube composite enhanced the catalytic signals significantly for the low detection limit. The parameters that could affect the immunosensor response, such as pH, temperature, and applied potential were optimized. A linear calibration plot for neomycin was obtained between 10 ng/mL and 250 ng/mL with the detection limit of 6.759 ng/mL.

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Electrochemical Characterization and Electrocatalytic Behavior of Silver Pentacyanonitrosylferrate Thin Film

허기영, *문성배

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The electrochemical characteristics of Silver pentacyanonitrosylferrate[$AgFe(CN)_5NO$] thin film were studied by CV, IR and EQCN. The electrocatalytic effects of $AgFe(CN))_5NO$ thin film in acidic solutions is shown. The results exhibit a linear relationship between the concentration of given materials and Iac or Ipc. Therefore, $AgFe(CN)_5NO$ thin film can be confirmed to be used as electrochemical sensors for the determination of some bio-materials, such as Pyridoxine, Nicotic acid, L-Alanine, Trichloroacetic acid, L-proline.

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Aminophenyl boronic acid for recognition of sugars

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3-amino phenyl boronic acid (APBA) layer was used for the detection of saccharides using the complexation reaction between boronic acid and cis-diol groups of these molecules. The sugar sensing surface was prepared by modifying the bare GCE by electro-polymerization of a terthiophen monomer bearing a carboxylic group, TTCA and then incubating it in APBA. It results in the formation of boronic acid attached TTCA polymer. The interaction of boronic acid derivative and sugars was studied by cyclic voltammetry, differential pulse voltammetry and quartz crystal microbalance techniques. Various experimental parameters like pH, temperature and reaction time were optimized with respect to the performance of the modified electrode towards oxidation of glucose. Preliminary results suggest a dynamic range of 1-20μM and a detection limit of 1μM for glucose.

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Electrochemical Detection of Sulfonamide Using $ZnSO_4$ Modified Carbon Paste Electrode

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부산대 화학과

Electrochemical detection of sulfonamide was carried out with chemically modified electrodes containing some metal compounds ($ZnSO_4$, $CoCl_2$, $CdCl_2$) by linear sweep voltammetry (LSV). The response of metal ions to sulfonamide was examined with the modified electrodes. The $ZnSO_4$ modified electrode was selected because it was most sensitive among them. To optimize experimental conditions, the following experiments were performed; the pH dependencies of peak height current, electrode composition, deposition temperature, and the effect of reduction time. Under the optimized conditions, the sulfonamide of real sample was detected and analyzed. The peak current increased linearly with increase of sulfonamide concentration in the range of 10^{-6} M ~ 7.7 x 10^{-5} M with correlation coefficient 0.99062.

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An *In Vitro* Immunosensor for Inducible Nitric Oxide Synthase (iNOS) Detection and Its Application toward Neuronal Cell Toxicity

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We report in this study the characterization of a chemically modified electrode by iNOS antibody immobilized on electropolymerized 2,2':5',5''-terthiophene-3'-benzoic acid (TTBA) film-covered gold nanoparticles for the determination of iNOS in aqueous solution. The obtained result showed a real-time amperometric determination of iNOS in aqueous solution. Under optimum conditions, the current response exhibits a linear relationship with the iNOS concentrations in the concentration range between 1 ng/ml and 20 ng/ml. The detection limit of nNOS was determined to be 0.2 ng/ml based on five-times measurement for the standard deviation of the blank solution (95% confidence level, k = 3, n = 5). The iNOS immunosensor showed high selectivity and sensitivity to iNOS determination in neuronal cells and should be promising for the in vitro measurement in deriving neuronal cell toxicity.

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DNA Aptamer based electrochemical sensor for daunomycin detection

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부산대 화학과

A DNA Aptamer functionalized electrode was prepared by immobilization of NH_2 modified DNA Aptamer on poly–(2,2':5',2"-terthiophene-3'-(*p*-benzoic acid)) (poly-TTBA). Detection of daunomycin by DNA /Apt/ poly TTBA was carried out by employing cyclic voltammetry (CV) and differential pulse voltammetry (DPV). Surface of the electrode was characterized by XPS, QCM, and AFM. Various experimental parameters, pH, temperature, applied potential and deposition time were optimized and performance of the daunamycin aptamer sensor was examined. The DNA /Apt/ poly TTBA based sensor exhibited a dynamic range of 0.9 -15μM and a detection limit of 0.5 (± 0.008.)μM.

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Electrocatalyst of oxygen reduction at nanoporous gold structures electrodeposited on gold electrode surfaces in acid and base conditions

최경민, 최수희, 김종원

충북대 화학과

Electrocatalytic reduction of oxygen was investigated at nanoporous gold structures electrodeposited on gold electrode surfaces. These nanoporous gold (NPG) structures were made by electrodeposition of Au-Ag mixed solution, where the different Au-Ag ratio led to the various nanoporous structures on the surfaces. The presence of these pores affects the change of the surface area, which result in enhanced electrocatalytic effect in oxygen reduction in acid and base conditions. The number of electrontransfer, concerned with the improvement of electrochemical activity of oxygen reduction, was measured by Rotating disk electrode (RDE). The pore size of the NPG electrode and the structures of the gold nanoparticles were examimed by scanning electron microscope (SEM). The relationship between the morphology of nanoporous gold nanoparticles and catalytic activity of oxygen reduction in acid and base conditions is discussed.

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Electrochemical Properties of three-dimensional Gold film Electrodes

현명희, 최수희, 김종원

충북대 화학과

금막이 형성된 microspheres(AuMS) 를 이용하여 3 차원 금막 전극의 전기화학적 특성과 그 응용을 연구하였다. AuMS 의 농도에 비례하여 Au oxide 의 면적이 증가하는데 이는 각각의 AuMS 가 전기적으로 연결이 되어 전기화학적 표면적이 증가한다는 것을 의미한다. 이렇게 형성된 전극은 다공성 전극의 특성을 띠는 것으로 관찰이 되었는데, 글루코오스의 산화 전류는 AuMS 의 농도가 증가함에 따라 증가하는 경향을 보이고, 반면에 아스코르브산이나 $Fe(CN)_6^{3-}$ 와 같이 전자전달이 비교적 빠른 물질들은 AuMS 의 농도에 상관없이 전류의 크기가 거의 변하지 않는다. 이러한 특성들을 응용하여 비효소적인 방법으로 글루코오스를 방해인자의 영향을 받지않고 측정할 수 있었다. 또 이 전극을 이용하여 순수한 금 필름에 비해 산소 환원 봉우리는 (+) 방향으로 이동하고 과산화수소 산화 봉우리는 (-) 방향으로 이동하는 것을 확인할 수 있었다. 이에 따라 글루코오스 센서와 과산화수소 센서 등으로 응용가능함을 알 수 있었다. 이 연구는 지역혁신 인력 양성사업의 도움을 받아 수행되었다.

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Heterogeneous Electron Transfer at Polyoxometalate-modified Electrode Surface

서보라, 최수희, 김종원

충북대 화학과

전극 표면에서 불균일 전자전달은 전기적촉매와 전기화학적 센서와 같은 전기분석 응용에 많이 연구되어왔다. 전자전달은 산화환원 활성종과 전극 표면에 의존한다. Polyoxometalate(POM) 는 금, 은, 그리고 탄소와 같은 다양한 전극표면에 자발적으로 흡착된다. 특히 Keggin type POM 은 잘 배열된 단분자층을 형성한다. 본 연구에서는 glassy carbon(GC), highly orientated pyrolytic graphite(HOPG), 그리고 금 전극 표면에서 Keggin type POM 인 $SiMo_{12}O^{4-}$ 의 자가조립 단분자층을 통한 전자전달을 관찰하였다. 산화환원 활성종으로 다른 전하를 띄는 (양성, 중성, 그리고 음성) 세 가지 분자를 사용한다. $SiMo_{12}O^{4-}$ 층이 형성된 전극에서 전자전달 속도는 (-) 전하를 띄는 $Fe(CN)_6^{3-/4-}$ 의 경우 감소하고, (+) 전하를 가진 $Ru(NH_3)_6^{3+/2+}$ 의 경우 증가하며, 전하를 띄지 않는 1,1'-ferrocenedimethanol(FDM) 의 경우 영향을 받지않는다. 이러한 전하 종에 따른 전자전달 효과는 세 가지 다른 전극 표면에서 비슷한 경향을 보이지만 효과의 정도는 GC < Au < HOPG 의 순으로 증가한다. 이 연구는 지역혁신 인력 양성사업의 도움을 받아 수행되었다.

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Formation of organic-inorganic hybrid self-assembled monolayers and their electrochemical properties

추연이, 최수희, 김종원

충북대 화학과

POM (polyoxometallate) 와 Thiol 은 전극표면에 자가조립 단분자층 (self assemble monolayer) 을 형성한다. 전극표면에 형성된 Thiol 단분자층은 전자전달을 방해한다. 이 연구에서는 유기 자가조립 단분자층을 형성하는 thiol 과 무기 자가조립 단분자층을 형성하는 POM 계열의 $H_4SiMo_{12}O_{40}$ 화합물을 사용하여, 전극 표면 위에서 각각의 thiol 과 POM 이 동시에 흡착된 단분자 막을 형성하고 이의 전기화학적인 특성을 살펴 보았다. Thiol 을 먼저 표면 위에 흡착시킨 후 POM 을 흡착시켜 전하가 다른 산화환원 활성종 ($Fe(CN)_6^{3-}$, $Ru(NH_3)_6^{3+}$) 을 통해 전자전달의 특징을 Cyclic voltammetry (CV) 와 Electrochemical impedance spectroscopy (EIS) 를 이용하여 전기화학적인 방법으로 알아본다. Alkanethiol 의 alkyl 사슬 길이에 따라 thiol 과 POM 이 흡착된 전극 표면에서의 경쟁적인 전자전달 특징이 다르게 나타난다. 이를 통해 유기 자기조립 단분자층과 무기 자기조립 단분자층이 동시에 존재하는 경우의 표면 전자 전달 특성을 비교 분석하였다. 이 연구는 지역혁신 인력 양성사업의 도움을 받아 수행되었다

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Electrodeposition and Stripping Analysis of Bismuth Selenide Thin Films Using Combined Electrochemical Quartz Crystal Microgravimetry and StrippingVoltammetry

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Combined stripping voltammetry and electrochemical quartz crystal microgravimetry were employed for the compositional analysis of electrodeposited bismuth selenide (Bi-Se) thin films. Electrodeposited films contain free Bi and free Se in addition to the targeted Bi_2Se_3 compound and the amount of these "impurity" phases depends on the electrodeposition variables. Thus the free Se content was determined using the reduction peak of Se to Se^{2-} obtained during the cathodic scan of films in 0.1 M Na_2SO_4 blank electrolyte. The Se content obtained during the cathodic stripping of Bi_2Se_3 to Bi + Se^{2-} was used for the determination of Bi_2Se_3 content using the assumption of 2:3 compound stoichiometry. Finally, the total Bi content was obtained from the anodic scan and the free Bi content was calculated from the difference between total Bi and the Bi present in Bi_2Se_3. The compositional assays thus obtained from the combined use of stripping voltammetry and EQCM are presented as a function of electrodeposition potential and electrolyte composition. The Bi_2Se_3 content decreased as the deposition potential was decreased (made more negative) and was highest when the electrolyte contained the same molar ratio of Bi^{3+} and Se^{4+}species. Unlike the Bi_2Te_3 previously studied by us, electrodeposition of Bi_2Se_3 was not efficient at potentials more negative than -0.5 V because of Se stripping and hydrogen evolution.

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코발트/폴리피롤/카본나노튜브의 합성과 고분자 전해질 연료 전지의 산소극 촉매 활성에 대한 연구

복혜미, 김현종

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연료전지는 석탄, 석유를 대체하여 높은 전기적 효율과 연료가 계속해서 공급되는 한 연속적인 출력생산이 가능하다는 장점이 있어 청정에너지 전환 장치로서 많은 연구가 진행되고 있다. 그 중에서도 최근에 연구가 활발히 진행되며 상업적으로도 가장 근접한 분야는 고분자 전해질 연료전지이다. 특히, 비백금계 촉매는 현재 널리 사용되고 있는 고가의 백금 촉매를 대체할 수 있기 때문에 새로운 연구 분야로 각광받고 있다. 본 연구에서는 고분자 전해질 연료전지의 비백금계 촉매로서 코발트/폴리피롤/카본나노튜브 복합체를 합성하였다. 폴리피롤/카본나노튜브 복합체는 삼염화철의 존재하에서 피롤의 화학적인 산화 중합 반응(Chemical oxidation polymerization)을 거쳐 얻어진다. 그리고 이 복합체의 특성은 퓨리에 변환 적외선(FT-IR) 분광기와 X-ray 회절(XRD)에 의해 분석되었다. FT-IR 스펙트럼에서 C-N 신축 모드에 따른 피크를 보여주고 있어 카본나노튜브 표면에 폴리피롤이 잘 코팅되어 있음을 확인하였고, XRD 패턴을 분석한 결과, 폴리피롤의 넓은 피크(2Θ=25°)와 카본나노튜브의 강한 흡수 피크(2Θ=26°)를 확인할 수 있었다. 또한, 코발트/폴리피롤/카본나노튜브의 표면과 통 모양의 구조는 전자현미경을 통해 확인되었다. 이러한 코발트/폴리피롤/카본나노튜브 촉매의 전기화학적 산소 환원 반응(Oxygen reduction reaction; ORR)은 회전디스크 전극을 사용하여 측정되었다. 촉매의 onset potential 은 대략 0.6 V (NHE)이며, 전기화학적 촉매 활성은 각각의 코발트 이온과 피롤의 몰 비율에 의존해서 변화한다. 그러므로, 코발트 이온과 폴리피롤의 질소 원자와의 상호작용이 촉매 활성을 결정하는 중요한 역할을 한다고 볼 수 있다.

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Synthesis of $LiFePO_4$ with using alcohol carbon precursor in solid-state reactionChi Ho Yoo, Na-Ra Han, Ji Eun Park, Youngil Lee*Department of Chemistry, University of Ulsan, 680-749 Ulsan, Korea

유치호

울산대 화학과

Lithium ion batteries are used widely for laptop, camcorder and hybrid electric vehicle as well as in many other applications. Olivine-structured $LiFePO_4$as a candinate cathode material for lithium ion batteries has received a lot of because it is low cost, non toxic, environmentally and relatively high theoretical capacity (approximately 170 mAh g^{-1}). But one of the main problems for $LiFePO_4$ to be a commercial material is its low conductivity. For overcoming this problem, many studies have been tried such as metal doping, reduce particle size and carbon coating. $LiFePO_4$ of its carbon composites were prepared by solid-state reaction of FeC_2O_4-$2H_2O$, $(NH_4)_2HPO_4$ and Li_2CO_3 with addition of alcohol carbon precusor. In this work, the effect of carbon composite and structural characterization of $LiFePO_4$/C composite have been investigated.

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The Study of Contribution Effects on Phot to Electrical Conversion Efficiency of Fabricating Parameters of Dye-Senstized Solar Cells Based on Liquid Electrolytes

최찬수

대전대 응용화학과

This study has been performed to find contribution effects on photo to electrical conversion efficiency of fabricating parameters of dye-sensitized solar cells (DSSCs) consisting of N3 or N719 sensitized nanoporous TiO_2 on the FTO glass plate, liquid electrolytes containing 0.6 M PMII, 0.05 M I_2, and 0.1 M LiI in the mixture of acetonitrile and valeronitrile (8:2 by volume), and Pt-coated FTO glass plate. To estimate the parameter effects a Taguchi method was applied. We chose different layers of TiO_2 slurry, TiO_2 particle sizes, and drop number of titanium(IV) butoxide solution as fabricating parameters. 67% from the TiO_2 slury layer, 32% from the particle size, and 0.9% from the titanium(IV) butoxide solution drop were found to be contributed to the photo to electrical conversion efficiency improvement. Under our experimental conditions, as the thickness of TiO_2 slurries becomes thin, the amount of titanium(IV) butoxide solution applied is small, and the size of TiO_2 particle is small, the photo to electrical conversion efficiency becomes higher. The efficiency of our best device was found to be 3.0% under AM 1.5 with an light intensity of 100 mW/cm^2.

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In situ X-ray absorption study of $Li(Mn_xFe_{1-x})PO_4$ as cathode material for Li-ion battery

한나라, 박지은, 이영일

울산대 화학과

Olivine structure composite, space group Pnma of $Li(Mn_xFe_{1-x})PO_4$ (x = 0, 0.6) has been studied with *In situ* X-ray absorption spectroscopy (XAS) as cathode material in lithium ion battery (LIB). For *In situ* XAS study, pouch type of cell was constructed to observe the change of olivine structure during charge and discharge process. *In situ* XAS measurements were conducted on the cell at 0.1 C rate using operating voltages 2.5-4.5 V versus Li/Li+. As well known, the low conductivity of olivine structure composite makes difficulty to apply a commercial cathode material. For overcoming, super-P has been applied to increase conductivity, and high energy milling of sample for 2 h performed to normalize particle size. Fe and Mn K-edge X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS) of $Li(Mn_xFe_{1-x})PO_4$ have been observed to characterize the changes of oxidation states (Fe(II)/Fe(III) or Mn(II)/Mn(III)) and the bond lendth on Fe or Mn atom, respectively.

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Study of The Local Activity of Mesoporous Pt Electrocatalyst for Oxygen Reduction Reaction Using Scanning Electrochemical Microscopy

양지혜, *이종목, **이영미

*이화여대 화학나노과학전공 *이화여대 화학과 **이화여대 자연과학대학/화학전공*

Pt is currently used as a popular electrocatalyst for sluggish oxygen reduction reaction (ORR) in polymer electrolyte membrane fuel cells (PEMFC) because it shows the best ORR activity. To improve the efficiency and to minimize the content of expensive Pt in electrocatalyst, it is of great interest to control the microstructure. Therefore, we prepared porous (not structure-controlled) as well as mesoporous (structure controlled) Pt electrocatalysts and then characterized the corresponding ORR activities using scanning electrochemical microscopy (SECM) in comparison with the one of bare solid Pt. Potential dependency of these differently structured Pt electrocatalysts was also examined. The corresponding morphologies of these electrocatalysts were obtained using SECM by measuring SECM feedback currents when the tip is scanned over the electrocatalysts in the solution of reversible electroactive species (e.g., $Ru(NH_3)_6^{3+}$, $Fe(CN)_6^{4-}$). The observed morphology and the local ORR activity are compared and analyzed.

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Electrochemical Nitric Oxide and Oxygen Dual Microsensor: Characterization and Biological Application

박선아, *이영미

*이화여대 화학 나노과학과 *이화여대 자연과학대학/화학전공*

An electrochemical nitric oxide (NO) and oxygen (O_2) dual sensor was prepared. The sensor is composed of a planar dual platinized Pt microdisk working electrode (each Pt disk diameter = 25 μm, distance between two Pt disks > 330 μm) and a Ag/AgCl counter/reference electrode. Working and reference/counter electrodes immersed in an optimized internal solution (30 mM NaCl and 22.4 nM NaOH in water) were covered with polytetrafluoroethylene (PTFE) membrane for gas selectivity of the sensor. The working electrode potentials were +0.75 V and -0.4 V (vs. Ag/AgCl) for electrochemically measuring NO and O_2, respectively. Cross-talking between the two disks of the sensor working electrode was also examined and no interference induced by the cross-talking was confirmed. The sensitivities of the sensor for NO and O_2 were 0.18 ± 0.08 nA/μM and 0.19 ± 0.03 nA/μM, respectively and the detection limit of NO was under 5 nM. The prepared NO/O_2 dual microsensor was applied for simultaneous and quantitative measurements of the co-dynamic relationships between NO and O_2 contents in rat brain *in vivo*.

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Development of an Electrochemical Gas Microsensor Based on a Micropore electrode

도현경, *이영미

*이화여대 화학나노과학 *이화여대 자연과학대학/화학전공*

Due to many important physiological and biological functions of nitric oxide (NO) and oxygen (O_2), the demand for the real-time determination of NO and O_2 in biological conditions has been increasing. In terms of analytical performance such as selectivity, sensitivity, durability and spatial resolution, an electrochemical sensor based on micropore electrode has some advantages over general Clark-type and/or disk-type sensors. Therefore, we developed NO or O_2 microsensor based on micropore working electrode (pore opening < 5 μm). By etching a planar microdisk electrode, micropore electrode is fabricated. Then the pore of the electrode is filled with porous Pt black by electrochemical platinization in chloroplatinic acid solution. The platinization of the electrode enhances the sensor sensitivity to both NO and O_2 due to the enlarged surface area while the electrode still possessing a quite small dimension. The prepared sensor is employed to detect either NO or O_2 levels in biological environments.

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A Novel Synthesis Approach of Supported Pt-Ru/CNT Catalysts for Proton Exchange Membrane Fuel Cell

김민식, *김정호, **Nitin Chaudhari, **kiran chaudhari, **김민우, **임신묵, **송민영, 유종성

*고려대 신소재화학과 *고려대 신소재 화학과 **고려대 소재화학과*

A novel approach called homogeneous deposition (HD) was employed to synthesize carbon nanotube (CNT)-supported Pt-Ru (60 wt%) catalysts under various pH conditions. In this method, urea was used as a precursor of precipitating agent to generate in-situ hydroxide ions, resulting in homogeneous deposition of Pt-Ru species on the CNT support. In addition, it was found that the pH value in the staring solution has significant influence on the Pt-Ru metal particle size and the catalytic activity of the supported Pt-Ru catalyst. Under most pH values investigated (i.e., higher than 5~6), the CNT-supported Pt-Ru catalysts prepared by the HD approach have shown smaller metal particle size with better particle dispersion and demonstrated greatly improved anode catalyst performance over the one prepared by impregnation-NaBH4 reduction at pH 7~8 in proton exchange membrane fuel cell. The results presented in this study highlights that the HD approach is straightforward and extremely effective for synthesis of carbon-supported high metal loading Pt-based catalysts with small metal particle size and uniform particle distribution for improved fuel cell performance.

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Multi-walled carbon nanotube (MWCNT) linking using gold nanoparticles

박선미, 김잔디, 김혜령, 김세철, zhangting, *류재철, *김혜란, **권기현, 이충균

*충남대 화학과 *충남대 분석과학기술대학원 **한국기초과학지원연구원 전자현미경연구부*

탄소 나노튜브는 나노미터의 소재로 나노재료에 적합하고 전기전도도, 열전도 등의 특성으로 인해 여러 분야에서 많은 연구가 수행되고 있다. 이에 따라 본 연구에서는 금 나노입자를 사이에 두고 평행하게 연결된 탄소 나노튜브를 만들어 나노파이프와 같은 새로운 나노물질을 개발하고자 하였다. 우선 탄소 나노튜브의 연결을 효과적으로 관찰하기 위해서 탄소 나노튜브를 산화반응과 볼밀을 사용하여 약 300nm 의 길이로 잘라주었다. 그리고 탄소 나노튜브의 표면을 금 나노입자와 결합할 수 있도록 thiol 로 결합된 탄소 나노튜브로 만든 후, dodecanthiol 로 안정화된 약 1.4nm 의 금 나노입자를 도입시켰다. 탄소 나노튜브의 연결을 확인하기 위해서 연결의 형태를 single, cross, parallel 3 가지로 정의하고 각각의 개수를 세어 통계를 내고 비교하였다. 산화한 탄소 나노튜브, thiol 이 결합된 탄소 나노튜브, 금 나노입자가 도입된 탄소 나노튜브의 연결 형태 개수를 세어 비교해 본 결과, 금 나노입자가 도입될수록 parallel 형태가 증가하고 single 형태가 감소함을 알 수 있었다. 이 결과는 탄소 나노튜브가 연결할 때 금 나노입자의 영향이 있음을 보여준다. 하지만 cross 형태가 존재하는 문제점이 있으므로 parallel 한 결합력을 증가시키기 위해 계속 연구하고 있다.

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Observation of selectively bonded gold nanoparticles and multiwall CNTs on mixed SAMs with CFM and AFM

김잔디, 김혜령, 박선미, 김세철, **zhangting**, *류재철, *김혜란, 이충균

*충남대 화학과 *충남대 분석과학기술대학원*

3 차원 나노구조체를 만들기 위해 알킬 체인 길이가 다른 3 가지의 mixed SAMs 를 Au(111)에 각각 형성시키고 CFM(chemical force microscope)으로 반응기(-SH)의 분포를 관찰하였다. 그리고 gold nanoparticle(GNP)을 도입하여 AFM 으로 관찰한 결과, CFM 으로 관찰한 반응기(-SH) 분포와 AFM 으로 관찰한 GNP 의 분포가 일치했고 이를 통해 GNP 가 반응기(-SH)에 매우 선택적으로 결합함을 알 수 있었다. 알킬 체인 길이가 다른 4 가지 SAMs 에 알킬 체인 길이가 다른 3 가지의 dithiolate MWCNT 를 각각 접근시킨 후 AFM 으로 CNT 의 결합 여부를 관찰하였다. 1,3-dithiolate CNT 는 1-propanethiol(3C thiol)의 SAM 에 결합하고 SAM 의 thiol 체인길이가 1-dodecanethiol(12C thiol)로 길어지면 결합하지 않았다. 하지만 긴 체인의 1,9-dithiolate CNT 는 1-dodecanethiol(12C thiol) 기질에 결합하였다. 이를 통해 SAMs 의 thiol 알킬체인 길이와 CNT 의 dithiol 알킬 체인 길이 간의 경쟁으로 CNT 가 기질에 선택적으로 결합함을 알 수 있었고 이를 응용해 CNT 를 패턴화하는 기술로 발전시킬 수 있을 것이다.

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Strategy for Low Background-Current Levels in the Electrochemical Biosensors Using Horse-Radish Peroxidase Labels

강현주, Aziz Abdul, 양해식

부산대 화학과

In electrochemical biosensors using horse-radish peroxidase (HRP) labels, background-current levels are generally high because of the redox reaction of the electroactive HRP substrate and H2O2. We describe an electrochemical strategy to achieve low background-current levels in HRP-based electrochemical immunosensors. The strategy consists of (i) the use of an HRP substrate/product redox couple whose formal potential is high and (ii) the use of an electrode that shows moderately low electrocatalytic activity for the redox couple. The strategy is met by a model biosensor consisting of an immunosensor using a catechol/o-benzoquinone redox couple and an indium tin oxide (ITO) electrode. The combined effect of high formal potential and moderately low electrocatalytic activity allows o-benzoquinone electroreduction with minimal catechol electrooxidation and H2O2 electroreduction. The detection limit for mouse IgG is 100 pg/mL, which is much lower than with an immunosensor using hydroquinone as the HRP substrate.

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Label-free electrochemical aptamer sensors: Feasibility of using ferrocene-modified silica nanoparticles as an electrochemical probe

한준희, 이지훈, 이지연, 최정연, 윤종해, *정인석, *정승현, 차근식, 남학현, 신재호

*광운대 화학과 *(주)아이센스 부설연구소 바이오센서 2팀*

An aptamer-based biosensor is known to detect lysozyme, ATP, and thrombin. In this study, a ferrocene-modified silica nanoparticle is introduced to the aptamer-based sensing system as an electrochemical probe for a simple, label-free detection of thrombin. The ferrocene-modified silica nanoparticle was synthesized by chemical coupling between ferrocene-carboxylic acid and aminated silica nanoparticle. The thiolated thrombin aptamer is immobilized on the gold electrode surface based on gold-thiol chemistry, followed by immobilization of 1-mercapto-6-hexanol on the electrode to prevent non-specific binding of thrombin. To measure the concentration of thrombin in the sample solution, cyclic voltammograms were performed in the range of 0 to +0.7 V with the scan rate of 100 mV s^{-1}, and square wave voltammograms were obtained at 15 Hz with a step potential of 0.004 V and the amplitude of 0.025 V in the range of +0.7 to 0 V. Both electrochemical experiments were done with the aptamer-modified gold electrode in the presence of the ferrocene-modified silica nanoparticle in the sample solution. Cathodic peak area was found proportional to the thrombin quantity specifically adsorbed onto the electrode surface. The thrombin binding aptamer based label-free aptasensor shows a reliable and sensitive electrochemical data with lower detection limit at 100 pM. Thrombin calibration curve is sigmoid as is typical for immunoanalysis. Linear range corresponds from 10^{-7} to 10^{-9} M thrombin concentration (R^2=0.9555).

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Alkanedithiol Self-Assembled Monolayers on Au(111)

Deyu Qu, *K.N. Shashikumar, **석진호, 이치우

*고려대 신소재화학과 *고려대 소재화학과 **고려대*

Self-assembled monolayers (SAMs) of organic thiols on gold have been extensively studied in past decades. They provide a good molecular candidate to be used in many application areas as well as a highly reproducible model system for understanding organic interface. The SAMs with -functional groups have been of particular interest. In this work, the structures of 1, n-alkanedithiol (n = 2, 4, 6, 8, 10) self-assembled monolayers (SAMs) on a Au(111) substrate were investigated by electrochemical measurements. The results of the experimental techniques indicated that the dithiols, except n = 2, showed an upright molecular structure in the SAMs, in which alkanedithiols were bound to the Au surface via only one thiol functionality and the other one faced up to the air.

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Preparation of Antibody-Au nanoparticles and its application to electrochemical amperometric immunoassay for hippuric acid

최영봉, 김혁한

단국대 화학과

The urinary HA, which is a major biological indicator in toluene-exposed human, is usually measured by colorimetric reaction, gas chromatography (GC), and high performance liquid chromatography (HPLC). However, the low specificity, complicated procedures, the length of time, a large number (volume) of samples, and high cost are limitations in these methods. The electrochemical immunoassay system for clinical diagnosis has several advantages such as, simple instrumentation, relatively low cost, miniaturization, portability, disposability, and fully automation. The electrochemical immunoassay system needs to label antigen or antibody with electro-active materials such as osmium complex and metal nanoparticles. The series of novel, electro-active antigen-HA-osmium complex was prepared and then characterized using electrochemical techniques. The electrochemical immunoassay comprised antibody-HA-Au nanoparticles and then applied antigen-HA-Os in the micro-tube. The electrical signals were measured by voltammetry technique. The resulting currents were linearly related with the concentration of antigen HA through the competitive reaction. A study of the electrochemical immunoassay offer the development of cheap, miniature devices capable of performing rapid immunoassays.

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Fabrication and characterization of nanostructured platinum and gold electrodes and their application to electrochemical immunoassay

홍성아, 성다연, 강영재, 권기학, 임은혜, 차근식, 남학현, 신재호

광운대 화학과

Carbon electrode used as working electrode in general. But carbon electrode has low sensitivity, biocompatability, and low signal. Herein we demonstrate a straightforward signal amplification technique by employing nanostructured electrode surfaces. Three different types of nanostructured metal surfaces (i.e., platinum black, gold black, and mesoporous platinum) will be investigated in terms of degree of signal amplification, stability, and reproducibility. In addition, a series of metal electrodes with different surface areas and nanostructures will be prepared by varying metal deposition conditions (e.g., metal salt concentration, deposition time/temperature, and type/concentration of surfactants). Platinum black is one of electro deposition method using cyclic voltametry. And the mesoporous pt electrode was fabricated by using an electrodeposition technique with nonionic surfactant and hydrogen hexachloroplatinate hydrate (HCPA). Gold-black was deposited by reduction of gold chloride hydrate in solution. Finally we apply such nanostructured electrodes to electrochemical immunoassay of a cardiac biomarker, B-type natriuretic peptide (BNP).

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Bioengineered recombinant single-chain fragment variable (scFv) antibody for electrochemical immunoassay of B-type natriuretic peptide (BNP)

이지연, 정연호, 한준희, 최정연, *최문희, *임승민, 차근식, 남학현, 신재호

*광운대 화학과 *(주)아이센스 부설연구소 바이오센서 2팀*

B-type natriuretic peptide (BNP) is one of the most important biomarker in early diagnosis of congestive heart failure. A rapid measurement of BNP in the emergency department is critical in the treatment of patients with acute dyspnea. In this presentation, we demonstrate an electrochemical BNP immunosensor by employing a recombinant single chain fragment variable (scFv) antibody to develop a early diagnostic tool for heart failure. Recombinant BNP scFv antibody consists of small heterodimers of 240 amino acids (MW 26 kDa) with the antibody variable heavy (V_H) and light (V_L) pairs. A peptide linker is used to stabilize the V_H-V_L pairs. The use of the scFv antibody to prepare BNP immunosensing devices allows for high density of effective antigen-binding sites on the electrode, eventually yielding a highly sensitive BNP immunosensor.

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Sensor application of disulfide-terminated molecular layers on electrode surfaces

김현진, 김규원

인천대 화학과

Recently, many kinds of organic molecular layers have been developed for chemical and bio-sensors application. In this presentation we report a synthesis of disulfide-terminated organic linker molecule that can form monomolecular layers on indium-tin-oxide (ITO) electrode surfaces. The molecular layers have been characterized by using X-ray photoelectron spectroscopy and cyclic voltammetry. It is also presented the use of the molecule for the electrochemical detection of metal ion and for the direct immobilization of antibodies. The surface resulting from the latter use is applied to antigen detection based on fluorescence and electrochemistry.

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Use of formylbenzenediazonium (FBD) salt for micropatterning of biomolecules and immunoassay application

Al-Monsur Jiaul Haque, 김규원

인천대 화학과

We report a simple method to produce formyl group terminated electrode surfaces for the selective immobilization of biomolecules. This was achieved by the electrochemical reduction of 4-formylbenzenediazonium cation (FBD) on indium-tin-oxide (ITO) microarray electrode surfaces. We show for the first time the synthesis through simultaneous diazotation of amine group and deprotection of aldehyde group. FBD modified surfaces were characterized by cyclic voltammetry, X-ray photoelectron spectroscopy (XPS) and fluorescence microscopy. The application of FBD for selective patterning of diverse biomolecules by successive electrodeposition of FBD and immobilization of biomolecules to fabricate multi-analyte immunosensors is demonstrated.

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Electrochemical galactose biosensors based on a screen-printed, disposable sensor strip

권기학, *임은혜, 이재선, 김영국, 차근식, 신재호, 남학현

*광운대 화학과 *광운대 화학*

Galactosemia is a rare genetic metabolic disorder that cannot convert galactose to glucose. If galactosemia is not treated, infants may develop a kidney problem and a brain damage. Every newborn should be tested for galactosemia which can be indicated by high galactose level (>240 μM) or lack of galactose-1-phosphate uridyl transferase (GALT) activity. While the tests are conventionally made with the samples eluted from dried blood spots, there have been demands for a point-of-care testing (POCT) of total galactose level. In principle, the blood galactose level may be determined conveniently with a strip-type biosensor similar to that for blood glucose determination. In this study, we introduced a quick and simple biostrip technique for detection of galactose.

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Electrochemical deprotection of disulfide functionalized silane on indium-tin-oxide electrode surfaces

권승용, 김규원

인천대 화학과

Spatially selective immobilization of biomolecules is essential to construct multi-functionalized surfaces for biosensors. We newly synthesized electrochemically active and protected disulfide functional group-terminated molecules that can form self-assembled monolayer (SAM) through silanization process on indium-tin-oxide (ITO) surfaces. ITO has been widely used because of its transparent and conductive characteristics that rely mainly on optical microscopic observation techniques. ITO microarray electrodes were used to activate the monolayer selectively on the electrodes of interest. The monolayer on the ITO electrodes was partially modified by an electrochemical oxidation which resulted in two types of thiol terminated molecules. In this presentation, we demonstrate partially controlled immobilization of biomolecules on indium-tin-oxide and its application based on fluorescence.

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Immobilization of Osmium Complexes to the Current-Dependent Deposited Gold Nanoparticles on the Screen Printed Carbon Electrodes(SPEs) using Glucose Sensor.

전원용, 최영봉, 김혁한

단국대 화학과

A series of novel, electro-active osmium complexes were prepared and then characterized using electrochemical techniques The newly synthesized redox mediators presented here are described in shorthand as $[Os(bpy)_2(mc\text{-}py)Cl]^{+/2+}$ and $[Os(dme\text{-}bpy)_2(mc\text{-}py)Cl]^{+/2+}$, linked with the gold nanoparticles onto the carbon electrodes. The electrical signals were measured by electrochemical technique and surface of the Au-deposited screen printed carbon electrodes(SPEs) were identified by SEM image. Also, the catalytical currents were amplified by GOx which are electrically mediated by new osmium redox films, converting the films into an electrocatalysts for the electro-oxidation of glucose. The the resulting catalytical currents were linearly related with the concentrations of and glucose.

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pH-dependent immobilization of bio-ligand molecules on chemically and electrochemically-modified indium-tin-oxide (ITO) surfaces

박혜진, 김규원

인천대 화학과

Immobilization of organic linker molecules on solid surfaces is essential for biochips. Development of the linker having a new function is important to improve an efficiency of the biochips. We synthesized a new linker that has electrochemically active group, 1,3-dithiane and can form self-assembled monolayer (SAM) on ITO surface. Electrochemical oxidation of 1,3-dithiane on the SAM results in aldehyde group which can react with amine-terminated bio-ligand molecules or biomolecules. In this presentation, we report pH-dependent immobilization of bio-ligand molecules on the linker-modified ITO surfaces. It is also demonstrated that the results can be applied to detect proteins.

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Modification of size controlled Pt nanoelectrodes using irreversible adsorption of Bi for formic acid oxidation

zhangting, 김세철, *류재철, 김잔디, 박선미, 김혜령, *김혜란, 이충균

*충남대 화학과 *충남대 분석과학기술대학원*

본 연구에서는 다양한 크기의 Pt 나노전극을 담지시킨 Pt/C 촉매를 제조하고, 크기가 다른 Pt/C 촉매에 비가역적으로 Bi 를 흡착시켜 Bi/Pt/C 촉매를 제조하였다. PCNF(Platelet Carbon Nano Fiber) 위에 1.14~6 nm 의 Pt 나노전극을 담지시키고, Bi 를 비가역적으로 흡착시킨 후, 전기화학적으로 환원시켜 Bi adsorbed Pt on PCNF(Bi/Pt/PCNF) 촉매를 만들었다. 이 촉매는 Cyclic voltammetry 와 Chronoamperometry 를 통해서 개미산의 산화 전류 특성을 측정하였고, CO 벗김 실험을 통해서 전기화학적 유효 표면적을 측정하였다. Pt 나노전극의 크기가 감소함에 따라 개미산 산화 활성이 증가하지만 1.8 nm 이하에서는 산화 활성이 감소한다. Bi 흡착 농도가 증가 할수록 Bi 에 의하여 개미산의 촉매독 생성이 억제 되어 개미산 산화의 효율이 1.8 nm Pt/PCNF 촉매는 0.5 kA/g, 같은 크기의 Bi/Pt/PCNF 는 0.25 kA/g 을 나타내며 최대 5.5 배까지 개미산 산화 활성이 증가하였다.

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The molecular-ruler fabrication of nano structures for nano scale devices :1.Dielectric layer-by-layer structures.

이은교, *손용근

*성균관대 화학 *성균관대 화학과*

An organic nano-scale dielectric layer for OTFT (Organic Thin Film Transistor) was synthesized by using the molecular-ruler method. In this process, 16-MHDA (16-Mercaptohexadecanoic acid) layers were used to form SAM on Au substrate. Copper(Ⅱ) was also used for linker ion between 16-MHDA (16-Mercaptohexadecanoic acid) layers. SAM(Self-Assembled Monolayer) of alkanethiols on gold substrate have ability to form well ordered organic film with high stability because they have bonding character between sulfur and gold and the Vander Waals interactions between alkyl chains. 16-MHDA and copper(Ⅱ) perchlorate were selected to build up this multilayer system between gold electrodes seperated by nano-gap on Si wafer. The thiols attached only to the gold made SAM layer first and then the carbonyl end group easily connected to the linker Cu ions. This Cu layer is ready to make second layer of 16-MHDA and so on. Therefore 16-MHDA and copper(Ⅱ) were fabricated to form layer by layer structure on the Au substrate. The thickness of the multilayer structures can be simply controlled by varying the numbers of multilayers in this structure. As a result, dielectric properties of OTFT is controlable easily that is the remarkable advantage of this study. Multilayers of 16-MHDA and copper(Ⅱ) perchlorate was fabricated and their dielectric properties were tested. XRF(X-ray fluorescence), XRD(X-ray Diffraction), CV(Cyclic Voltammetry), IR(Infra-red) and SEM(Scanning Electron Microscope) methods were utilized in this study.

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Phenol Sensors Adopting Conducting Polymer Microtubule Structure.

백승진, 손용근

성균관대 화학과

The determination of concentrations of phenolic compounds is of great importance due to their toxicity and persistency in the environment. In this work, an amperometric sensor for the determination of phenolic compounds in waste water was developed adopting microtubule structure of conducting polymer. The microtubules were manufactured by the electrochemical polymerization of EDOT into a polycarbonate template membrane having 1.2μm pore. The hollow tubules were loaded with aqueous tyrosinase solution to immobilize the enzyme. To prevent tyrosinase from escaping from the containers, the tubule openings were sealed with PEDOT/PSS composite. The microtubule worked as a container retaining water soluble electro-active materials as well as a current collector for the electrochemical reaction of species retained inside. Enzyme species could be stored inside the tubule structure to convert the phenolic substrates into quinones. Phenolic compounds are oxidized by tyrosinase to form a detectable product, which was determined at -100mV vs. Ag/AgCl reference electrode. The calibration curve showed its linearity 2~8μM range. The Sensitivities of the biosensor for catechol were 2.05μA/μM·cm^2. In summary, A phenol sensor and it showed good selectivity was achieved.

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Simultaneous Detection of Cd (II), Pb (II), Cu (II), and Hg (II) Ions in Dye Waste Water Using a Boron Doped Diamond Electrode with DPASV

윤장희, *양지은, *심윤보, 원미숙

*한국기초과학지원연구원 부산센터 *부산대 화학과*

The simultaneous detection of Cd (II), Pb (II), Cu (II), and Hg (II) ions in aqueous medium using a boron doped diamond (BDD) electrode with differential pulse anodic stripping voltammetry (DPASV) is described. X-ray photoelectron spectroscopy (XPS) was used to characterize the chemical states of trace metal ions deposited on the BDD electrode surface. Various experimental parameters that affect response, such as pH, deposition time, deposition potential, and pulse amplitude were carefully optimized. Using DPASV, the logarithmic linear response range for the Cu (II), Cd (II), Pb (II), and Hg (II) ions were in the range of 10 ppb to 100 ppb. The detection limits for Cd (II), Pb (II), Cu (II), and Hg (II) ions were 22 ppb, 10 ppb, 0.4 ppb and 3 ppb, respectively. Other metal ions did not interfere with the detection of Cd (II), Pb (II), Cu (II), and Hg (II) ions. The response of the BDD electrode was 10 times higher than that for a GC electrode. We also investigated the applicability of the BDD electrode on the electrochemical pretreatment of organic compounds for the detection of Cd (II), Pb (II), Cu (II), and Hg (II) in dye waste water.

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Heterogeneous electron-transfer kinetics for PQQ SAM in the presence of diluents

홍희정, 박원철, *김성현

*건국대 생명공학과 *건국대 특성화학부생명공학과*

Effect of diluents on the heterogeneous rate constant between the electrode and the redox active group has been studied by cyclic voltammetry. Pyrroloquinoline quinone(PQQ) as an electroactive group was attached on the aminoalkanethiol($NH_2(CH_2)_nSH$, n=6). Alkanethiols of various length (n = 4, 6, 8, and 11) were co-adsorbed with PQQ. PQQ showed $2e^-/2H^+$ redox reactions and its redox reactions gradually became irreversible as the chain length of diluents increased. This was attributed to the less accessability of protons to the PQQ moiety. Heterogeneous electron transfer rate constant exponentially decreased with the chain length.

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Comparative Study of Two Poly(thionine) Films on Glassy Carbon Electrode For The Determination of Dopamine in The Presence of Ascorbic Acid And Uric acid.

Ahammad A.J Saleh, *김성현, **이재준

*건국대 신소재공학과 *건국대 특성화학부생명공학과 **건국대 응용화학과*

A comparison of two different poly(thionine) films on glassy carobn (GC) electrode has been discussed based on the determination of dopamine in the presence of ascorbic acid and uric acid. Poly(thionine) modified electrode was obtained electrochemically in two different ways. The first one was prepared by one step anodic polymerization by applying a cycling in the wide electrochemical potential range, while the second one by two steps which consist of electrochemical anodization of GC at sufficiently positive potential followed by a polymerization by potential cycling within a relatively narrow potential range. The electrodes were characterized by cyclic voltammetry (CV), differential pulse voltammetry (DPV), and atomic force microscope (AFM). The two different type electrodes exhibited a different electrocatalytic activity towards the oxidation of DA, ascorbic acid (AA), and uric acid (UA) in 0.1 M phosphate buffer solution (pH 7.0). The first one showed an enhanced electrochemical response of DA while it significantly suppressed the signal of the ascorbic acid (AA) and uric acid (UA). On the other hand, voltammetric response of DA could be separated from that of AA and UA with second type electrode. The detection limit (S/N = 3) of 0.2 μM and 0.7 μM were obtained for DA using first and second type electrodes respectively. This results implies that a simple variation of electrochemical polymerization dramatically change the electrochemical catalytic properties of the electrode and therefore we can easily prepare the detection system of DA, AA, and UA depends on the experimental condition.

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Sandwich electrophoretic anchoring of MWCNTs into TiO2 photoelectrode for efficient dye-sensitized solar cells (DSSCs).

NaraYan ChanDra Deb, *Ahammad A.J Saleh, **subrata sarker, **이재준

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AbstractDye-sensitized solar cells (DSSCs) having sandwich incorporating of multiwall carbon nanotubes (MWCNTs) into TiO2 photoelectrode, constructed by electrophoretic deposition were efficiently studied. Usually, the electron transport across the TiO2 semiconductor particle network dominates the performance of these solar cells. So, the introduction of MWCNTs in mesoporous TiO2 film of DSSCs increases charge transport through the grain boundaries of TiO2 nanoparticles. Simultaneously, the open circuit voltage decreases due to the positive shifting of apparent Fermi level of mixed system. To minimize the lowering of open circuit voltage, we designed optimum conditions for the construction of sandwich type MWCNTs mixed TiO2 photoelectrode. Then, the enhancement of photocurrent density dominated over the little lowering of open circuit potential and resulted the higher overall power conversion efficiency than that of reference. Field-Emission Scanning Electron Microscope (FE-SEM), spectrophotometry, Voltammetry, IPCE measurement system, Electrochemical Impedance Spectroscopy (EIS) tools were used to characterize these electrodes. The sandwich CNTs in the junction of multilayer TiO2 film, acts as excellent charge collecting channels to increase the electron diffusion coefficient across the photoelectrode.

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Multi-wall carbon nanotubes incorporated TiO2 photo-electrodes in dye-sensitized solar cells (DSSCs)

subrata sarker, *NaraYan ChanDra Deb, **Ahammad A.J Saleh, 이재준

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AbstractThin films of multi-wall carbon nanotubes (MWCNTs) were deposited on fluorine doped tin oxide (FTO) glass substrates in two different ways: electrochemical deposition and transfer-printing technique with vacuum filtration. MWCNTs thin films were incorporated with TiO2 films in dye-sensitized solar cells (DSSCs). It has already been reported that carbon nanotubes (CNTs) increase short-circuit current (Isc) while decrease open circuit voltage (Voc) resulting in overall efficiency almost unchanged. The increase in Isc results from the beneficial role of conducting nature of CNTs. On the other hand, decrease in Voc is attributed to the movement of the apparent Fermi level to a more positive potential when Fermi level of TiO2 is equilibrated with that of CNTs film. To explore the characteristics of CNTs modified TiO2 electrodes to a greater extent we have prepared TiO2 film mixing with MWCNTs in different ways and studied the photovoltaic characteristics of the DSSCs. The TiO2 photo-electrodes were characterized using scanning electron micrograph, UV-visible absorption spectrum, electrochemical impedance Spectrum and cyclic voltammogram.

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ConcepTests의 활용이 학업 성취도와 학습태도에 미치는 영향

문숙희, 이상좌

목포대 화학과

이 연구는 ConcepTepts 를 활용하여 학생들을 유기 화학 수업의 학습 과정에 참여하게 함으로써, 활동적인 수업을 유도 하여 학업 성취도가 향상될 수 있는지의 여부 및 학습 태도에 긍정적인 영향을 미치는 지를 알아보고자 한다. 연구대상은 전라남도 소재 대학 2 학년 학생들을 학과별로 각각 실험집단 및 통제 집단으로 구성하였다. ConcepTepts 는 매 단원별로 시행하였으며 사후 검사를 2 회 실시하여 이 결과를 학업 성취도 검사로 사용하였다. 또한 실험 집단에만 태도 검사를 실시하였다. 연구 결과는 학과 별로 조금 상이하였으나 사후 2 차 시험에서 통계적으로 유의미한 결과를 도출할 수 있었고, ConcepTepts 에 참여도가 높은 학생일수록 화학 공부에 기여하는 바도 크고, 화학에 대한 이미지도 좋아진 것을 확인 할 수 있었다. 학생들은 기본 개념을 익힐 수 있었고, 책을 더 볼 수 있는 계기가 되어 도움이 되었다고 답하였다. 학업성취도와 상관 관계가 높았던 단원은 Aromatic compound 와 Carbonyl compound 를 다루는 단원이었으며, 전반적으로 학생들의 긍정적인 태도를 이끌어 낼 수 있었다.

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한국과학영재학교 일반화학실험 운영의 발전

천만석

한국과학영재학교 화학

교육과정으로의 일반화학실험은 일반화학 강의와 연계하여 운영이 되고 있으며 그 동안 많은 운영의 변화가 있었다. 일부 대학에서 학점으로 인정을 받는 과목으로 대학수준에 준하는 시간(2 시간/주)과 방법으로 운영이 되고 있으며, 화학에 관심을 가진 학생들이 선택하여 수강하고 있다. 한국과학영재학교 일반화학실험의 다양한 접근법의 변화를 소개하고, 운영의 특징이나 문제점에 대해서 정리하고, 대학 일반화학실험과의 비교를 통하여 발전된 운영형태를 찾고자 한다.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

최근 화학교육 연구의 경향: 국내외 화학교육 연구 비교

이상철, *한재영

*충북대 교육대학원 화학교육전공 *충북대 사범대학 화학교육과*

최근 국내외 화학교육 연구의 경향을 살펴봄으로써 향후 화학교육 연구의 방향을 논의하고자 한다. 최근 10 년 동안 대한화학회지(Journal of the Korean Chemical Society)와 미국의 Journal of Chemical Education 에 실린 화학교육 관련 논문을 수집하였다. 논문의 주제와 내용, 연구 대상, 연구 방법 등에 대하여 두 저널에 실린 논문을 비교 분석하였다. 논문은 NARST 의 학술발표 분류 항목을 참고하여 화학 학습(이해와 개념변화), 화학 학습(환경, 상호작용, 학습자 특성), 초등 화학교육, 중고등 화학교육, 대학 화학교육, 비형식 화학교육, 예비 화학교사 교육, 현직 화학교사 교육, 반성적 사고, 교육과정 및 평가, 사회-문화-성차, 교육공학, 화학사-철학과 화학사회학, 정책연구 등으로 구분하였다. 또한 조사연구, 실험연구, 양적연구, 질적연구 등으로 구분하여 비교였다. 이후 한국의 과학교육학회지에 수록된 화학교육 논문과, 외국의 우수한 과학교육 저널(Journal of Research in Science Teaching, International Journal of Science Education, Science Education 등)에 게재된 화학교육 관련 논문들도 분석할 예정이다.

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Green tea diet; inhibitory effects on three digestive enzymes, alpha-amylase, trypsin and lipase.

유승윤, 박인영, 한문정

숙명여자고

Green tea is famous for its effectiveness in weight-loss diet. In order to confirm the common knowledge, we first try to observe the inhibitory effect against digestive enzymes. First, total green tea extract from water showed a little inhibitory effect on alpha-amylase activity while that from DMSO showed no inhibitory effect at all. We also investigated what kinds of components of green tea have the highest inhibitory effects on three typical digestive enzymes; alpha-amylase, lipase, and trypsin. Catechin, caffeine, and theaflavin were chosen as the most representative components of tea extracts. Catechin showed modest inhibitory effect on alpha-amylase; however, it had no inhibitory effects on trypsin or lipase. Meanwhile, caffeine did not inhibit any alpha-amylase or lipase activity, but showed a little inhibition on trypsin. Theaflavin showed the most profound inhibitory effect on alpha-amylase, but showed a little and no effect on lipase and trypsin, respectively. It seems that catechin and theaflavin have similar inhibitory effects; both are mainly effective on alpha-amylase. On the other hand, caffeine showed no significant effects on alpha-amylase.

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일반화학실험에서 maple과 mathematica를 활용한 양자화 현상 및 원자 오비탈의 이해

천만석, *이광우, *양동현, *김발해

*한국과학영재학교 화학 *한국과학영재학교*

maple 이나 mathematica 를 활용하여 함수의 그래프를 쉽게 그릴 수 있다. 일반화학 교재에 나오는 상자속 입자, 조화 진동자, 원자 오비탈에 대한 그래프를 직접 그려 경험하면서 양자현상 및 원자 오비탈을 보다 더 이해하고자 한다. 일반화학 수준에서 나오는 기초 양자 부분의 함수인 상자속 입자의 형태를 1 차원, 2 차원, 3 차원으로 직접 그려 보면서 양자화된 과정을 경험한다. 또한 조화진동자를 사용한 함수를 이용하여 양자화된 현상과 터널링에 대한 개념을 그래프로 그려 이해를 증진한다. 또한 원자 오비탈의 함수를 이용하여 s-, p-, d-, f- 오비탈을 표현하고 노드의 갯수와 상대적인 위치를 확인한다. 또한 파동함수와 파동함수의 제곱의 차이에 대해서 이해한다.

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화학I 교과서의 물 단원 어휘의 적절성 분석

조미주, *박종석

*다사중학교 *경북대*

과학 교과의 내용은 과학 용어를 통해 기술되며 과학 수업은 교사와 학생간의 언어를 매개로 한 의사소통과정이다. 과학 교과서는 이러한 교수.학습과정의 기준을 제공하고 있으므로 학습자의 수준에 맞는 적절한 과학 용어를 사용해야 한다. 이에 본 연구는 표준국어대사전에 등재된 어휘를 바탕으로 화학 I 교과서 물 단원에 사용된 모든 어휘들을 분석한 후, 이들 어휘 수준과 11 학년 학생들의 어휘 발달 수준과의 적절성 여부를 파악하였다. 사용된 어휘의 등급 분포를 분석한 결과 연어휘수와 개별어휘수 모두 1 등급 어휘가 가장 많았고 2, 3, 4, 5 등급 어휘 순서로 그 수가 감소하였다. 어휘를 과학전문어와 비과학전문어로 분석한 결과는 전체 어휘 중 비과학전문어의 비율이 과학전문어의 비율에 비해 약 5 배 정도 높게 나타났음에 비해, 평균빈도의 경우는 비과학전문어에 비해 과학전문어가 더 높게 나타났다. 특히 과학전문어는 등급 외 어휘가 다른 등급에 비해 그 수가 압도적으로 많은 것으로 나타났다. 반면 비과학전문어는 연어휘수와 개별어휘수 모두 1 등급 어휘가 다른 등급의 어휘에 비해 압도적으로 그 수가 많았으며, 평균빈도 역시 1 등급어에서 가장 높게 나타났다.한편, 화학 I 교과서 물 단원에 사용된 어휘 수준과 11 학년 학생들의 어휘 발달 수준과의 적절성 여부를 파악한 결과 과학전문어의 경우 5 등급 어휘의 21%, 등급 외 어휘의 25%, 비과학전문어의 경우 5 등급 어휘의 41.1%, 등급 외 어휘의 16.8%가 사용 부적절한 어휘인 것으로 나타나, 11 학년 학생들의 어휘 발달 수준에 적절하지 않은 어휘가 상당량 사용되었음을 알 수 있었다. 뿐만 아니라 해당 어휘에 대한 부가적인 설명이 주어져 있지 않았기 때문에, 학생으로 하여금 추상적이고 생소한 과학 용어 또는 과학책에 등장하는 낱말들로부터 발생하는 과학 공부의 어려움을 더욱 가중시킬 것으로 판단된다.따라서 교과서 편찬 시 해당 학년 학생들의 어휘량 발달 수준에 적절하지 않은 어휘의 사용을 지양하고 적절한 대체 어휘를 선택할 필요가 있다. 불가피하게 어려운

어휘를 사용해야 할 경우에는 해당 어휘에 대한 부가 설명을 첨부해서 과학 학습에서 학생들이 가지는 어려움을 줄여주어야 한다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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모델링 실험 과정에서 대학생의 반응 및 상호작용 분석

장은경, 강성주

한국교원대 화학교육과

이 연구는 본교 일반화학실험 수강생을 대상으로 모델링 실험을 실시하고, 그 과정에서 일어난 학생들의 반응 및 상호작용을 분석하였다. 모델링 실험을 수행하는 동안의 녹음 자료, 실험보고서, 관찰노트, 그리고 실험 후 실시한 인터뷰 자료를 분석하였다. 모델링 실험은 '기체의 확산', '산염기의 전도도', '이온의 이동' 총 3 가지 주제로 진행되었다. 그리고 각 모델링 실험은 '탐색', '모델제안', '모델검증', '모델형성', '모델통합'의 5 단계를 거치며 각 단계에서 학생-학생, 학생-교사 사이의 상호작용을 통하여 피드백을 하게 되었다. 그 결과 학생들마다 모델을 세우고, 검증하고, 수정하고, 통합하는 과정에서 큰 차이를 보였다. 또한 모델링 실험을 거듭할수록 글로 서술하던 모델을 수식으로 설명하는 등 모델을 더욱 구체적이고 정교하게 표현하는 능력이 향상되었다. 이 연구는 과학 탐구 실험에서 학생들의 사고 과정을 알 수 있으며, 학생들의 탐구 능력을 배양하기 위한 전략의 기초를 제공할 것으로 기대된다.

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중학 과학영재의 비판적 사고력과 물질의 본질에 대한 과학사적 이해 과정의 차이 분석

허진휴, 이영민, *최용석

*전북대 화학교육과 *호남제일고*

비판적 사고력은 논리적이고 체계적인 사고 기능으로 문제를 객관적으로 분석하고 그 결과를 평가하는 고차원적 사고과정이며 문제를 명료화하고 가능한 방안들의 타당성을 검토한 후 문제를 조직적으로 해결하는 능력이므로 영재교육에서 중시되어야 한다. 본 연구는 과학 영재교육에 참여하고 있는 중학 과학영재의 비판적 사고능력의 특성을 분석하였는데, 비판적 사고 기능은 사실부분과 가치부분을 구분하기, 제시된 근거의 타당성을 평가하기, 객관적 근거에 의해서 평가하기, 다른 관점에서 바라보기, 숨겨진 과정과 의도를 찾아내기와 같은 능력이 포함된다. 이러한 사고기능과 관련된 수업을 위해서 물질의 근원과 물질관의 발전에 대한 고대 그리스 자연 철학에서부터 중세, 근대에 이르는 과학사적 내용을 바탕으로 하는 영재교육 자료를 개발하여 활용하였으며, 수업 활동지에 나타난 과학영재(화학반)의 과학사적 이해에 대한 특징을 분석하였다. 분석 자료를 바탕으로 비판적 사고력과 과학사의 이해 과정에 대한 영재아의 특징을 도출하고 영재교육을 위한 교육 자료 개발과 비판적 사고력 향상을 위한 구체적인 방안을 모색하였다.

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우리나라 과학교과서에서 나노개념에 대한 분석 및 나노교육의 필요성

장낙한

공주대 화학교육과

세계적으로 과학에서 나노과학에 대한 많은 연구 성과와 소식들이 전문 학술지뿐 아니라 대중 매체에도 많이 소개되고 있다. 그러나 우리나라 학생들은 나노기술이란 말을 텔레비전이나 신문에서 자주 봤지만 무슨 뜻인지는 모른다는 말한다. 현재 우리나라 과학교과서에서 언급된 나노개념에 대한 분석과 학생 및 교사들에 대한 나노교육의 필요성을 제안하였다. 또 외국의 나노교육에 대한 사례 및 교육과정도 소개하고 분석하였다.따라서 우리나라 학생들의 나노개념 확산을 위해 나노교육에 적합한 교육과정이 개발되어야 하며 초등학교부터 나노과학에 관한 교육이 시작되어야 한다.

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발표분야: 환경화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

한국연안에 존재하는 새로운 방오도료제의 농도변화 분석 (2006년, 2009년)

이성언, 성락규, 박천호, 이동섭

삼육대 화학과

2003 년을 기점으로 하여 유기주석화합물의 사용이 전면 금지되었다. 이에 따라 전세계적으로 대체도료로써 몇몇의 new antifouling agents 가 소개 되었으며 한국에서도 이들이 TBT 대체 도료로 사용되고 있다. 본 연구실에서는 2006 년도에 한국의 주요 만을 대상으로 하여 바닷물 중에 3 가지의 대체 방오도료제의 농도를 조사 하였으며 변화를 확인하기 위하여 2009 년도에 동일지역을 대상으로 측정을 하였다. 2006 년도에 검출된 new antifouling agents 의 경우 Chlorothalonil 은 N.D.-4.19 ng/L 의 범위로, Dichlofluanid 은 N.D.-61.69 ng/L 의 범위로, Irgarol 1051 은 N.D.-23.80 ng/L 의 범위로 검출되었다. 2009 년도에 Chlorothalonil 은 N.D.-80.30 ng/L 의 범위로, Dichlofluanid 은 N.D.-114.03 ng/L 의 범위로, Irgarol 1051 은 N.D.-432.11 ng/L 의 범위로 검출되었다. 비교결과 2006 년도에 비하여 2009 년도에 3 가지 화합물의 농도가 전부 증가 추세에 있는 것으로 나타났으며 이들 화합물에 대한 위해성에 대한 조사가 필요한 것으로 판단이 된다.

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발표분야: 환경화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

THE ROLE OF IODIDE IN THE PHOTOOXIDATION OF As(III) UNDER 254 nm IRRADIATION

여지만, 최원용

포항공과대 환경공학부

Arsenic is one of the most significant water contaminants of natural origin and a large population in the developing country is at health risk because of widespread arsenic pollution of groundwater. Among the two commonly occurring arsenic compounds, arsenite, As(III), is more toxic, more mobile, more difficult to remove by coagulation/precipitation due to its low affinity for adsorbents than arsenate, As(V). Therefore, the preoxidation of As(III) to As(V) is a highly desirable process to increase the removal efficiency of arsenic in water treatment. In this work we propose the photooxidation of As(III) in the presence of iodide and 254 nm irradiation as a new preoxidation method. Iodides are photochemically active under 254 nm irradiation. Light absorption by iodide in water generates a caged complex containing an iodine atom and an electron (I·, e-) through the charge transfer. The caged complex may dissociate into an aqueous electron and an iodine atom and preferably in the presence of an electron acceptor. The following reactions of iodine atoms lead to the generation of iodine, iodine anion radical, and triiodide. Such unique photochemistry of iodide can be coupled with the oxidation of As(III). In this study, the role of iodide in the photooxidation of As(III) and the mechanism of the newly proposed process were investigated in detail.

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Refinery of the Copper Powder in the Etching Waste of PCB

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This research paper provides the investigation and experimental results of the copper powder recovery in the wastewater produced during PCB manufacturing process. During the etching process, it discharges hazardous but precious resource since PCB being used to hold and attach electronic components has been made using laminated with copper. We used both dry and wet techniques to measure the weight percent of copper in the wastewater, and measured the purity of copper recovered by centrifuge after combining with several metals like ferrous, zinc, aluminum, and magnesium. We analyzed the recovered copper in terms of how much it contributes to achieve the goal of this experiment, which is to explain the economical benefits. In such ways, we recovered the copper power with 99.5wt% purity after twice refinery process, also it will be possible to use as the material for powder metallurgic products or electrode materials.

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Titania Containing Zeolite Catalyst for Selective Photocatalysis

zhangguan, 최원용

포항공과대 환경공학부

The superior photocatalytic performance of titanium dioxide(TiO2) has been widely investigated for almost 40 years, while this superior redox ability is non-selective for the cleavage of chemical bonds during the reaction. While the application of selective photocatalysis is of particular interest because it might open new potential fields of applications such as separation process. Here, we report “charge-selective” photocatalytic activity of titania containing zeolites, which promotes a positive charge selective photocatalytic degradation of pollutants. This catalytic property is triggered by a combination of titania active species located in zeolites and the negative charge framework system of zeolites.

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Dioxygen Reduction by Zero-Valent Aluminum for Oxidation of Organic Pollutants

Alok D. Bokare, 최원용

포항공과대 환경공학부

The reduction of molecular oxygen (O2) by zero-valent aluminum (ZVAl) for oxidative degradation of aquatic organic contaminants was investigated. In acidic conditions, corrosion of Al metal is accompanied by electron transfer to O2, which led to simultaneous generation of Al3+ and hydrogen peroxide (H2O2). Subsequently, hydroxyl radicals (HO•) were generated by electron transfer from Al0 to H2O2, which initiated oxidation of 4-chlorophenol (4-CP), a model substrate. The oxidation process was only initiated after an induction period (~2 h) during which the surface oxide layer was removed. The HO•-mediated oxidation reaction was completely quenched in the presence of methanol acting as radical scavenger. The effects of ZVAl loading, pH, and surface oxide content revealed that 4-CP oxidation was crtitically dependent on the oxide layer dissolution. Compared to zero-valent iron (ZVI/O2) system, ZVAl/O2 exhibited a higher oxidation capacity because of the stability of aquo-complexed Al3+ ions over a wider pH range. The degradation of other organic pollutants like phenol, nitrobenzene, and dichloroacetate was also successfully achieved with ZVAl.

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Visible Light Induced Pollutants Degradation by Organic-dye sensitized TiO_2

박이슬, 최원용

포항공과대 환경공학부

This study reports an example of visible-light photocatalyst based on TiO_2 modified by organic-dye sensitizers and compares their property with ruthenium-complex sensitized TiO_2system for the pollutant degradation. To minimize costs and to obtain the higher extinction coefficients, attention has been drawn toward organic dyes in the dye-sensitized solar cell system. Therefore, we applied these good properties for the pollutant degradation under visible light. The photodegradation of 4-chlorophenol and Cr(VI) was used as a probe reaction for evaluating the visible light activity of the photocatalyst under the illumination of > 420nm. Organic-dye sensitized TiO_2 showed a drastically increased photocatalytic reactivity for the Cr(VI) reduction and a similar photocatalytic reactivity for the 4-chlorophenol degradation compared with Ru-complex dye sensitized TiO_2 system. Futhermore, the stability of the organic-dye/TiO_2 were tested for the 4-chlorophenol degradation at various pH. The organic-dye/TiO_2 maintained their photocatalytic reactivity independently on pH, whereas, the Ru-complex dye/TiO_2 showed a drastically reduced photocatalytic reactivity at the basic pH. This strong interaction between organic dyes and TiO_2 could be confirmed through the comparison of UV-DRS spectrums.

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POM/SiO2 Acting as Heterogeneous Photocatalyst: Oxidation of gaseous acetaldehyde

이재선, 최원용

포항공과대 환경공학부

Acetaldehyde in air is known to be one of the principle indoor air pollutants and the most abundant carbonyl compounds in the atmosphere, so the photocatalytic oxidation (PCO) reaction of gaseous acetaldehyde was frequently studied. The performances of silica-immobilized polyoxometalates (POMs) on the PCO of gaseous acetaldehyde under the ambient air conditions were investigated in this study. Polyoxometalates and insoluble silica-immobilized POMs are used as effective homogeneous and heterogeneous photocatalysts in the oxidation of organic pollutants in water, respectively. Catalysts were prepared using tetraethoxysilane as a silica precursor and commercial POM powders without further purification by the sol-gel hydrothermal technique according to a method described elsewhere. After the acetaldehyde adsorption equilibrium was attained on the catalysts in the dark, the irradiation of UV light was immediately followed and the concurrent generation of carbon dioxide was measured. The amount of acetaldehyde and carbon dioxide was monitored by GC analysis. All pure POM powders, synthetic bare silica, and silica-immobilized POMs were compared for the adsorption and degradation of acetaldehyde. The silica-immobilized Na3O40PW12, H3Mo12O40P, and H4O40SiW12 markedly improved the decomposing of pre-adsorbed acetaldehyde compared to pure Na3O40PW12, H3Mo12O40P, and H4O40SiW12 powders. The adsorption of acetaldehyde and the conversion of pre-adsorbed acetaldehyde into carbon dioxide on the silica-immobilized POMs were highly enhanced compared to synthetic bare silica.

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